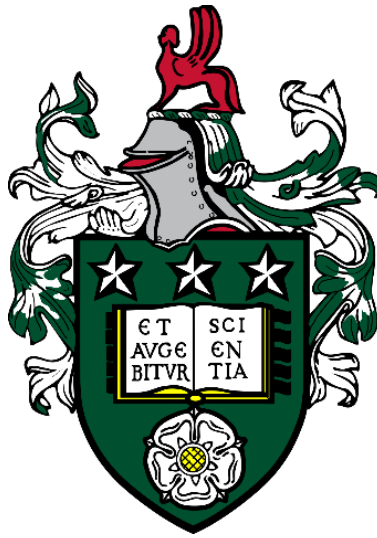

Leveraging GPS-based trip diaries for modelling individual mobility behaviour



Submitted in accordance with the requirements
for the degree of Doctor of Philosophy
by
Panagiotis Tsoleridis

University of Leeds
July 2022

Intellectual property and publications

The candidate confirms that the work submitted is his/her own, except where work which has formed part of jointly-authored publications has been included. The contribution of the candidate and the other authors to this work has been explicitly indicated below. The candidate confirms that appropriate credit has been given within the thesis where reference has been made to the work of others.

Five papers have been produced from the research that was undertaken in the context of the current thesis. Each paper is listed below including its location in the thesis and a full reference where appropriate. Also for each paper, an author contribution statement is provided.

The work in Chapter 2 of this thesis appeared in publication as follows:

Tsoleridis, P. Choudhury, C.F. Hess, S. 2021. *Utilising activity space concepts to sampling of alternatives for mode and destination choice modelling of discretionary activities*. Journal of Choice Modelling. 42(1), p.100336. [10.1016/j.jocm.2021.100336](https://doi.org/10.1016/j.jocm.2021.100336).

I developed the main idea for this work, performed the modelling work and wrote the manuscript. Charisma Choudhury and Stephane Hess provided recommendations on the modelling and comments on the results. The manuscript was improved by comments from all the co-authors.

The work in Chapter 3 of this thesis is manuscript under review:

Tsoleridis, P. Choudhury, C.F. Hess, S. (under review). *Deriving Values of Travel Time estimates using emerging Revealed Preference data*.

I developed the main idea for this work, under the guidance of both Charisma Choudhury and Stephane Hess. I performed the modelling work and wrote the manuscript. Charisma Choudhury and Stephane Hess provided recommendations on the modelling and comments on the results. The manuscript was improved by comments from all the co-authors.

The work in Chapter 4 of this thesis is manuscript under review:

Tsoleridis, P. Hess, S. Choudhury, C.F. (under review). *Accounting for distance-based correlations among alternatives in the context of spatial choice modelling using high resolution mobility data*.

I developed the main idea for this work, under the guidance of Stephane Hess. I performed the modelling work and wrote the manuscript. Stephane Hess and Charisma Choudhury provided recommendations on the modelling and comments on the results. The manuscript was improved by comments from all the co-authors.

The work in Chapter 5 of this thesis is manuscript under review:

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I developed the main idea for this work, under the guidance of Charisma Choudhury. I performed the modelling work and wrote the manuscript. Charisma Choudhury and Stephane Hess provided recommendations on the modelling and comments on the results. The manuscript was improved by comments from all the co-authors.

The work in Chapter 6 of this thesis is manuscript to be submitted shortly:

Tsoleridis, P. Choudhury, C.F. Hess, S. (in preparation). *Probabilistic choice set formation incorporating activity spaces into the context of mode and destination choice modelling.*

I developed the main idea for this work, performed the modelling work and wrote the manuscript. Charisma Choudhury and Stephane Hess provided recommendations on the modelling and comments on the results. The manuscript was improved by comments from all the co-authors.

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Abstract

The new emerging passively-collected data sources of the recent years have been increasingly providing new avenues for research due to their high spatio-temporal granularity. Datasets captured from GPS, mobile phone, location-enabled social media, smart-card payments etc., falling under the general term of Big Data, have the ability to provide mobility information at an unprecedented volume, velocity and variety, even if they were not initially collected with that purpose in mind. Despite the benefits they offer, however, they also pose new challenges for their analysis and the skills and knowledge required to derive value out of them, which transcend into different scientific fields. On one hand, that has largely limited their use in aggregate descriptive analyses and inference of general insights about mobility behaviour. Those studies offer valuable information and insightful comparisons with traditional Revealed Preference data, however they lack in their ability to generalise their findings and make them suitable for policy analysis. A significant reason for that is the often missing contextual information in terms of the trip makers' sociodemographic characteristics and any information regarding the observed mode and trip purpose, all of which are important inputs to any model of disaggregate mobility behaviour. On the other hand, even in the presence of additional semantic information, the overall complexity of those datasets has been proven to be challenging for traditional econometric specifications. That has led to the increasing popularity of Machine Learning, which generally excels at identifying patterns within complex datasets. Nonetheless, Machine Learning methods, typically described by non-parametric algorithms have limited ability to provide insights useful for policy analysis hindering their adoption for real-world policy making. Furthermore, the limited case studies of behavioural modelling using emerging datasets do not provide any systematic comparison with traditional data sources to properly assess the benefits and drawbacks of both data collection methods. The current thesis aims to address the three aforementioned overarching literature gaps utilising a specific form of emerging dataset, namely a semi-passive GPS-based trip diary collected from a sample consisting of recruited participants. The collected dataset was complemented with a background household survey capturing the individuals' important sociodemographic information and minimal input from the trip makers regarding the chosen mode of the trip and the activity purpose at the destination. Further enhancing that GPS trip diary with data derived from APIs and other openly available data sources can be sufficient to make the dataset usable for estimating a behavioural model. In the studies presented in this thesis, a general methodology is outlined on how to transform the initial GPS traces into useful inputs for behavioural models, which are able to uncover realistic sensitivities and trade-offs in accordance with the ones already proposed in the literature. More specifically, behaviourally accurate Values of Travel Time estimates have been derived from a mode choice model utilising such a dataset similar to the official values currently used for appraisal in the UK, which are derived from large-scale Stated Preference studies. In addition, a range of studies has been proposed aiming to address common research questions in spatial choice models, such as sampling of alternatives to reduce their computational complexity, accounting for the latent nature of the consideration choice set and capturing spatial correlation among alternatives, in all of which geography-derived concepts are also being implemented. Furthermore, the current thesis aims to focus on the integration of Machine Learning and Choice Modelling,

rather than their comparison, by proposing a combined framework in which Machine Learning is used to identify patterns in the dataset, while Choice Modelling is implemented in order to understand individual mode and location choice behaviour, thus taking advantage of the best of both approaches, which offers significant improvements over traditional econometric specifications without compromising the microeconomic interpretation of the outputs. The overall purpose of the current thesis is to enhance the confidence of the research community in the use of similar emerging datasets and to promote the integration of data-driven and econometric specifications. This is expected to provide useful insights about expanding the discussion moving forward into more advance combined specifications of capturing individual behaviour.

Contents

Intellectual property and publications	iii
Acknowledgements	vii
Abstract	ix
List of Tables	xv
List of Figures	xvii
1 Introduction	1
1 Theoretical background	1
1.1 Types of emerging data sources	2
1.2 Studies using GPS data	3
2 Research gaps	4
3 Objectives	6
3.1 Methodological objectives	6
3.2 Applied objectives	8
4 Thesis outline	9
References	12
2 Utilising activity space concepts to sampling of alternatives for mode and destination choice modelling of discretionary activities	19
1 Introduction	20
2 Methodology	23
2.1 Activity spaces - general literature	23
2.1.1 Detour Ellipse	23
2.1.2 Standard Deviatonal Ellipse	25
2.1.3 Familiarity buffers	26
2.2 Applying AS approaches to destination sampling	26
3 Empirical application: data and model specification	29
3.1 Data	30
3.1.1 Original GPS data	30
3.1.2 Processing of data into trip chains	31
3.1.3 Definition of shopping areas	31
3.1.4 Data enrichment: level-of-service information and mode availability assumptions	32
3.2 Full choice set model	33
3.3 Sampling strata formation	34
3.3.1 Creation of Detour Ellipses	34
3.3.2 Detour Factor modelling framework and outputs	34
3.3.3 Creation of Standard Deviatonal Ellipses	36

	3.3.4	Creation of Familiarity Buffers	37
	3.4	Definition of sampling protocols	37
4	Results	38
	4.1	Full choice set model outputs	38
		4.1.1 Variable selection	39
		4.1.2 Estimated parameters	40
		4.1.3 Value of Travel Time estimates and demand elasticities	40
	4.2	Sampling protocol evaluation/comparison	43
		4.2.1 Fit statistics comparison	44
		4.2.2 Sampled estimate comparison	45
		4.2.3 Evaluation of sampled VTT estimates and demand elasticities	47
5	Conclusions	55
	References	55
	Appendix	62
3	Deriving Values of Travel Time estimates using emerging Revealed Preference data		71
1	Introduction	72
2	Literature review	74
	2.1	Studies on Values of Travel Time estimates	74
	2.2	GPS data for transport research	76
3	Data	77
	3.1	DECISIONS data	77
	3.2	NTS dataset	81
4	Modelling framework	81
5	Modelling results	84
6	Values of Travel Time estimates	87
7	Discussion	91
8	Conclusions	94
	References	95
4	Accounting for distance-based correlations among alternatives in the context of spatial choice modelling using high resolution mobility data		102
1	Introduction	103
2	Methodology	107
3	Data	111
	3.1	Background	111
	3.2	Initial data processing	112
	3.3	Definition of general shopping areas	113
	3.4	Data enrichment	114
	3.5	Locational variables	115
	3.6	Direction of travel	116
4	Results	116
	4.1	Destination model outputs	116
	4.2	Joint mode and destination model outputs	120
	4.3	Demand elasticity analysis	124
		4.3.1 Destination elasticities	124
		4.3.2 Joint mode and destination elasticities	126
5	Conclusions	126
	References	127
5	Augmenting Choice Models with Machine Learning techniques to capture the heterogeneity in Travel Behaviour		132
1	Introduction	133

2	Methodology	135
2.1	Latent Class Choice Model	135
2.2	Clustering - Latent Class Choice Model	136
3	Data	140
3.1	DECISIONS dataset	140
3.2	London travel demand survey	141
4	Results	141
4.1	Case study 1: Yorkshire mode choice	142
4.1.1	Model specification	142
4.1.2	Model outputs	142
4.2	Case study 2: Yorkshire shopping destination choice	146
4.2.1	Model specification	146
4.2.2	Model outputs	146
4.3	Case study 3: London mode choice	151
4.3.1	Model specification	151
4.3.2	Model outputs	151
5	Conclusions	153
	References	154
6	Probabilistic choice set formation incorporating activity spaces into the context of mode and destination choice modelling	158
1	Introduction	159
2	Forms of Activity Spaces	163
2.1	Detour Ellipse	163
2.2	Standard Deviatonal Ellipse	165
3	Methodology	166
4	Data	168
5	Results	172
5.1	Detour Ellipse outputs	172
5.2	Standard Deviatonal Ellipse outputs	173
5.2.1	Home-SDE centroid distance outputs	173
5.2.2	Home-SDE centroid angle outputs	176
5.2.3	SDE orientation outputs	177
5.2.4	SDE minor/major axis ratio outputs	178
5.2.5	SDE area outputs	179
5.3	Latent Class Choice Model outputs	179
6	Conclusions	187
	References	188
7	Discussion and conclusions	193
1	Summary	193
2	Objectives and contributions	195
3	Outlook	199
	References	201

List of Tables

2.1	Modelling outputs of the DF model for <i>O-S-D</i> trip chains	35
2.2	Modelling outputs of the travel distance model for <i>O-S-O</i> trip chains	36
2.3	Modelling outputs of the full choice set model	41
2.4	Value of Travel Time estimates of full choice set model	43
2.5	Demand elasticities of full choice set model	44
2.6	Fit statistics of sampling protocols	45
2.7	Estimate evaluation of sampling protocols	48
2.8	Comparison of sampling protocols	49
2.9	Evaluation of VTT estimates of sampling protocols	52
2.10	VTT comparison of sampling protocols	53
2.11	Evaluation of demand elasticities of sampling protocols	54
2.12	Demand elasticity comparison of sampling protocols	54
2.13	Evaluation of Random sampling protocol for choice sets of 10, 50 and 100 alts	63
2.14	Evaluation of Random sampling protocol for choice sets of 150, 200 and 250 alts	64
2.15	Evaluation of AC sampling protocol for choice sets of 10, 50 and 100 alts . .	65
2.16	Evaluation of AC sampling protocol for choice sets of 150, 200 and 250 alts .	66
2.17	Evaluation of TC sampling protocol for choice sets of 10, 50 and 100 alts . .	67
2.18	Evaluation of TC sampling protocol for choice sets of 150, 200 and 250 alts .	68
2.19	Evaluation of TAC sampling protocol for choice sets of 10, 50 and 100 alts .	69
2.20	Evaluation of TAC sampling protocol for choice sets of 150, 200 and 250 alts	70
3.1	Number of DECISIONS and NTS trips per mode and purpose	82
3.2	Outputs of base MNL and mixed MNL models	85
3.3	Distance band distributions and distance-based correction factors per mode .	89
3.4	Official VTT estimates per mode, purpose and distance band based on the latest SP survey (Batley et al., 2019) and the respective derived GPS-based VTT estimates (£/hour) (2016 prices)	91
3.5	Confidence intervals and standard errors of the mean estimates for the overall official VTT estimates per mode and purpose (Batley et al., 2019; Hess et al., 2017) and the respective derived GPS-based VTT estimates (£/hour) (2016 prices)	92
4.1	Chosen mode and general locations	115
4.2	Fit statistics and nesting parameters of destination choice models	118
4.3	Modelling outputs of the proposed CNL destination choice model	119
4.4	Fit statistics and nesting parameters of joint mode and destination choice models	121
4.5	Modelling outputs of the proposed CNL joint mode and destination choice model	122
4.6	Distance multipliers and allocation probabilities per mode combination	124
4.7	Individual level demand elasticities for forecasting scenario 1	125
4.8	Individual level demand elasticities for forecasting scenario 2	126
5.1	Fit statistics of the Yorkshire mode choice models	143

5.2	Modelling estimates of LCCM and H-LCCM models for the Yorkshire mode choice context	143
5.3	Estimated parameters of clustering covariates for the Yorkshire mode choice model	145
5.4	Values of Travel Time estimates (£/hr)	146
5.5	Fit statistics of the Yorkshire shopping destination choice models	149
5.6	Modelling estimates of LCCM and H-LCCM models for the Yorkshire shopping destination choice context	149
5.7	Estimated parameters of clustering covariates for the Yorkshire shopping destination choice model	150
5.8	Fit statistics of the London mode choice models	152
5.9	Modelling estimates of LCCM and H-LCCM for the London mode choice context	152
5.10	Estimated parameters of clustering covariates for the London mode choice model	153
5.11	Willingness-to-pay estimates (£/hr) for the London dataset	153
6.1	Modelling outputs of the DF model for <i>O-S-D</i> trip chains	174
6.2	Modelling outputs of the distance (km) model for <i>OSO</i> trip chains	175
6.3	Modelling outputs for the distance of the Standard Deviational Ellipse centroid from the home location ($dist_{hc}$)	176
6.4	Modelling outputs for the angle between the Standard Deviational Ellipse centroid and the home location (θ_{hc})	177
6.5	Modelling outputs for the orientation of the Standard Deviational Ellipse (θ_{sde})	178
6.6	Modelling outputs for the minor/major axis ratio of the Standard Deviational Ellipse ($\frac{b_{sde}}{a_{sde}}$)	179
6.7	Modelling outputs for the area of the Standard Deviational Ellipse (A_{sde}) . .	180
6.8	Fit statistics and estimated parameters of the modelling specifications	184
6.9	Comparison of Values of Travel Time estimates across models (£/hr)	187
6.10	Comparison of demand elasticities across models	187

List of Figures

2.1	Two-dimensional projection of time-space prisms (Demsar and Long, 2016)	24
2.2	Weighted standard deviational ellipse around observed/visited destinations (Schönfelder, 2003)	26
2.3	Example of sampled choice set specification	29
2.4	User interface of smartphone application used for the trip diary (Calastri et al., 2020)	30
2.5	Allocation of retail polygons located within overlapping shopping clusters (OpenStreetMap contributors, 2021)	32
2.6	Improvements of evaluation measures across sampling protocols and choice set sizes	50
2.7	Plots for β_{time}^{base} estimates for each sampling realisation across sampling protocols	51
2.8	Plots for β_{cost}^{base} estimates for each sampling realisation across sampling protocols	51
3.1	User interface of smartphone application used for the GPS trip diary (Calastri et al., 2020)	78
3.2	Spatial distribution of interzonal flows between MSOAs across the UK	79
3.3	Spatial distribution of interzonal flows between MSOAs across the region of Yorkshire	79
3.4	Comparison approach between SP and GPS-based VTTs	88
3.5	Box plots of GPS-based Car VTTs per purpose	92
3.6	Box plots of GPS-based Bus VTTs per purpose	93
3.7	Box plots of GPS-based Rail VTTs per purpose	93
4.1	NL structures for joint mode and destination choice model	106
4.2	Existing CNL nesting structure for a joint mode and destination choice model (Ding et al., 2014)	107
4.3	Proposed CNL nesting structure for destination choice model	109
4.4	Proposed CNL nesting structure for the joint choice model	110
4.5	User interface of smartphone application used for the trip diary (Calastri et al., 2020)	112
4.6	Allocation of retail polygons located within overlapping shopping clusters	114
4.7	General area of shopping destinations in the study area	114
4.8	Segmentation of destination alternatives based on their administrative area	117
4.9	Demand cross-elasticities of CNL-dest model for each destination alternative based on their distance from the target alternative for forecasting scenario 1	125
5.1	Schematic diagram of the LCCM framework and its constituent components	136
5.2	Schematic diagram of the H-LCCM framework and its constituent components	137
5.3	Flow chart of the H-LCCM algorithm	139
5.4	Class-specific average values of covariates across LCCM and H-LCCM for Yorkshire mode choice model	147

List of Figures

5.5	Class-specific average values of covariates across LCCM and H-LCCM for Yorkshire shopping destination choice model	150
5.6	Class-specific average values of covariates across LCCM and H-LCCM for the London mode choice model	154
6.1	Weighted standard deviational ellipse around observed/visited destinations (Schönfelder, 2003)	165
6.2	User interface of smartphone application used for the trip diary	169
6.3	Home locations segmented in quartiles relative to their position from Leeds CBD (black circle)	170
6.4	Index of Multiple Deprivation for 2015	172

Chapter 1

Introduction

1 Theoretical background

In recent decades, the advancements in Information and Communication Technologies (ICT) together with the significant market penetration and the increasing reliance on devices with embedded sensors, such as smartphones, has resulted in data being generated at an exponential rate (Evans, 2011). Recent reports have predicted that the generated data from sensors will double its size every two years from 2005 to 2020 (Gantz and Reinsel, 2012).

Emerging datasets generated by new ubiquitous sensors, also commonly termed as Big Data, are generally defined by their volume, variety and velocity (Laney, 2001), which differentiate them from traditional data sources, such as household trip diaries, field surveys and road-side interviews (Banik and Bandyopadhyay, 2016). Despite their sheer *volume*, new forms of data have the added features of being dynamic in nature (*velocity*), since they are generated in real-time and they can arrive in different formats (*variety*), i.e. structured, semi-structured and unstructured, with the latter being the most usual case (Gandomi and Haider, 2015).

For transportation research, new emerging data sources are steadily gaining importance over traditional sources, such as transport-related surveys. Those data sources offer new avenues for research and policy making, but also bring together new challenges regarding their analysis and ways to derive value out of them with significant research being currently under constant development for that purpose (Grant-Muller et al., 2021). Emerging data sources have been used in studies of road safety, road infrastructure maintenance, transport planning and mobility pattern analysis (Antonioni et al., 2019). The advantages they provide in terms of the lower cost, the increased sample size and spatio-temporal coverage (Calabrese et al., 2013) compared with the low update rate of census data (conducted every 5 to 10 years) and respondents' misreporting in surveys (non-recalled trips, overstated travel times etc.) make them a viable alternative data collection method (Yang et al., 2015). Furthermore, traditional data collection methods include small-scale roadside or more detailed household surveys, the former resulting in possible low response rates and the latter in respondents' cognitive fatigue (Ma et al., 2017). In contrast, emerging datasets can capture a more comprehensive view of individual mobility behaviour resulting in more trips per day and larger panels per individual compared to traditional trip diaries leading to less cognitive fatigue to the respondents.

Furthermore, conventional fixed sensors, such as loop detectors, despite being widely used in transport research, they tend to provide a limited spatio-temporal coverage, are susceptible to adverse weather conditions and are subject to high installation and maintenance costs (Leduc, 2008). On the other hand, emerging data sources provide a more efficient source of longitudinal data, important to assess behavioural change and the impact of policy measures (Kusakabe and Asakura, 2014). The past problems of data scarcity have been redefined in the sense of how to make value out of the current abundance of data either by adopting new

methodologies or by adapting existing ones.

Despite those benefits, however, it is also important not to ignore certain pitfalls and drawbacks. The majority of the data generated from sensors are not purpose-specific, hence important variables for Travel Demand Modelling are usually missing, such as gender, age or income level (Calabrese et al., 2013). In that sense, Big Data can be said to be “big” in numbers, but “thin” in semantic information (Zhao et al., 2018). Furthermore, the underlying complexity of the data and its multidimensional spatio-temporal characteristics require significant pre-processing analysis to distinguish the signal from the noise and end up with meaningful variables/features (Kim and Mahmassani, 2015) or transform unstructured data (e.g. text or images) into inputs for demand modelling, while the data complexity also challenges well-established methods and modelling frameworks. That in turn led to the need for developing further skills and expertise on methods and approaches of other research domains, a common theme in transport research, with Computer Science being this time on the focus. Indeed as these new emerging datasets are gaining increasing research interest among the transport research community, so do Data Science and Machine Learning techniques and algorithms that are now considered almost necessary for deriving value out of those data sources. A range of different tools and techniques, such as database management, cloud computing, data-driven algorithms etc. have become part of the everyday data analysis pipeline.

Concerns on ethics and privacy protection have also been raised with the increased resolution of the collected data creating possibilities for the identification of distinct individuals and their home locations. Actions to mask the home locations have been implemented in very granular datasets, such as GPS, where noise is being added in the traces at a certain buffer zone around home locations to conceal their exact location. The possibility of individual identification, however, still cannot be excluded completely especially in contexts of low populated geographic zones. Ownership of the data raises additional concerns, since the analysts and researchers who are using the data are usually not the ones collecting the data in the first place. Therefore, any consent provided by the individuals when their private data was collected should also include its potential analysis at a later stage. In response to those ethical questions about the data, their use and the need for privacy protection of the individuals under examination the European General Data Protection Regulation (GDPR) (European Parliament, 2016) was established setting guidelines for future data collection and its analysis for research.

1.1 Types of emerging data sources

A vast array of different new emerging sources is currently being used in transport research that can be categorised in the following groups and are further analysed in the subsequent paragraphs (Willumsen and Picornell, 2016):

- Data collected for other purposes (e.g. fare collection and billing purposes, fitness checks etc.), which can also be used to derive mobility insights, such as GPS (Marchal et al., 2004; Marchal et al., 2011; Bierlaire et al., 2013; Hess et al., 2015) offering information on individual mobility behaviour at the highest level of spatio-temporal resolution, mobile phone (Iqbal et al., 2014; Tolouei et al., 2017; Bwambale et al., 2017; Bwambale et al., 2019b; Bwambale et al., 2019a), which can offer a representative depiction of daily urban mobility due to the high market penetration of smartphones, but inference is usually required to identify movement between successive cell tower interceptions and smart-card data (Batty, 2013; Batty et al., 2013) captured from passengers’ daily transactions which can also offer a general view of the demand state of the system.
- Data collected from fixed-located sensors, such as Bluetooth sensors (Barcelo et al., 2010; Crawford et al., 2018; Kottayil et al., 2020) capturing distinct MAC addresses of Bluetooth-enabled devices of passing vehicles and road-side cameras (ANPR) (Fox et

al., 2010; Hadavi et al., 2020) capturing number plates of passing vehicles and further analysing them with image-processing algorithms, both of which being used in analysing vehicle trajectories.

- Location Based Social Network (LBSN) data derived from social media platforms and including individual geolocated text messages or check-ins revealing the individuals' activity. Due to the misrepresentation of certain population subgroups (older or lower income individuals) and the tendency for more leisure-related check-ins compared to other trip purposes, LBSN data are not considered suitable for forecasting travel demand on their own, but they can be used effectively as a complementary source of information (Chaniotakis et al., 2016).

1.2 Studies using GPS data

GPS data arguably provide the highest spatio-temporal resolution from the aforementioned emerging data sources. The level of detail of data derived from mobile phone, bluetooth and ANPR data heavily rely on the density of their respective infrastructure, i.e. cell towers (Chen et al., 2014), bluetooth sensors (Mitsakis et al., 2017) and road-side cameras (Fox et al., 2010). Furthermore, smart-card data e.g. for public transport only capture the tap-ins and/or tap-outs without any additional information on the rest of the trip (Zannat and Choudhury, 2019), which could be a significant limiting factor for understanding mobility behaviour for multi-modal trips, while social media data would rely solely on the frequency of the location-enabled check-ins, tweets etc. Contrary to those, a GPS tracking device will capture the traces of the trip maker at a high frequency with each trace having a unique pair of latitude/longitude coordinates.

Consequently, GPS is probably the only data source out of the aforementioned ones that is most likely to be captured as part of a mobility-related survey, i.e. purpose-specific. Nonetheless, Vij and Shankari (2015) have argued that due to the absence of mode and trip purpose information and the significant errors associated with their inference, fully passively-collected GPS data will never replace surveys with active input from the participants for accurate demand estimation. As a result, a GPS-based travel survey is likely to include additional steps to make the data usable for behavioural modelling with policy making in mind. Those additional steps could include a background household survey to capture the most important socio-demographic attributes of the participants, while also minimum input from the participants is usually required with regard to the chosen mode and trip purpose at the end of each trip. The drawback in those cases is the smaller sample size and the limited survey period (limited longitudinal data) compared to data from other sources, such as mobile phone or smart-card, which can have data for millions of users over multiple years.

That trade-off between higher level of detail-smaller sample size is to be expected since no form of data could be considered sufficient on its own to answer planning questions with reasonable accuracy. At present -and likely in near future- the optimum solution hence lies either in the fusion of different data sources or in the use of semi-passive data sources, where some additional active input from the participant is necessary to enrich the value of the data manifold. GPS data currently can be safely considered as the most suitable type of emerging data sources to be used for behavioural modelling and in fact they have been used extensively in transport research since mid-1990s. Mobility-related surveys based on GPS were first performed mostly with GPS-enabled devices installed in vehicles to track their movements (probe vehicles). That provided a sound representation of the traffic network and allowed transport planners and traffic engineers to better understand travel demand and delays occurring within the network. Those studies, were limited, however, since they were capturing only moving private vehicles and hence ignoring other transport users. That led to the second generation of GPS-based surveys performed with GPS-loggers, which are devices that participants carry or wear to log their daily trips. Those studies were able to capture non car trips too, however they were subject to certain limitations, such as individuals

forgetting to carry them during their daily trips or charge them sufficiently (Bohte and Maat, 2009). The third generation of GPS trip diaries involved the use of smartphones with trips being captured either through the phone’s GPS sensor or through applications dedicated for that task. It is argued in the literature that individuals are less likely to forget their smartphone when leaving their premises compared to a GPS logger, thus making them a more effective data collection method leading to more captured daily trips (Calastri et al., 2020). Nonetheless, both survey methods can be subject to signal issues or privacy protection issues with individuals switching them off to conceal parts of their daily mobility.

A number of studies have been performed utilising GPS data in a range of different application contexts. The most significant use of GPS data has arguably been in the context of route choice, however, those models often require significant pre-processing efforts to match the GPS traces with the underlying road network and provide meaningful paths, a process known as map-matching (Quddus et al., 2003; Bierlaire et al., 2013). Such examples are the studies of Li et al. (2005) and Hess et al. (2015), who analysed the route choice behaviour during morning commute and for freight trips, respectively. Traces captured from fitness applications, such as Strava (Jestico et al., 2016) and Endomondo (Schirck-Matthews et al., 2022), have also been used to track the routes of individuals using them and were compared with conventional methods to assess their validity. Caution is required, however, when extrapolating the findings of those studies to the wider population, since they usually refer only to a specific group of individuals. In the context of trip generation, Wolf et al. (2003) and Hossan et al. (2018) have reported significant discrepancies between the reported trips from GPS and traditional surveys, highlighting the significant implications that could arise with biased estimates cascading to the later stages of travel demand modelling. Specifically, Wolf et al. (2003) noted the significant differences in vehicle miles travelled and estimated travel times resulted from traffic assignment as a result of the initial misreporting of trips. In a similar notion, Gallotti et al. (2015) identified differences in travel time budgets obtained from GPS trip diaries compared to traditional surveys. Li et al. (2004) using descriptive statistics analysed variability patterns of departure time and route choice for commuting trips with results suggesting that significant variation exists for departure time, while trip chaining with the presence of intermediate stops might affect the variability for route choice, which otherwise shows significant signs of stability across commuters. GPS data were used to understand departure time for freight over a 24-hour period in the study of Vegelian and Dugundji (2018). Schuessler and Axhausen (2009) used raw GPS data without any additional information for developing pre-processing methodologies for mode detection, while with regard to understanding mode choice behaviour, Calastri et al. (2018) utilised GPS trip diaries combined with a household survey to capture latent availability and consideration effects in a mode choice context. In the same mode choice context, there are also the studies of Montini et al. (2017) and Huang et al. (2021), who analysed mode choice behaviour together with route and trip chaining behaviour, respectively. Finally, a limited number of location choice models is currently present in the literature with prominent examples being the studies of Huang and Levinson (2015) and Huang and Levinson (2017), who utilised GPS data to analyse the choice of single and consecutive non-work destinations, respectively.

2 Research gaps

Despite the aforementioned studies and the wealth of new research opportunities provided by the implementation of GPS data, there are still a lot of areas where established practices and general inertia hinder the adoption of new approaches. GPS data can be used to address some of the issues in the behavioural transport modelling domain that could not be resolved with traditional RP data, which are described in the following.

RG1: Limited use of GPS trip diaries for spatial disaggregate behavioural modelling.

According to the previous section, despite GPS data having been used in transport research for more than two decades, their utilisation is still to a large extent limited to studies of descriptive statistics of daily urban mobility with only a few examples taking advantage of their benefits over traditional data sources for behavioural modelling. Particularly limited has been their adoption in the specification of behavioural models in spatial contexts. The high spatio-temporal resolution, despite being one of the main advantages of GPS data, could also be considered one of its main drawbacks hindering their wider use in spatial choice modelling due to the larger choice set sizes they provide. Using traditional data sources for the specification of spatial choice models, such as location models of discretionary activities, usually require some form of aggregation to reduce the choice set size by combining elemental alternatives into aggregated ones, usually within traffic analysis or geographic zones, (such as MSOA or LSOA zones in the UK), which forms the alternatives included in the choice sets used for estimation. The increased spatial resolution of emerging datasets will only exacerbate that computational complexity by creating the need for finer levels of aggregation, i.e. smaller aggregation of alternatives, in order to take better advantage of GPS data. To add to that problem, there is also an inherent difficulty in discerning the arrow of causality between mode and destination choices and there is still not a general consensus as to which choice dimension comes first during the individuals' decision making process. That is also evident in aggregate four-stage travel demand modelling approaches, where trip distribution (destination choice) and modal split (mode choice) can change order between stages 2 and 3, while commonly preceded by trip generation in stage 1 and followed by trip assignment (route choice) in stage 4 (Ortuzar and Willumsen, 2011). That uncertainty has led many researchers arguing in favour of studying these two choice dimensions together in joint models of mode-destination choices better capturing the interrelations between them, which of course provide additional computational complexity with choice set sizes of $J_m * J_d$, where J_m and J_d are the total mode and destination alternatives presented in the study area. That also requires additional information to be obtained for the non-chosen alternatives that is necessary to estimate the corresponding behavioural model. The high granularity of GPS data allows to calculate that information at a higher level of accuracy compared to traditional data. The current thesis focuses to a large extent on such spatial contexts of joint mode-destination models, which have so far been neglected in the literature of utilising GPS data for transport-related behavioural modelling. As a result of that, several research questions commonly applied to simpler mode choice contexts have never been addressed in a spatial context or only to a limited extent, such as accounting for correlation among alternatives and uncovering latent choice set formation mechanisms.

RG2: Lack of a systematic comparison between estimates derived from GPS and other traditional data sources.

Comparison between GPS and traditional data sources has so far been limited on emphasising the ability of the former to capture a more representative depiction of daily mobility. Wolf et al. (2003) extended that initial observation to quantify the emerging differences in the stage of trip assignment. Nonetheless, due to the lack of more studies investigating the impact of those discrepancies for different aspects of travel demand and on different choice contexts, it is still uncertain whether differences in trip misreporting or in the granularity of the utilised datasets, will materialise in significant improvements for the models estimated and also in what aspects, e.g. in model fit, in better capturing unobserved heterogeneity etc. It can be argued that one of the reasons hindering their wider adoption for behavioural modelling is not only that those types of datasets might offer higher computational complexity, but also because researchers are uncertain of the potential added benefits that would justify their collection and subsequent analysis. Furthermore, previous experiences with traditional Revealed Preference (RP) data accumulated over the years and documented in the literature have led to the adoption of certain practices favouring Stated Preference (SP) data and responses to hypothetical scenarios over real ones. On that front, a comparison of traditional approaches over GPS-based specifications could provide empirical

evidence on the validity of GPS trip diaries that is currently lacking from the literature.

RG3: Current literature focusing on contrasting Machine Learning and Discrete Choice Modelling rather than combining the two approaches.

Currently, there is much discussion around the use of Machine Learning (ML) supervised learning algorithms as an alternative approach to traditional econometric behavioural modelling, such as Discrete Choice Modelling (DCM). An increasing number of studies in the literature comparing the two approaches are highlighting the increased prediction accuracy of ML over DCM. There is also concern, however, that the results obtained from ML might not be suitable for policy-oriented transport planning and demand modelling since they are mostly data-driven and not grounded on microeconomic theory of human behaviour. That has hindered the wider adoption of ML methods in behavioural transport modelling, missing additional opportunities to benefit from using those approaches in areas in which they excel. In response to that, in recent years there has been a slow shift of focus more on the integration of the two methodological paradigms. Sfeir et al. (2022) and Sfeir et al. (2021) have made significant contributions towards that direction by combining ML algorithms with DCM models within an integrated Latent Class Choice Modelling (LCCM) framework for analysing mode choice behaviour. Nonetheless, both of those studies were based on traditional RP and SP data and it would be interesting to see how a GPS trip diary would perform in a similar integrated ML-DCM framework, but based on different ML approaches. Furthermore, it could be worth testing an ML-DCM integration in different choice contexts, as well, such as location choice, and also assess its ability to uncover behaviourally intuitive latent profiles compared to traditional econometric specifications.

3 Objectives

The broad aim of the thesis is to enhance the validity of GPS data for behavioural modelling and the research community’s trust in utilising them. A 2-week GPS trip diary captured through a smartphone application is being used as the main dataset utilised to address the key research gaps listed above. The GPS trip diary is also benchmarked and cross-compared against two secondary traditional datasets, namely the SP data used in the official VTT study (Batley et al., 2019) and the London Passenger Mode Choice (Hillel et al., 2018). Several methodological and applied objectives have been pursued in the thesis, described in the following.

3.1 Methodological objectives

M1: Provide a more detailed representation of individual mode and location choices for discretionary activities (addressing RG1 and RG3).

The primary objective of the thesis is to study the problem of mode and location choice for discretionary activities more in depth taking advantage of the utilised GPS trip diary. The higher granularity of the observed choices can allow for smaller aggregations of elemental shopping locations to form the final choice set to be defined. Utilising a clustering algorithm to group together elemental shopping locations within a certain maximum distance threshold among them can help to not limit the analysis within the usual geographical boundaries. Furthermore, the study acknowledges that the choice of a shopping location would also depend on the following activity and the mode chosen to travel to that. Consequently, in the current thesis an additional layer of complexity is added by studying in conjunction the choice of an intermediate shopping location, as well as the two modes travelling to and from there for the two trip legs. Thus, the analysis is performed at the level of the trip chain from an initial origin O to the shopping location S and finally to the following destination D . A core motivation for that analysis is to understand whether the intermediate shopping location

is more likely to be closer to O or D , what would be the most likely detour from the straight OSD path to reach the shopping location and what role the direction of travel might have in the individuals' decision making, among others.

M2: Examine concepts around choice set formation in a spatial context (addressing RG1).

The thesis aims to take advantage of the higher granularity of individual mobility behaviour and the large panels of trips per individual to better address issues of choice set formation, which are a central theme for spatial choice modelling. Choice set formation is an issue relevant to different approaches of spatial choice modelling, namely sampling of alternatives and modelling frameworks of probabilistic choice set formation. Sampling of alternatives has been proposed as an empirical tool with significant practical value, which is often utilised for the purpose of creating smaller sampled choice sets used for estimation. On the other hand, probabilistic choice set formation frameworks provide a more behaviourally realistic approach aiming to capture latent constraints during individual decision making. For both of those cases, the aim is to utilise the geography-derived concepts of Activity Spaces (Hagerstrand, 1970) in the form of detour ellipses (Justen et al., 2013; Leite Mariante et al., 2018) and standard deviational ellipses (Brown and Moore, 1970; Horton and Reynolds, 1970; Horton and Reynolds, 1971; Yuill, 1971; Schönfelder and Axhausen, 2003; Schönfelder and Axhausen, 2004; Schönfelder and Axhausen, 2010; Manley, 2016) as proxy measures of trip-specific space-time and individual-specific spatial awareness/cognition constraints, respectively. The use of those types of Activity Spaces, will help to provide additional structure for the development of more efficient protocols of sampling of alternatives than the ones currently presented in the literature (Leite Mariante et al., 2018) in the case of large global choice sets, and assist to uncover instances of latent mechanisms employed by individuals leading to the formation of their actual choice set under consideration when making joint choices of mode and shopping locations (Manski, 1977; Swait and Ben-Akiva, 1986; Swait and Ben-Akiva, 1987; Calastri et al., 2018).

M3: Propose an efficient framework for capturing spatial correlation among locations by treating space as continuous (addressing RG1).

The fourth objective aims to propose an efficient and operational specification for the purpose of capturing spatial correlation among destinations of discretionary activities. Despite the widespread use of the Multinomial Logit model (MNL) (McFadden, 1973) in the domain of behavioural modelling (McFadden, 2000), the assumption of independent and irrelevant alternatives (IIA principle) has been identified as its main limitation since its initial inception. Accounting for unobserved correlation is important for estimating unbiased parameters and behaviourally realistic demand elasticities. As a result, the Generalised Extreme Value (GEV) family of models (Ben-Akiva and Lerman, 1985) was formulated to account for correlated alternatives with the Nested Logit (NL) model (Williams, 1977) being its prominent example, where the choice set is segmented into a finite number of disjoint nests including alternatives with common unobserved attributes. The inherently complex spatial context, however, requires a different type of analysis and the need to treat space as continuous rather than discrete acknowledging the true continuous nature of correlation across locations. The relevant approaches currently proposed in the literature are characterised by high computational complexity and estimation times, causing researchers and practitioners to follow simpler specifications, which unavoidably leads to biased estimates and demand elasticities or estimating models on smaller choice sets thus still not properly capturing correlation across the whole space in the study area. As a result, proposing a modelling framework able to account for correlation among all location alternatives in a more efficient way is of great importance to provide researchers with an operational tool to properly capture spatial correlation and realistic substitution patterns.

M4: Explore potential benefits arising from the integration of Machine Learning and Choice Modelling (addressing RG3).

Contrary to the majority of the studies in the literature, the current thesis aims to shift the focus on the efficient integration of Machine Learning and Choice Modelling, rather than their comparison. The thesis will aim to illustrate the benefits of integrating concepts from Machine Learning with an emphasis on taking advantage of their strong points over DCM specifications, namely identifying patterns within complex data and to enhance their performance. For that purpose, various clustering algorithms are utilised both as part of pre-processing analysis and also as an integral modelling component of advanced DCM specifications. More specifically, ML clustering algorithms are being used to provide finer groupings of elemental shopping destinations into general shopping neighbourhoods, which form the alternatives in the choice set. That allows the analysis to be performed in a more detailed geographical resolution and not be limited in the pre-defined geographical boundaries or traffic analysis zones. In addition, a combined ML-DCM framework is proposed, where each component is utilised in the context in which they excel. Specifically, a data-driven ML algorithm is used to more effectively identify patterns in the data, while DCM is used to understand individual mobility behaviour. The proposed specification can thus take advantage of the best of both worlds, while also extending the suitability of Machine Learning for policy making.

3.2 Applied objectives

A1: Focus on the practical applicability of proposed modelling frameworks by reducing their computational cost (addressing RG1).

A core applied objective of the thesis is to provide novel modelling frameworks that besides the additional policy insights they could provide, they should also provide more efficient specifications to reduce their computational cost and estimation times. The high estimation times of spatial choice models have arguably been one of the main drawbacks leading to more simplified frameworks being applied in practice that have the potential for not accurately capturing individual behaviour. Examples like that can refer to cases of implementing inefficient random sampling protocols for reducing choice set sizes, avoiding to treat space as continuous in order to capture spatial correlation across locational alternatives and ignoring the inherently latent nature of choice set formation in revealed preference data on spatial choices, among others. Those simplifications could have the potential danger of leading to biased estimates with adverse effects for policy making. Therefore, proposing new more efficient specifications with the focus on being able to be used in practice could have the potential of closing the gap between academia's state-of-the-art and industry's state-of-practice approaches.

A2: Provide a systematic comparison of behavioural models and their respective estimates utilising GPS trip diaries and traditional data sources (addressing RG2).

A third objective of this thesis is to shed light in the existence of any potential discrepancies of estimates derived from GPS trip diaries and SP surveys and traditional trip diaries. Emphasis is given in the estimation of GPS-derived Values of Travel Time estimates and the quantification of their statistical difference with official VTT values derived from SP. Part of this objective is to stress the importance of accounting for real-world choices in VTT estimation given their significance for the appraisal of future transport projects, while also highlighting the need to increase researchers' trust to emerging data sources for use in policy making as they are becoming increasingly more popular (Daly et al., 2014). Analysis also focuses on the ability of behavioural models estimated on GPS data to capture unobserved heterogeneity more effectively or in a range of different dimensions compared to models estimated on traditional sources. That finding could provide empirical evidence on the added value of the higher resolution, the larger panels of individual mobility behaviour and the longer survey durations of GPS-based data collection methods. On the other hand, traditional

trip diaries, which usually capture smaller panels and for durations of up to one week are expected to be less effective in capturing heterogeneity among individuals.

4 Thesis outline

The thesis is structured into seven chapters. The current chapter offers an Introduction on the topic analysed, the identified research gaps and the overarching aims of the thesis, while in the remaining chapters several approaches proposed to address those gaps are analysed. In the last chapter, the conclusion of the thesis are summarised.

Chapter 2 presents a paper titled *"Utilising activity space concepts to sampling of alternatives for mode and destination choice modelling of discretionary activities"*. The purpose of that study is to take advantage of the high resolution of GPS data to more precisely create different strata to sample alternatives and reduce the computational complexity of a joint mode-shopping location choice model. Sampling of alternatives has been proposed as a method to reduce the choice sets of models. Random sampling of alternatives in particular has been proven to be a very popular approach due to its simplicity, which also guarantees estimating parameters with negligible differences from the ones estimated using the full choice set (McFadden, 1978). Despite its simplicity, however, random sampling can also be a less efficient protocol compared to others since it is likely to include a high number of alternatives in the sampled choice sets that are irrelevant to the underlying choice process of each task, thus not adding any useful information for model estimation. Importance sampling offers a more informed alternative sampling protocol, in which certain alternatives are prioritised over others, i.e. are being sampled with a higher probability and hence are more likely to be included in the final sampled choice sets. Caution is, however, required since an additional sampling correction term needs to be included in the utility function to account for the sampling bias arising from importance sampling and to guarantee unbiased estimates (Guevara and Ben-Akiva, 2013a; Guevara and Ben-Akiva, 2013b). Keeping a well-balanced variation among higher and lower prioritised alternatives is also important for sampling efficiency, i.e. achieving outputs close to the full choice set model by using smaller sampled choice sets. The majority of studies implementing sampling of alternatives has been focused in residential choice models with protocols prioritising location alternatives in certain areas of the city relative to others (Farooq and Miller, 2012; Guevara and Ben-Akiva, 2013a; Guevara and Ben-Akiva, 2013b). A different approach, however, has to be implemented for creating sampled choice sets for location choice models of discretionary activities, since those choices might be subject to the individuals' spatial awareness, as well as their space-time constraints. Therefore, alternatives adhering to those constraints might provide more useful information for the underlying choice process compared to the remaining locations. A limited number of studies have implemented sampling protocols based on space-time constraints, but they have neglected to account for cognitive constraints. Therefore, there is potential in improving the efficiency of sampling protocols by including another layer of information during their implementation and by taking advantage of the high precision of GPS data to define proxy measures of spatial awareness and space-time to accomplish that. The importance sampling protocol proposed in this study gives higher priority to alternatives located within the stratum referring to space-time constraints followed by the stratum capturing constraints of spatial awareness. Finally, alternatives from the remaining area of the case study should also be sampled albeit with a smaller probability, so as to each alternative in the global choice set will have a non-zero probability of being included in the final sampled choice set, thus acknowledging the uncertainty around the strata creation. The proposed sampling protocol is compared with other importance and random protocols on an increasing number of choice set sizes and on a range of different realisations per protocol and choice set size to test sampling efficiency and stability.

Chapter 3 presents a paper titled *"Deriving Values of Travel Time estimates using*

emerging Revealed Preference data". The study utilises a 2-week GPS trip diary captured through a smartphone application as part of a survey conducted between October 2016-March 2017. The purpose of the study is to derive behaviourally accurate VTT estimates and compare them with the current official SP-based values currently used for appraisal purposes in the UK. For comparison purposes and to ensure consistency with the official VTT study reported in Hess et al. (2017) and Batley et al. (2019), the methodology developed in those studies was followed as closely as possible. Consequently, the analysis is based on a mixed Logit mode choice model in which unobserved heterogeneity among individuals is captured by specifying a range of log-uniformly distributed level-of-service parameters. Scaled utilities were also specified with additional scale parameters as a function of distance to capture the heterogeneity and the increased randomness arising in trips of longer distances. The estimates of the mixed Logit model, estimated on the GPS trip diary (estimation data), were then applied on the NTS data of 2015-2017 (application data) and were further weighted by distance based on the mode-specific travel-to-work trip distances from the latest Census of 2011. Standard errors for the GPS-based VTTs are computed using simulation, which allowed the calculation of confidence intervals and t-statistics of their difference with the official VTT values. That process resulted in GPS-based VTT estimates with no statistically significant differences with the official values at a 95% confidence level. Furthermore, the estimates are consistent with previous empirical findings in the literature (Wardman et al., 2016) suggesting the presence of increasing VTT values with distance, higher values for rail and business trips and also in general lower values for other non-work related trips. That study is the first who performs a systematic comparison between GPS-SP VTT estimates and the results suggest that new emerging data collections methods are suitable for providing behaviourally reasonable VTTs. The fact that the GPS values are statistically equal with the SP-based values should actually be considered as validation for the SP study and the rigorous efforts of the researchers involved in that study. It is also worth noting that the GPS-based VTTs were estimated on smaller samples than the SP values, both for estimation and application datasets, indicating that smaller samples and less expensive data collection efforts could be sufficient when using GPS data of higher spatio-temporal resolution. In that study it is suggested that GPS data should be considered as a realistic alternative or at least be used to complement SP surveys for VTT estimation. The potentially smaller required GPS sample could lead to more frequent GPS surveys for the purpose of capturing significant variations from the official values as we are entering in a period of constant change in the transport sector significantly influencing individual behaviour.

Chapter 4 presents a paper titled *"Accounting for distance-based correlations among alternatives in the context of spatial choice modelling using high resolution mobility data"*. The study proposes a Cross-Nested logit (CNL) model to capture unobserved spatial correlation among location alternatives based on Tobler's First Law of Geography postulating that *"Everything is related to everything else, but near things are more related than distant ones"* (Tobler, 1970). More specifically, a CNL nesting structure is specified, such that each destination is a nest of its own. The allocation probability to every nest is specified as a negative exponential function of distance, thus each destination is allocated with a non-zero probability to all nests, but with a higher allocation probability to its own nest. The proposed specification is the first application of a CNL model for a destination choice model. Previous attempts were based on variants of the Paired Combinatorial Logit (PCL) model (Chu, 1989; Bhat and Guo, 2004; Sener et al., 2011) and the Error Component model (Weiss and Habib, 2017), which due to their computational complexity are limited to being implemented in models of smaller choice sets. PCL, for instance, requires the specification of a nesting structure with nests for every possible pair of alternatives with the number of nests increasing as $\frac{J!}{(J-2)!(2)!}$, where J is the total number of alternatives in the choice set. Furthermore, the EC specification requires simulation during estimation, which significantly increases estimation times. The more flexible nesting structure of the proposed CNL specification for the destination choice model, allows its easy extension to more complex choice contexts, such

as a joint mode-destination model with an even larger choice set. For that joint model, a mode-destination alternative is allocated to mode and destination nests, but the allocation to destination nests further takes into account the distance among them as previously described for the destination model. In the current study, the proposed methodology is empirically tested on a destination and a joint mode-destination choice model of shopping activities utilising a GPS trip diary. For the destination choice model, the proposed specification is compared to a base MNL model that does not account for the presence of unobserved correlation among alternatives, a range of Nested Logit (NL) models nesting together destinations of similar geography and an equivalent PCL model with nests equal to the number of all possible pair combinations of alternatives. Similarly for the joint mode-destination choice model, the proposed specification is compared against a base MNL model, a NL model where mode alternatives of the same destination are nested together (Destination-over-Mode), a NL model where destinations reached by the same mode are nested together (Mode-over-Destination) and a CNL model in which each joint mode-destination alternative is equally allocated to destination- and mode-specific nests, but without accounting for the distance effect on the correlation among them. A PCL model could not be implemented for the joint model and an EC model could not be tested in general for the current choice models due to computational reasons, which are indicative of the limitations of those two approaches. In both contexts, the proposed CNL specifications manage to outperform the remaining models, while also being able to uncover significant unobserved correlation based on spatial proximity among destinations.

Chapter 5 presents a paper titled *"Augmenting Choice Models with Machine Learning techniques to capture the heterogeneity in Travel Behaviour"*. The current study presents an integrated framework combining an ML clustering and an MNL choice model for the purpose of capturing inter-individual heterogeneity for mode and destination choices. More specifically, the aim is to utilise a clustering algorithm at the upper level to allocate individuals probabilistically into latent clusters, while a choice model for each cluster is used to analyse their behaviour at the lower level. The two described components are estimated jointly, thus making the proposed specification a case of a Latent Class Choice Model (LCCM), where the clustering algorithm takes the role of class allocation commonly used in the traditional econometric LCCM specification. In order to achieve a proper integration between ML and DCM in an LCCM framework, the clustering component (class allocation) needs to be able to account for the probabilistic allocation of individuals into clusters (classes). The K-means clustering algorithm is utilised for that purpose, which is a deterministic clustering method aiming to minimise the distance of data points allocated to the same cluster, while at the same maximising the distance from the remaining ones. The transition to a probabilistic K-Means is achieved by considering the fact that there are still non-zero distances of data points from their allocated cluster centroids. Thus, the allocation probabilities of every point is calculated based on its distance to each centroid. The same principles around the transition from deterministic to probabilistic clustering can be applied to other similar algorithms, as well. The proposed specification is tested on two datasets, namely a GPS and a traditional pen-and-paper trip diary, and on a range of mode and destination choice models. It is also compared with a traditional econometric LCCM specification in which an MNL model takes the role of class allocation. The proposed integrated ML-DCM framework outperforms the traditional econometric LCCM in terms of model fit in all cases and more importantly it is able to provide a more intuitive behavioural profiling of the estimated latent clusters and also more realistic Values of Travel Time estimates. In addition, it excels particularly in cases of larger sample sizes, while it is also worth noting that it is easier to capture additional heterogeneity in the GPS data than the traditional RP data with the estimation of additional latent classes and the inclusion of more covariates in the class allocation/clustering component. Overall, the study clearly illustrates the benefits that can be achieved by combining the two approaches and it also provides opportunities for ML methods to be more widely adopted for policy making.

Chapter 6 presents a paper titled *"Probabilistic choice set formation incorporating*

activity spaces into the context of mode and destination choice modelling". Choice models typically are estimated by assuming that all alternatives are available to the decision makers. It has long been argued, however, that individuals might not be in a position to equally evaluate all the alternatives included in the global choice set, but rather use certain latent screening rules either due to cognition or due to space-time constraints. An important strand in the literature focused on analysing that aspect is mainly based on the framework proposed by Manski (1977), who first proposed decomposing the choice set generation from the choice itself. It has also been argued that misspecifying the choice set is another form of model misspecification with the same adverse effects, i.e. biased estimates, welfare and valuation measures (Williams and Ortuzar, 1982; Li et al., 2015). Empirical applications of probabilistic choice set generation have been applied almost exclusively in the context of mode choice, which generally offers a well-defined and limited choice set, while the problem is mostly ignored or avoided in spatial choice models due to their high computational complexity. That study aims to address that gap by focusing on the need to account for the inherently latent nature of the choice set in a spatial choice model by presenting an implementation of a probabilistic choice set formation approach suitable for a joint mode-destination choice model of shopping activities. The proposed specification is a Latent Class Choice Model (LCCM), in which individuals are probabilistically allocated into three classes by acknowledging that different sources of latent constraints might coexist at the same time affecting the individual's decision making process. As a result, each class has a different choice set as captured by a range of estimated proxy measures of different Activity Space forms, which largely refer to space-time constraints within a specific trip chain/tour and the individuals' general knowledge/awareness of the space around them and the opportunities within it. Contrary to past studies focusing on capturing spatial awareness and space-time constraints utilising traditional pen-and-paper trip diaries (Schönfelder and Axhausen, 2003; Schönfelder and Axhausen, 2004; Axhausen, 2007; Schönfelder and Axhausen, 2010), thus being subject of the aforementioned limitations (limited survey duration, recalled and often omitted trips), the 2-week semi-passively collected GPS trip diary utilised in the current study provides a richer and more suitable dataset in order to capture them more accurately. More specifically with regard to the specified latent classes, class 1 contains alternatives within estimated detour ellipses, which are used as proxy measures for capturing space-time constraints. Class 2 contains alternatives within estimated standard deviational ellipses, which are used as proxy measures for capturing spatial awareness. The last class includes all feasible alternatives from the global choice set, thus it has the purpose of capturing individuals who are more free to roam around the space within the study area. Different sets of parameters are also specified across classes for specific variables, thus inter-individual heterogeneity is captured both at the choice set and at the sensitivity level. The proposed specification is empirically tested on an MNL and an LCCM specification where heterogeneity is captured only based on the sensitivities of the different classes, without accounting for different choice sets across classes, outperforming both in terms of model fit. More importantly, however, significant insights are derived from such a framework, which could have a significant impact for proposing more effective policy measures on addressing the specific needs of individuals, while at the same time acknowledging the constraints they face.

Finally, **chapter 7** contains the discussion and the conclusions derived from the research presented in the previous chapters, while further avenues for future research are being discussed.

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Chapter 2

Utilising activity space concepts to sampling of alternatives for mode and destination choice modelling of discretionary activities

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Abstract

Choice models estimated or applied to datasets with large numbers of alternatives present significant challenges, leading to rapidly expanding computational cost, as well as potential behavioural realism issues since many of the alternatives included in the model may not be considered by the individuals. Sampling of alternatives has been a well-known method proposed to overcome the computational limitations mostly applied to choice models of residential location. Nonetheless, sampling protocols for destination choice models of discretionary activities require a different type of analysis, since the choice may depend on time-space constraints and familiarity on the alternatives in the choice set. The present paper makes the case that observing the general areas of travel for a period of days can provide important information of the individuals' whereabouts and the areas that they are more likely to visit, which can be used to better infer their choice sets. New emerging data sources, such as GPS tracking, can provide such information at a very high spatial resolution, which was not possible with traditional transport-related surveys. The present study, taking advantage of such a dataset, proposes a more behaviourally realistic sampling protocol to reduce the choice set utilising the geography-based concepts of activity spaces. Differential importance sampling rates are applied depending on the activity space and trip chain of the person making the resulting sampled choice set a function of person-specific spatial awareness and mode-specific time-space constraints. The performance of the sampling protocol developed is assessed using a model estimated on the full choice set and compared with random sampling and several other importance sampling protocols. The modelling outputs show that the proposed approach, incorporating both time-space constraints and individual spatial awareness, is able to produce less biased estimates, achieve higher sampling stability and statistical efficiency, while also avoiding overfitting.

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1 Introduction

Mathematical models capable of predicting the destinations of travellers are important for estimating transport demand levels. First introduced by McFadden (1973) and later expanded by Daly (1982), discrete choice models have emerged as the prominent tool for modelling disaggregate level destination choices. The large number of potential alternatives, however, poses two issues, namely behavioural realism and computational complexity.

Considering the full choice sets has the risk of leading to a behavioural misrepresentation of the individual-level decision making process, since in reality, the decision makers are highly unlikely to equally evaluate all the alternatives in the global choice set. Some of the areas of a city, for example, may just not be of interest to a given traveller, while some destinations may in fact be unknown (Fotheringham, 1988). The key problem is that the analyst is usually unable to observe or extract the true choice set evaluated by the decision makers and only assumptions can be made about it (Thill, 1992).

The problem of choice-set specification and its significance is well documented in the literature (Thill, 1992; Pagliara and Timmermans, 2009). In fact, estimating a model using an inaccurate choice set can be considered a case of model misspecification leading to biased estimates (Swait and Ben-Akiva, 1987). Pellegrini et al. (1997) showed that estimated parameters can depend significantly on the spatial distribution of the alternatives in the choice set and that it could vary among different market segments. Probabilistic choice set generation based on the theoretical foundations of Manski’s model (Manski, 1977) has been proposed as an approach of decoupling the choice problem into a choice set generation and an alternative choice sub-problem (Thill, 1992; Horni et al., 2011). Specifically, the final choice is defined as a two-stage process, where the probability that individual n will choose alternative i depends on the conditional probability of choosing alternative i from a choice set C and the probability of choosing choice set C from the universal choice set G , as shown in Equation 2.1.

$$P_{in} = \sum_{C \in G} P_n(i | C) P_n(C) \quad (2.1)$$

Manski’s formulation requires an exhaustive enumeration of all possible non empty choice sets, a process that quickly increases exponentially in complexity with the addition of more alternatives. Despite its appealing behavioural principles, it is generally considered not applicable in cases of large choice sets, such as in spatial choice models (Pagliara and Timmermans, 2009). Several variants based on the principles of Manski’s model have been proposed over the years aiming to relax the computational complexity (Swait and Ben-Akiva, 1987; Ben-Akiva and Boccara, 1995). Nonetheless, in many cases these modelling formulations adversely impact the behavioural realism of choice set generation (e.g. independent availability of alternatives) negating the main purpose of this modelling approach (Thill, 1992). Other Manski-inspired frameworks focused on introducing penalties in the utility function to minimise the probability of selecting alternatives exceeding certain upper/lower bounds on certain trip- and individual-specific constraints (Cascetta and Papola, 2001; Martinez et al., 2009; Haque et al., 2019). In addition to being critiqued on whether these models are able to replicate Manski’s principles (Bierlaire et al., 2010), they again rely to some extent on analyst assumptions (especially in terms of defining constraints), while the increased number of model parameters and the non-concavity of the log-likelihood function have also hindered their adoption in spatial choice models (Thill, 1992).

Despite the ongoing efforts to decouple choice set formation from the choice itself (Thill and Horowitz, 1997a), there have been critics of the importance of the choice set generation issue suggesting that the notion of model misspecification only has theoretical grounds (Lerman, 1985; Thill, 1992). It is argued that in an empirical setting, the choice probabilities of alternatives that are not in the actual choice set of an individual are likely to be negligible

provided the utility function is correctly specified (Thill and Horowitz, 1997b). On the other hand, if there are any significant omitted variables in the utility specification, for instance a latent time constraint, the correlation among the error term and the omitted variables will lead to non-intuitive results, such as yielding sign violations or high standard errors for the estimated parameters. In contrast, the behaviourally accurate estimates from an unconstrained model using the full choice set could still be considered as a sufficient representation of reality.

The above approaches are concerned with seeking to *understand* the choice process. Aside from relying on analyst assumptions, they do not address the second issue of working with large choice sets, namely the computational burden. In fact, especially for the Manski model, the computational cost is further increased. Even with much simpler models, and those that do not seek to incorporate any element of choice set formation, the computational cost of working with very large choice sets can be prohibitive in estimation, as well as application.

Sampling of alternatives has been proposed as a way to overcome the computational limitations of estimating choice models with a large number of alternatives, thus reducing the choice set and in turn the computational cost. McFadden (1978) showed that constraining a choice set by sampling of alternatives still yields unbiased estimates, if the true model is an MNL, by adjusting the utility function with the inclusion of an additional term, called the sampling correction term (*SC*). The bias in the estimated parameters, defined as the difference between the sampled estimates and the estimates obtained using the full choice set, will decrease as the size of the sampled choice set keeps increasing (Guevara and Ben-Akiva, 2013b). The specific choice set size beyond which only marginal improvements are observed in the accuracy of the sampled estimates is to be determined as a result of the analysis. As mentioned in Guevara and Ben-Akiva (2013b), the process of identifying the minimum required choice set size to achieve estimation stability is equivalent to the process of finding the required number of draws for the same purpose in a simulated Maximum Likelihood estimation for a mixed Logit modelling framework.

The additional SC term has the purpose of adjusting the utility function to account for the sampling bias, since the spatial distribution of the sampled alternatives will now depend on the sampling protocol developed and it may differ substantially among individuals. The additional term is computed as $\ln\pi(D_n|i, x_n)$, which is the logarithm of the probability of creating the choice set D_n given that alternative i was chosen for individual n . That can be also considered as a penalty added to the utility, since the $\pi(D_n|i, x_n)$ will always be between 0 and 1 and its logarithm will always be negative. In other words, the smaller the probability of sampling that choice set D_n given that alternative i is selected, the bigger the penalty applied. In that case the choice probabilities are modified as shown in Equation 2.2 and the *SC* term for stratified importance sampling without replacement is defined in Equation 2.3 (Ben-Akiva and Lerman, 1985; Guevara and Ben-Akiva, 2013a).

$$P(i | \beta, x_n, D_n) = \frac{e^{V(x_{in}, \beta) + \ln\pi(D_n|i, x_n)}}{\sum_{j \in D_n} e^{V(x_{jn}, \beta) + \ln\pi(D_n|j, x_n)}} \quad (2.2)$$

$$\pi(D_n | i, x_n) = \frac{J_{r(i)n}^*}{J_{r(i)n}} \quad (2.3)$$

where $J_{r(i)n}^*$ is the number of alternatives sampled from stratum r of alternative i and individual n and $J_{r(i)n}$ is the total number of alternatives in that stratum. The SC is calculated for each alternative i per choice task as if that alternative was chosen. It is clear to see that in cases of random sampling with a uniform probability from the global choice set, where $\pi(D_n | i, x_n) = \pi(D_n | j, x_n)$, the additional SC term remains the same across alternatives and hence it drops out (Nerella and Bhat, 2004). No correction is thus needed

with random sampling, but that is not the case with importance sampling. Guevara and Ben-Akiva (2013a) and Guevara and Ben-Akiva (2013b) extended this theory for stratified importance sampling in GEV and mixed logit models, respectively.

Given the need for corrections when using importance sampling, random sampling provides an easier to implement sampling protocol compared to the former. The limitation of random sampling, however, is that it leads to more deterministic models, since the sampled alternatives can be topologically not relevant to the chosen alternative. Therefore, the model will assign higher choice probabilities to the chosen alternative compared to the rest diminishing the explanatory power of the model. The insufficient number of close substitute alternatives to the chosen one, for small choice set sizes, leads a random sampling protocol to require choice sets of generally larger sizes in order to achieve the same level of estimate accuracy compared to an importance sampling protocol, making the former a less efficient approach. Various importance sampling techniques have been proposed in the literature, as opposed to a pure random sampling, aiming to create a reduced choice set that would best represent the individual’s trip-specific constraints (Li et al., 2005; Scott and He, 2012; Leite Mariante et al., 2018). Defining a realistic sampled choice set that would be in accordance with the individuals’ time-space constraints in the sample is of great importance to produce unbiased parameters (Landau et al., 1982), while also being more efficient than random sampling (smaller sampled choice sets). That can also provide the advantage of moving to more advanced modelling specifications that were not possible to be estimated using the full choice set. Examples can be found in empirical studies of mainly residential location choice (McFadden, 1978; Farooq and Miller, 2012; Guevara and Ben-Akiva, 2013a; Guevara and Ben-Akiva, 2013b). The implementation of importance sampling in a destination choice of discretionary activities, however, will require a different type of handling from a residential location choice, since the chosen alternatives will be subject on some degree to travel impedance and time-space constraints (Daly et al., 2014). Evidence also shows that availability-consideration of alternatives depends not only on time-space constraints, but also on the familiarity/awareness of those destinations (Landau et al., 1982; Thill and Horowitz, 1997a).

The current paper aims to propose a sampling protocol that utilises concepts of Activity Spaces (AS) from the time-space and behavioural geography literature, namely (1) Potential Path Areas based on detour factors around a previous origin O and a following destination D ; and (2) Ellipses incorporating a notion of the individuals’ awareness/knowledge of their surrounding space. The geography-derived notion of Activity Spaces is a tool capable of capturing time-space constraints and individual spatial awareness, and we use path areas and ellipses for creating person- and trip-specific spaces for importance sampling of mode-destination alternatives.

We rely on the notions of *Detour Ellipses (DEs)*, *Standard Deviatonal Ellipses (SDEs)* and *Familiarity Buffers (FBs)*, concepts that are looked at in detail in Section 3. To the best of our knowledge, SDEs and FBs have never been used before, on their own or in combination with DEs, for the purpose of delineating a choice set in a destination choice model, despite their extensive use in exploratory analysis studies of individual travel-activity behaviour. It is hypothesised that including an additional stratum delineated by SDEs and FBs would result in more accurate sampled choice set models (less biased estimates). That sampling protocol will result in constrained/sampled choice sets with most alternatives adhering to time-space constraints (within DEs) and also being familiar to the individual (within SDEs/FBs).

The remainder of the paper is as follows. In the following section, we give an overview of the relevant literature on time-space geography before expanding this to the context of sampling of destinations. In the third section, the modelling framework developed and the data utilised for the ensued practical application are presented. The results are presented next followed by a concluding section summarising the findings and setting the direction for future research.

2 Methodology

The present study aims to incorporate different forms of AS, namely DEs and SDEs/FBs in order to group the alternatives into three different spaces/strata for the purpose of stratified importance sampling. We will first review existing work on activity spaces in a general context, before extending this to destination sampling.

2.1 Activity spaces - general literature

Activity spaces (AS) originate from the work of time-space geography (Hagerstrand, 1970) and behavioural geography (Brown and Moore, 1970; Horton and Reynolds, 1970; Yuill, 1971) and they have been studied extensively since then for the purpose of understanding activity participation (Schönfelder and Axhausen, 2004; Schönfelder, 2006; Schönfelder and Axhausen, 2010; Kamruzzaman and Hine, 2012), trip chaining behaviour (Newsome et al., 1998), as well as physical activity (Zenk et al., 2011), instances of social exclusion (Schönfelder and Axhausen, 2003), intra-urban migration (Brown and Moore, 1970), criminal behaviour (Bichler et al., 2011) and even the potential spread of a virus (Yang et al., 2008). They are mainly used as a measure of describing the spatial distribution of visited locations and they incorporate a notion of individual spatial awareness (Manley, 2016) by providing invaluable information about the exposure to specific locations and activities that individuals might perform based on their usual mobility patterns and their time-space constraints. Due to the vast range of studies and application domains, there are several different forms of AS proposed in the literature depending on the aspect under examination in each case and the level of analysis. In a systematic review, Smith et al. (2019) summarised the different AS forms, which, amongst others include the following:

- Ellipses formed around two fixed points of a specific trip or trip chain, labelled here as *Detour Ellipses (DEs)*
- Ellipses formed around the observed trips of an individual during a survey period, most commonly known as *Standard Deviatonal Ellipses (SDEs)*
- Circles/buffer zones around frequently visited locations, labelled here as *Familiarity Buffers (FBs)*

We will now look at these three in turn.

2.1.1 Detour Ellipse

DEs is a form of what is known as Potential Path Areas (PPAs). PPAs originate from the time-space geography literature (Hagerstrand, 1970) and have been used extensively as the two-dimensional form of time-space prisms (Miller, 1991; Miller, 2005; Demsar and Long, 2016). A PPA, as depicted in Figure 2.1, is formed as an ellipse around two fixed locations, the foci of the ellipse represented as P_i and P_{i+1} , where these are usually the home and work locations, also referred to as *pegs* (Miller, 1991; Kamruzzaman and Hine, 2012). To complete the formation of the PPA, the available net time between the fixed activities performed in the two pegs is considered and an average travel speed is taken into account to identify the maximum area of potential travel within that time frame, while still having sufficient time to perform the intermediate discretionary activity (Miller, 1991). In a similar notion, however, other types of activity locations, except home-work, can be considered as the foci of the ellipse, as well, since there could be discretionary activities performed only in specific locations. A more sophisticated approach was proposed by Miller (1991) utilising real network travel speeds/times based on the time of day (e.g. peak/off-peak) and network constraints. The purpose of a PPA is to capture the reachable intermediate locations of discretionary

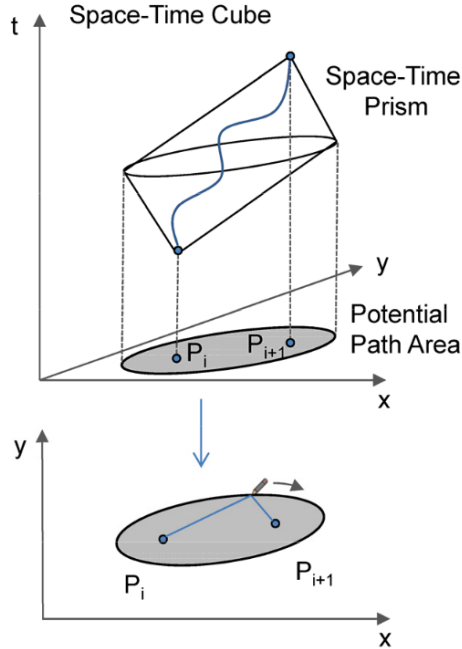


Figure 2.1: Two-dimensional projection of time-space prisms (Demsar and Long, 2016)

activities between the foci based on the individual’s time-space constraints, such as the chosen activity plan, activity duration and travel times.

The analysis for DEs/PPAs is performed at the level of trip/trip sequence, hence high resolution mobility data is required. As a consequence, the application of PPAs was initially limited due to the datasets available at that time (Miller, 1991; Newsome et al., 1998). That problem seemed to be resolved with the advances in GIS analysis (Miller, 1991) and more recently due to the increased data availability offered by emerging data collection methods, such as GPS, mobile phones etc. (Patterson and Farber, 2015). Some of the data limitations are however still relevant, described in Landau et al. (1982). Specifically, issues influencing time-space constraints and therefore the constrained choice set delineation, such as the preferred time spent in shopping location, departure/arrival time from previous/following fixed locations and even what type of activities can be considered fixed in space (e.g. social activities performed only in specific locations), cannot be resolved simply by using revealed preference data (Landau et al., 1982). Analyst assumptions are still required to overcome these issues.

The term *Detour Ellipse* is being used here instead of *PPA* to denote the method chosen to define them, which is based on the notion of *detour factor (DF)*. A DF is defined as the ratio of the sum of distances between O (previous origin)- S (shopping destination) and S (shopping destination)- D (next destination) and the distance between O - D , as defined in Equation 2.4 (Justen et al., 2013). In other words, a DF measures the deviation that an individual is willing to make to reach an intermediate shopping location S between the O - D (Leite Mariante et al., 2018) and it serves as a measure of spatial dependence among destinations in a trip/activity chain. It is also clear that $DF \geq 1$ should always hold. A DE explicitly accounts for time-space constraints without the need to make assumptions about the time allocation, hence it is not susceptible to some of the limitations outlined in Landau et al. (1982).

$$DF = \frac{l_{OS} + l_{SD}}{l_{OD}} \quad (2.4)$$

Previous studies have used fixed DFs for certain intermediate destinations to be considered along the path of observed O - D pairs (Cascetta and Papola, 2009). Newsome et al. (1998) created DEs based on the furthest visited intermediate location between home-work locations. Nonetheless, the DF would likely depend on the distance between O and D with longer OD distances resulting in smaller trip-specific DFs. That means that the individual would have reduced resources in terms of time and budget to deviate further away from the OD path. This relation between DF and OD distance has been taken into consideration in Justen et al. (2013), although their approach is limited by the fact that only average values per DF percentile are considered. Furthermore, it is likely that more factors could influence the DF besides the OD distance that have not been accounted for in their work, such as sociodemographic attributes of the individual, e.g. income, occupation status etc. and trip-specific characteristics, e.g. time of day.

2.1.2 Standard Deviational Ellipse

SDEs originate from behavioural geography (Brown and Moore, 1970; Horton and Reynolds, 1970; Yuill, 1971) and have been proposed as a measure of capturing the exposure of individuals to opportunities as a consequence of daily activities (Horton and Reynolds, 1971). ASs formed by SDEs are considered a subset of a larger latent *awareness space* (Brown and Moore, 1970; Patterson and Farber, 2015). In that sense, a SDE provides additional information on the individual awareness of certain destinations, that the DE/PPA is not able to provide. It should be noted, however, that the individuals would likely possess spatial knowledge that far exceeds the SDE formed around the observed destinations.

SDEs have been mainly analysed in social geography for the purpose of understanding human mobility patterns. Several measures can be extracted from a SDE that describe the mobility patterns of an individual, such as its shape (minor to major axis ratio), size (area, number of polygons located within etc.), orientation and eccentricity (Yuill, 1971). Temporal factors can also be taken into account, such as examining weekday/weekend differences (Srivastava and Schoenfelder, 2003; Smith et al., 2019) and their evolution over decades (Axhausen, 2007). Srivastava and Schoenfelder (2003) linked individual sociodemographic attributes with SDEs and found that workers tend to have more stable AS during weekdays with activities located between the two anchor points (home-work), while more variation is observed during weekends, similar to non-workers, as they seek to explore more discretionary activity options. Survey duration also plays an important role in the SDE creation. In a series of studies conducted by Schönfelder (2006) in his doctoral thesis on a number of datasets with different survey durations and from different countries, showed that surveys of longer durations are required in order to observe a stability in the mobility/activity patterns and hence to create more representative SDEs.

Contrary to DEs/PPAs, SDEs are formed around all of the visited locations (observed latitude/longitude coordinates) of an individual during the survey period. More specifically, a SDE is considered the two-dimensional equivalent of a standard 95% confidence interval. The procedure of defining a SDE requires the calculation of the covariance matrix of the latitude/longitude coordinates, the calculation of the rotation matrix and finally finding the points of the ellipse's perimeter (details can be found in Yuill, 1971). Weights can also be used for the latitude/longitude coordinates during the covariance matrix calculation for the creation of a weighted SDE based on trip frequency, activity duration etc. (Figure 2.2). The major axis of the ellipse indicates the axis of major dispersion and it is the regression line of latitude/longitude coordinates, while the orientation of the SDE depends on the correlation sign between them (Schönfelder, 2003). Destinations that are outside of a SDE are labelled

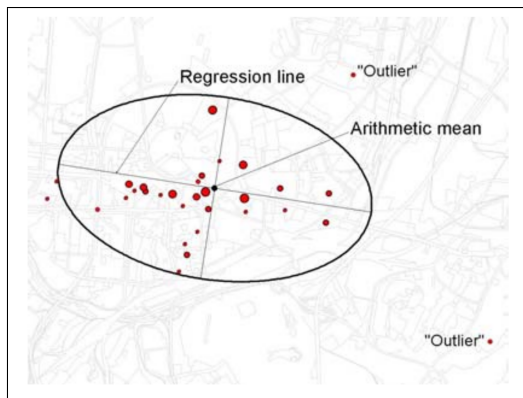


Figure 2.2: Weighted standard deviational ellipse around observed/visited destinations (Schönfelder, 2003)

as *outliers* and are generally considered as places that are not part of the usual movement areas of an individual .

2.1.3 Familiarity buffers

Buffer zones around frequently visited locations have been proposed as another form of AS used to capture the spatial awareness or the number and different types of services an individual is exposed to, similar to SDEs. Due to their ease of implementation, a large number of studies have implemented them. Among others, Larsen et al. (2009) defined buffers of 1.6 km and 500 m around school and home locations to define school neighbourhoods and the *immediate* home neighbourhoods, respectively, and identified factors of the built environment that might influence mode choice of children for their trips to school. van Heeswijck et al. (2015) specified buffers of approximately 20 minutes of walking distance (1.6 km) around visited destinations for the purpose of capturing the built environment within and how it might affect active travel specifically. Chaix et al. (2017) created buffers of 1 km (10-15 minutes of walking distance) around visited locations to capture the exposure of individuals to services located within those areas. Finally, Horni et al. (2011), in their conceptual choice set formation framework, proposed adding a buffer zone, equivalent to 15 minutes of walking distance, around home and work locations in a PPA ellipse formed between home-based work trips. Despite the aforementioned fixed buffers, an exposure weighting has also been applied for FB creation based on the type of activity performed, the visiting frequency or the time spent at those locations. An example is the study of Loebach and Gilliland (2016), where weighted buffers based on the time spent on locations around home were defined, labelled as the *habitual activity space*.

2.2 Applying AS approaches to destination sampling

Only a handful of studies, at least to the authors' knowledge, have combined time-space constraints and sampling of alternatives in order to further reduce computational complexity. Scott and He (2012) analysed shopping trips using real network travel times to create PPAs and to identify the reachable shopping destinations with a positive net activity time. Random sampling of the identified locations was applied to construct the final constrained choice set. This approach is subject to the limitations described earlier (Landau et al., 1982). Excluding destinations with a negative net activity time, by considering the observed departure/arrival times as fixed, fails to take into account the trade-offs the individual is willing to make in order to reach a certain destination. Even excluding the possibility of measurement errors and even if the analyst considers the activity scheduling choice dimension to precede the

choice of location, she cannot safely assume the same for the time allocation between those activity locations, such as departure-arrival time from/to different locations in a trip chain.

Leite Mariante et al. (2018) formed DEs (DF-based PPAs) for the purpose of sampling of alternatives for a destination choice model of different discretionary activity types. The DEs were defined based on the methodology described in Justen et al. (2013). The sampling protocol proposed involved selecting the chosen destination first and then sampling a number of alternatives from the space delineated by the DEs. In the case of not having enough sampled alternatives to reach the required choice set size, additional alternatives were sampled located outside the DEs. Mixed logit models were estimated utilising the methods proposed in Guevara and Ben-Akiva (2013a). The limitations of this study lie mainly on the sampling protocol developed and also on the DE formulation. Firstly, alternatives outside the DEs are sampled only in cases of an insufficient number of alternatives in the DEs. That means that many choice tasks will be estimated with choice sets containing alternatives only within DEs. That in turn can have significant implications on the estimation accuracy of parameters for spatial variables that generally lie in areas outside most of the DEs. Secondly, a problem could also arise in the case of small DEs. If we consider an example of a choice task/trip with a long distance between the previous O and the following D , then the chosen DF for the intermediate S would be small according to Equation 2.4 resulting in a small DE . Let us assume now that the created space within the DE contains only 2 alternatives, the chosen and an additional non-chosen destination, and the required choice set size is 50 alternatives (i.e. the largest choice set size in this study). That means that 48 additional alternatives will be randomly sampled from the remaining universal choice set, making that choice task/trip a case of almost pure random sampling from the universal choice set, which will result in choice sets with a large number of spatially irrelevant alternatives to the chosen one. Therefore, a more balanced sampling protocol would be required to address both issues. Finally, the created DEs depend only on the observed detour factors and on average values per quantile of the observed straight OD distances (previous O - following D) having an impact on the accuracy of the DEs both for chosen and non-chosen alternatives. Additionally, socio-demographic and trip characteristics that might influence the detour factor the individuals would be willing to choose in order to reach an intermediate shopping destination have not been taken into account.

The current study addresses the aforementioned limitations by formulating a range of stratified importance sampling protocols for shopping mode-destination alternatives and to provide a systematic comparison with random sampling. The main departure from the studies described so far, is to include SDEs and FBs alongside DEs and the corresponding activity spaces, to define strata for importance sampling. The space created within SDEs/FBs will provide an additional pool of alternatives to sample from and avoid the problems identified in Leite Mariante et al. (2018). In the case of small DEs, alternatives adhering to individual spatial awareness will be prioritised to be sampled in order to reach the required choice set size, instead of randomly sampling a large number of spatially irrelevant alternatives from the remaining global choice set. DEs for chosen/non-chosen alternatives are formed based on estimated DFs from an econometric model, thus being based on a more accurate representation of individual behaviour. Furthermore, we purposely refrain from excluding alternatives outside DEs and SDEs/FBs, in an attempt to accommodate extreme cases, to account for possible measurement errors during the DE and SDE/FB formation and finally to ensure that all alternatives will have a positive probability of being included in the sampled choice set. Therefore, regardless of the choice set size, alternatives outside DEs and SDE/FBs can still be sampled, albeit with a lower probability. Accounting for the fact that DEs and SDEs/FBs are just *proxy* measures of space-time constraints and spatial awareness, respectively, these will be used simply as *soft* constraints to create strata per individual from which to sample alternatives with a higher probability (importance sampling) and not to exclude alternatives outside of them.

The stratum constrained by the DE, labelled as T , aims to identify the most likely reachable destinations per mode combination (mode for first/shopping trip-mode for fol-

lowing trip). The stratum constrained by the SDE/FB (excluding the alternatives already within T), labelled as A , has the purpose of acting as a proxy for the individual’s spatial awareness/knowledge. That leads to the creation of a third stratum C , which is simply the remaining space outside T and A . The main assumption for the choice-set generation in this study is that alternatives that are more familiar and those that are in closer proximity to a specific trip chain between an O and D , are more likely to be considered and will contribute more in understanding individual behaviour than others. Therefore, the sampled choice set should include more alternatives from T , followed by alternatives from A and finally alternatives from C .

A simplified example is presented in *Figure 2.3* focusing on the context of the empirical application used later in the paper, which looks at destination choice for shopping activities. In the first subfigure, a choice task is presented, in which the individual starts from an origin (green cross) and during her trip to a destination (red cross), she chooses an intermediate shopping destination (purple circle) out of a set of available shopping destinations (blue circles). In total, there are 10 available destinations in the global choice set. The available transport modes for those two trips are combinations of car, public transport (PT) and walking. For simplicity, we assume that for that specific choice task, the only available mode combinations for the first/shopping and the following trip are *car-car*, *PT-PT* and *walking-walking*. Therefore, the global choice set consists of 30 mode-destination alternatives. In the second subfigure, the combined SDE-FB area of the individual is defined based on the observed destinations she visited during the survey period. Finally, in the remaining 3 subfigures, the estimated mode-specific DEs are defined for car-car, PT-PT and walking-walking, respectively, based on the modelling specification described in *Subsection 3.3.1*.

After the creation of the three strata (T , A , C) and the identification of the stratum of each mode-destination alternative, the following four different sampling protocols (without replacement) were compared with the model using the full choice set and were assessed in terms of parameter bias, sampling stability and forecasting performance:

- *Random sampling* with a uniform probability from the full choice set
- *AC* referring to sampling with a priority from A and then from C, such as $\pi(A) > \pi(C)$
- *TC* referring to sampling with a priority from T and then from C, such as $\pi(T) > \pi(C)$
- *TAC* referring to sampling with a priority from T, then from A and finally from C, such as $\pi(T) > \pi(A) > \pi(C)$

In the case of stratified importance sampling, a fixed number of alternatives is sampled per stratum with that number adhering to some notion of *importance* for a specific stratum relative to the rest. For that purpose and in order to avoid setting an arbitrary number of alternatives to be sampled per stratum, the stratum of each chosen alternative was identified by performing a spatial join between the strata and the observed mode-destination alternatives. The identified frequencies per stratum were then used as the *desired* share of alternatives from each stratum to be included in a choice set of a certain size. In the case of not having enough alternatives to reach that desired number per stratum, alternatives from the next stratum in line, as defined per sampling protocol, are sampled. The inclusion of a properly calculated SC term in the utility function will guarantee the estimation of unbiased parameters for sufficient choice set sizes, even when not reaching the desired number of alternatives from the respective strata. It is also assumed that alternatives that are being sampled and included in the reduced choice set are all considered equally by the individuals, hence no further consideration thresholds have been applied in the utility function (see for example Martinez et al. (2009)). The developed framework is summarised below:

1. Estimate a model using the full choice set to use as the base for evaluation comparison of the sampling protocols developed
2. Create PPAs based on estimated values derived from an econometric model

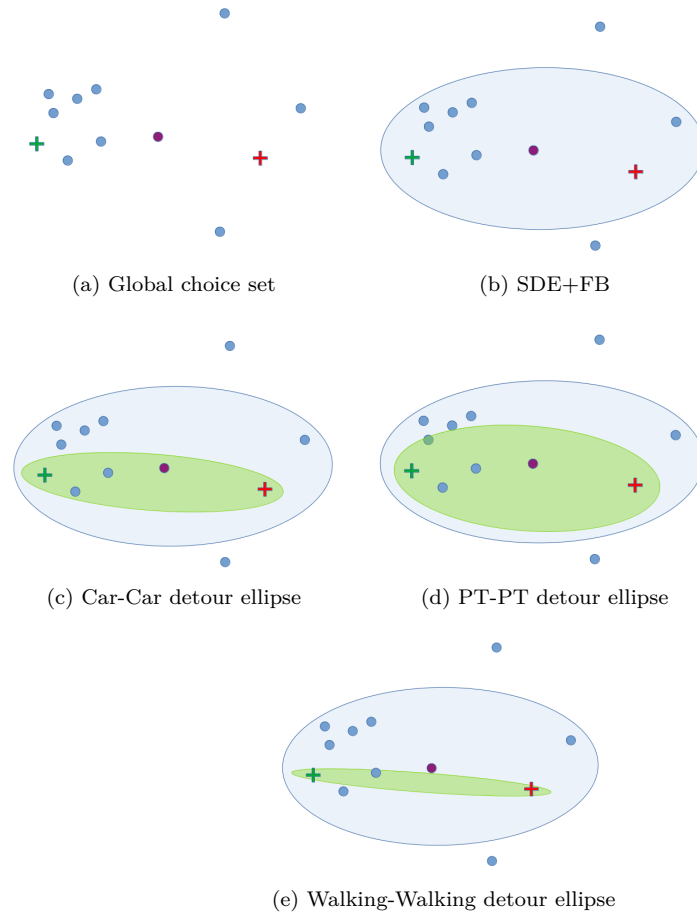


Figure 2.3: Example of sampled choice set specification

3. Create SDEs and FBs per individual using the observed destinations
4. Define the strata per choice task and individual
5. Define the sampling protocols to be compared
6. Perform sampling of alternatives from the respective strata for each sampling protocol and for different choice set sizes
7. Estimate models on the sampled choice sets using the same specification as in the full choice set model
8. Assess the performance of the sampled choice set models per sampling protocol and choice set size based on specific evaluation criteria proposed

3 Empirical application: data and model specification

This section discusses the data and its processing, before looking at model specification and the settings used for the AS approach to sampling of alternatives.

3. Empirical application: data and model specification

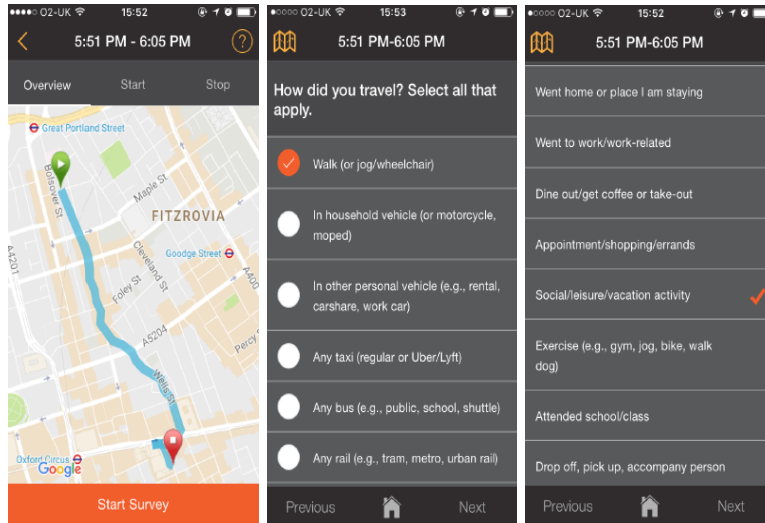


Figure 2.4: User interface of smartphone application used for the trip diary (Calastri et al., 2020)

3.1 Data

3.1.1 Original GPS data

The dataset used in the current study was collected as part of the research project “DECISIONS” carried out by the Choice Modelling Centre at the University of Leeds, during November 2016 and March 2017. The project aimed at observing individual decisions over a range of choice dimensions with an emphasis on travel, activities performed, both in-home and out-home, social networks and energy consumption over a period of 2 weeks. A detailed description of the survey and all of its different submodules (e.g. household survey, trip diary, energy consumption etc.) is presented in Calastri et al. (2020). For the purpose of the current study, only the trip diary and the household survey submodules were used. The trip diary includes all the trips that a participant made during the survey period. The trip diary was collected using a smartphone application that would record the GPS coordinates of each trip. The participants had to provide information regarding the chosen mode and the purpose of the activity performed at the end of each trip (Figure 2.4). In total, out of the 47,161 trips performed by 713 individuals, almost 75% of those were tagged with mode-purpose information. The majority of trips was within the region of Yorkshire and specifically around the city of Leeds. The household survey provided important sociodemographic information on the participants, such as gender, age, income, car ownership etc. which can be important explanatory variables in a behavioural model.

The analysis presented in the current study is focused on a specific type of discretionary activity, namely shopping. The study area was defined as the region of Yorkshire. Only individuals residing in the local authority of Leeds were selected, assuming they will have a similar knowledge of their surrounding shopping destinations having to adhere to the same spatial constraints (Thill, 1992). The purpose of the analysis is to understand where the individuals are more likely to go for shopping with respect to the previous and the following activity locations. Therefore, from the initial dataset, the shopping trips and their following trips were chosen for the subsequent analysis. The final dataset used in the analysis contained 1541 shopping trips and an equal number of following trips performed by 270 unique individuals (5.7 trips per individual, on average). Regarding the sociodemographic information of the individuals included in the sample, 64.1% were female, 32.2% between 30-39 years old and most of them employed (77%). The vast majority possessed at least one car in their household, while 20% had either a bus or rail season ticket.

3.1.2 Processing of data into trip chains

The shopping and their following trips were combined to create trip chains, which formed the basis of the analysis performed. Most trip chains, 66%, were from an origin O to an intermediate shopping destination S and then to another destination D , which will be referred to as O - S - D trip chain. The remaining trip chains, 34%, were from an origin O to a shopping destination S and then back to the origin O , which will be referred to as O - S - O trip chains. Shopping trips included three subcategories of shopping, namely grocery (82%), clothes (12.7%) and other types of shopping (5.3%), mainly for durables. The vast majority of following trips were trips going home (61.5%), while there was a small percentage (9.3%) of a consecutive shopping trip to a different shopping destination. From the remaining trips, 10.5% were for work/education, 11% for leisure/social and 7.7% were for other purposes. The present study is focused on a subset of modes of transports, namely car, public transport (PT) –as a combination of bus and rail– and walking. Most of the observed/chosen modes for the two legs of the trip chain were car-car (shopping-following trip) and walking-walking, namely 85.2%, while only 3% were PT-PT. Combinations of the three modes were also observed, such as car-PT, walking-car etc. and it was decided to include them in the analysis, despite their low mode share.

3.1.3 Definition of shopping areas

The shopping destinations for the study area were defined by clustering the elemental observed shopping trip destinations. Hierarchical Agglomerative Clustering (HAC) was implemented with a 800m distance threshold between the shopping trip destinations. The purpose of clustering the shopping destinations was to define general *shopping areas* and take advantage of the higher GPS data resolution, instead of limiting the analysis to the general geographical units in the UK (e.g. Middle or Lower Super Output Areas).

After defining the shopping clusters, their respective centroids were defined as the mean of the latitude/longitude coordinates of the elemental destinations in each cluster. The cluster centroids were then used to replace the original destination points of each shopping trip belonging to the cluster. Therefore, the main goal was to choose an appropriate distance threshold that would result in a small average distance difference between the original destination points of a cluster and its centroid. Because of that and after trying different distance thresholds between 500m-1000m, a 800m distance threshold was selected resulting in an average distance difference of 112m, while the maximum distance difference was 338m, which equates to between 4-5 minutes of walking (assuming a 5 km/h average walking speed). Larger distance thresholds resulted in distance differences of more than 5 minutes of walking distance, while smaller thresholds resulted in large shopping malls being split across two different clusters. In addition, visual inspection of the created clusters for different distance thresholds was performed in order to verify that distinct shopping areas were assigned to different clusters, with an emphasis on the main shopping areas of Leeds city centre. This procedure resulted in the creation of 176 general shopping clusters around the region of Yorkshire with most of them located around the city of Leeds. It is clear that shopping locations exist in other places within the study area, not captured by that process, mostly in areas outside the local authority of Leeds. Those shopping locations, which are never chosen by the individuals, are assumed to not having been considered by the individuals in the sample and hence are excluded from the subsequent analysis (Thill, 1992).

As a final step, a 400m buffer was created around the centroid of each shopping cluster to define the shopping areas. Therefore, a shopping area is defined as the space equivalent to 5 minutes of walking time around the cluster centroid. That high resolution of shopping area definition translates into having unique shopping malls, shopping districts etc. as separate destination alternatives. In the case of overlapping buffers, especially in Leeds city centre, the polygons within them were assigned to their closest cluster centroid (*Figure 2.5*). This ensured that each elemental shopping destination (in the form of polygons/individual stores)

3. Empirical application: data and model specification

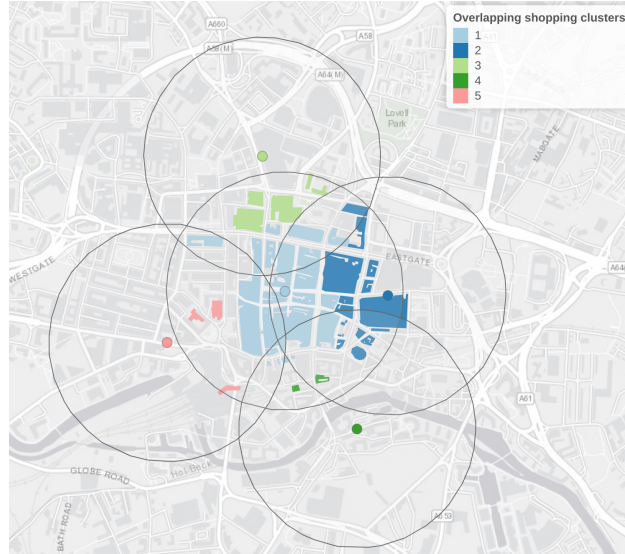


Figure 2.5: Allocation of retail polygons located within overlapping shopping clusters (OpenStreetMap contributors, 2021)

would belong to a single defined shopping area.

3.1.4 Data enrichment: level-of-service information and mode availability assumptions

In order to account for the fact that only travel times for chosen/observed alternatives were included in the dataset, travel times/distances were re-estimated both for chosen and non-chosen alternatives using the Bing Maps Routes API². The travel times/distances were recalculated also for the chosen alternatives for the sake of consistency (as also done in Calastri et al. (2018)). The total number of queries passed on the API were 1,627,296 (1541 trips \times 176 shopping destinations \times 3 modes \times 2).

For car travel cost, separate calculations for fuel and operating costs were performed using the UK's Transport Appraisal Guidance (WEBTag) specifications (Department for Transport, 2014). Parking cost was also calculated for trips with destinations in central areas/high streets across the region of Yorkshire based on information on hourly or fixed parking costs provided by the respective Local Authorities. Fuel, operating and parking costs were then added together to calculate the final car travel cost per trip. For PT, an average distance-based fare was used for bus and rail and a total PT cost was calculated per trip based on the information provided from the API regarding which leg was performed with bus or rail and what was its distance. Furthermore, a discount was applied for trips made by season ticket holders.

Deterministic mode availability was assigned in specific cases of trips based on the results obtained by the API. Such cases were PT trips in which the API returned only walking segments due to the small trip distance from the O or/and to the following D or the unavailability of PT services. For those trips, PT was assigned as unavailable. For the car trips, the availability was based on logical checks. For example, if a person chooses *Car* for the shopping trip, the grouping size is 1 and the following trip returns back to O (O - S - O trip chain), then only *Car* is available for the following trip. That is a clear indication that the individual is the driver and that she has to return her car back to O in the second trip.

²Details can be found here: <https://docs.microsoft.com/en-us/bingmaps/rest-services/routes/>

3.2 Full choice set model

In the current paper, it is assumed that a model estimated using the full choice set is considered the “true” model. Therefore, as a first step, a model using the full choice set is specified and estimated to act as the base for the assessment of the sampling protocols. Discrete choice modelling was used as the main methodological framework for the analysis (Ben-Akiva and Lerman, 1985). The analysis is performed at the level of the trip chain, which is defined as two consecutive trips, namely a shopping trip from an origin O to an intermediate shopping destination S with a mode k and a following trip to another destination D with a mode j . The behavioural model developed aims to understand the choices of modes k and j and of destination S for shopping trips in a joint fashion. In that context, the locations of O and D are considered as fixed for each choice task. Therefore, the full choice set consists of 3 modes for the first/shopping trip, 3 modes for the following trip and 176 shopping destinations, for a total of 1584 combined mode-destination alternatives. The choice of activity, i.e. travelling for shopping, is assumed that precedes the choice of mode-destination and is therefore considered exogenous. Furthermore, it is assumed that the choice of trip-chain complexity, i.e. perform a complex O - S - D trip chain by including a shopping trip on the way to work or perform a simple O - S - O trip chain, comes before the mode-destination choice dimension, a finding also described in Ye et al. (2007).

The specification proposed by Daly (1982) was utilised with the presence of level-of-service (LOS) variables, quality locational variables and lastly a number of size variables specified inside a composite log term (Equation 2.5). Deterministic taste heterogeneity is captured through the interaction of Alternative Specific Constants (ASCs) and LOS variables with sociodemographic covariates. Random heterogeneity has not been included (with the specification of mixed MNL models) due to the high estimation times of the full choice set model. Interactions with categorical sociodemographic variables were specified as shifts from the base level of the ASC, while non-linear interactions were specified for continuous sociodemographic variables, namely personal income interacted with travel cost and shopping duration interacted with travel time and walking distance.

$$V_{kj,S} = \sum_{r \in L} \beta_r x_{r,kj,S} + \sum_{r \in D} \beta_r y_{rS} + \phi \log(A_S) \quad (2.5)$$

where $x_{r,kj,S}$ is the r -th element of a vector L of LOS attributes for mode combination kj and shopping destination S , y_{rS} is the r -th element of a vector D of quality locational attributes for destination S and A_S is the composite size measure capturing the attraction of destination S defined as:

$$A_S = a_{1S} + \sum_{r>1} \exp(\gamma_r) a_{rS} \quad (2.6)$$

where a_{1S} is the attraction attribute used as a base with a γ parameter normalised to 1.0, a_{rS} are the additional attraction attributes of destination S relative to the base attribute and γ_r are the parameters to be estimated capturing the effect of those attributes on the attraction of that destination. The γ_r parameters are constrained to be positive by specifying them inside an exponential function.

The attraction of neighbouring destinations, at various distances away of the visited destination, has also been included in the size of the visited destination to capture the effects of trip chaining behaviour (Kitamura, 1984; Kristoffersson et al., 2018). It is believed that a destination with more surrounding shopping destinations will be perceived as more attractive compared to a more isolated destination, all else held equal.

3.3 Sampling strata formation

In the current subsection, we focus on the steps taken in order to form the different strata used for the subsequent practical application.

3.3.1 Creation of Detour Ellipses

For the DE creation, the limitation to overcome was having information only for the observed DFs referring to the chosen mode combination and shopping destination. Different mode combinations, however, would likely result in different space-time constraints and hence lead to different DFs. For instance, a mode combination of walking-walking is expected to result in a smaller DF compared to car-car, all else held equal. Furthermore, sociodemographic and trip-specific attributes could also influence the deviation an individual is willing or able to make in order to reach an intermediate shopping destination. Because of those reasons, the observed DFs and a number of trip-related, locational and sociodemographic explanatory variables were used to estimate a continuous model for DFs. The purpose of the estimated linear regression based DF model was to produce predicted values for the DFs for all of the 9 mode combinations per trip, both chosen and non-chosen, thus overcoming the limitation of having DFs only for the observed mode combinations while ensuring consistency. The estimated DFs were then used to produce DEs that are based on mode-specific, trip-specific and individual-specific time-space constraints of the participants in the sample and not simply on the observed/visited intermediate shopping locations. The DF modelling framework is described in further detail in *Subsection 3.3.2*.

3.3.2 Detour Factor modelling framework and outputs

Prior to the DF model specification, the trip chains were grouped into those starting-finishing at the same location, i.e. *O-S-O*, like a simple *Home-Shop-Home* tour, and those starting-finishing at different locations, i.e. *O-S-D*, such as a typical *Home-Shop-Work* trip chain. Therefore, two different continuous models were estimated for each case using Maximum Likelihood estimation.

For *O-S-D* trip chains, it was assumed that the observed DFs follow a lognormal distribution. In addition, the model specification has to guarantee that the estimated DFs will always be above 1.0. As a result, the specification in *Equation 2.7* was proposed to account for that, where y_i is the observed DF for trip i , x_i is a vector of mode-specific, trip-specific (including the straight *OD* distance), locational and sociodemographic explanatory variables and b_{x_i} are the respective parameters to be estimated. The disturbance term for the log-transformed DF is assumed to follow a normal distribution with $N(0, \sigma)$, where σ is the standard deviation that is estimated alongside the rest of the parameters. For the predicted DFs, the term $\frac{\sigma^2}{2}$ is added to the rest of the model as the unbiased estimator of the standard deviation.

$$\log(y_i - 1) = \Sigma b_{x_i} x_i + \sigma \Rightarrow E(y_i) = 1 + e^{(\Sigma b_{x_i} x_i + \frac{\sigma^2}{2})} \quad (2.7)$$

Since the aim of this part of the analysis was to produce as accurate predictions as possible for the DFs, Bootstrap sampling (Daly et al., 2020) was used in addition to MLE for a more robust assessment of the standard errors. After trying different numbers of Bootstrap samples and checking the differences between the mean of the Bootstrap estimates and the MLE estimates, it was decided to use 500 samples for the *OSD* model, since at that number of samples the average of the Bootstrap estimates showed only negligible average absolute percentage differences from the MLE estimates, namely 0.018. The t-ratios were then calculated as the ratio of the MLE estimate and the Bootstrap sampling standard deviation.

Table 2.1: Modelling outputs of the DF model for *O-S-D* trip chains

Parameters	MLE Estimates	Bootstrap sampling st.dev.	t-ratios
<i>Constant</i>	-0.8363	0.1734	-4.82
<i>Natural logarithm of O-D straight distance (km)</i>	-1.3253	0.0701	-18.92
<i>Car-Walking</i>	-1.8934	0.3206	-5.91
<i>PT-PT</i>	1.0609	0.3722	2.85
<i>Walking-Car</i>	-1.4617	0.3946	-3.70
<i>Walking-PT</i>	-0.6875	0.2904	-2.37
<i>Walking-Walking</i>	-1.6766	0.2425	-6.91
<i>Shopping: Clothes - Other</i>	0.6526	0.1895	3.44
<i>Household size: 3-4 members</i>	0.4733	0.1750	2.70
<i>Part time workers</i>	-0.3908	0.1726	-2.26
<i>Occupation: Students</i>	0.5936	0.3216	1.85
<i>Occupation: Other</i>	0.4199	0.2322	1.81
<i>Time of day: Weekend morning</i>	0.7590	0.2158	3.52
<i>Parking areas 400m around shopping cluster</i>	0.0182	0.0033	5.59
<i>Sigma</i>	2.0252	0.0613	33.03

The estimated parameters and the standard errors, presented in Table 2.1, refer to the Maximum Likelihood estimates and the standard deviation of the respective Bootstrap parameters. The best-performing model resulted in a Root Mean Square Error (rmse) of 4.35, a mean absolute error of 1.09 and a correlation between predicted and observed DFs of 0.69. Regarding the estimated parameters, the larger the *OD* distance (log) the smaller the DF, as expected due to the time limitations to reach those destinations and participate in the respective activities. All of the mode combinations would result in a smaller DF compared to the base mode combination of car-car. The only exception is PT-PT that results in a larger DF than car-car, all else held equal. Worth-noting is also the finding that individuals going for clothes shopping or for other types of durable shopping are willing to deviate more from the direct *OD* route compared to travelling for groceries. That is in accordance with prior expectation, since clothes shopping is an activity generally performed in more “relaxed” days of the week and times of day, hence there is more freedom to roam around the urban environment. Likewise shopping for durables usually requires going to specialised stores (e.g. IKEA), hence the individuals are willing to choose larger DFs to reach those destinations. On the other hand, grocery shopping is considered mostly a necessity and the individuals are usually trying to fit that in their everyday or weekly schedule with smaller deviations from their routing plan.

For *O-S-O* trip chains, a different modelling approach had to be formulated, since for those cases the $l_{OD,i}$ is 0, hence the DF cannot be defined. Consequently, the straight distance (in km) $l_{OS,i} = l_{SD,i}$ was selected as the dependent variable for those trip chains, which again it is assumed that follows a lognormal distribution. As a result, the modelling formulation of Equation 2.8 is proposed, where y_i is the observed straight distance $l_{OS,i}$ for trip i and as previously x_i is a vector of mode-specific, trip-specific, locational and sociodemographic explanatory variables and b_{x_i} is a vector of parameters to be estimated. As in the DF model, the unbiased estimator for σ was used for the predicted distances.

$$\log(y_i) = \Sigma b_{x_i} x_i \Rightarrow E(y_i) = e^{(\Sigma b_{x_i} x_i + \frac{\sigma^2}{2})} \quad (2.8)$$

A similar Bootstrap sampling approach was performed for *O-S-O* trip chains, as well, with 500 samples resulting in a very small mean absolute percentage error of 0.025. The

Table 2.2: Modelling outputs of the travel distance model for *O-S-O* trip chains

Parameters	MLE Estimates	Bootstrap sampling st.dev.	t-ratios
<i>Constant</i>	0.3664	0.0951	3.85
<i>Walking-Walking</i>	-1.4375	0.0797	-18.76
<i>Shopping: Other</i>	0.5167	0.1667	3.32
<i>Time of day: Night</i>	-0.3542	0.1527	-2.41
<i>Following purpose: Social-Leisure</i>	-0.7769	0.1999	-4.01
<i>Age: 18-24</i>	-0.2366	0.0617	-3.71
<i>Parking areas (linear)</i>	0.0047	0.0016	2.89
<i>Retail areas (log)</i>	0.0821	0.0244	3.29
<i>Household Income: 40000-50000 GBP/year</i>	-0.2008	0.0894	-2.44
<i>Household Income: No reporting</i>	0.4776	0.1500	3.54
<i>Shopping activity duration</i>	0.2078	0.0537	4.30
<i>Sigma</i>	0.6526	0.0327	20.61

best-performing model, presented in Table 2.2, resulted in an rmse of 1.99, a mean absolute error of 1.13 km and a correlation of 0.68. Only the mode combination of walking-walking showed significant differences to car-car (base) indicating a lower distance as expected for trips made by walking in both legs. Other types of shopping, i.e. durables, resulted in a higher accepted distance, while smaller distances are accepted for trips chains where the following trip is for social/leisure purposes. Finally, individuals who did not report their household income were found to accept larger distances.

The mode-specific predicted DFs and straight distances produced from the aforementioned procedure, were used to construct the DEs (detour ellipses and circles), representing the boundaries of potentially reachable areas or PPAs for a specific trip and mode combination with fixed *O*s and *D*s. For *O-S-D* trip chains, the predicted DFs were used to create DEs following the procedure described in Justen et al. (2013). For *O-S-O* trip chains, the predicted distance was simply used as the radius of a circle with its centre being the location of *O*.

3.3.3 Creation of Standard Deviatonal Ellipses

As mentioned before, SDEs were defined for the purpose of capturing spatial familiarity or awareness of the individual’s surrounding space. The SDEs were constructed using all of the observed destinations during the 2-week survey period. To achieve the most accurate representation of the AS of a participant, the untagged trips were used, as well. For this study, due to the high resolution of GPS data, latitude/longitude coordinates for all trips were unique even if a specific destination was visited more than once. Therefore, by using all of the observed destinations, the calculation of SDE was similar to a weighted SDE based on trip frequency. As a result, the created SDEs are shifted towards destinations that are more frequently visited.

After the SDE creation per individual, various metrics can be derived describing their mobility patterns during the survey period with the most important being the ratio between the minor/major ellipse axis (b/a). A ratio close to 1.0, i.e. $b = a$, would lead to an ellipse closely resembling a circle indicating that either an individual tends to roam more randomly around space or that the survey duration was probably not enough to capture the regularity of her travel. On the other hand, a small ratio, leading to an ellipse resembling a straight line, would indicate that this person has a quite tight schedule or limited resources to deviate from her usual axis of travel. It would be useful to note that on average the b/a ratio is 0.39 indicating that well-balanced spatial distributions of individual mobility patterns were captured even in the arguably limited 2-week survey duration. It may be noted that

the mobility patterns and hence the axes of the SDEs are expected to be functions of the sociodemographic characteristics of the person. For instance, the b/a ratio of workers is likely to be smaller than part-time workers or non workers due to their potentially non-flexible schedules.

3.3.4 Creation of Familiarity Buffers

In addition to the SDE, FBs are also defined around each destination, mainly inspired by the previous work of Horni et al. (2011), described in *Subsection 2.1.3*. FBs had to be defined around each unique destination. For that purpose, the initial GPS destinations had to be clustered to define unique visited locations per individual. The GPS latitude/longitude coordinates were clustered using HAC with a 200m distance threshold. The distance threshold of 200m means that on average the points assigned to a cluster will have a distance difference of around 100m between them. Only in the extreme case of a cluster with 2 points, those points would have a distance difference of 200m. Different thresholds were tested between 50m-300m, with 200m resulting in the most accurate results following a visual inspection of the clusters created in each case. From that process, home-work clusters/locations were identified based on the purpose of trips assigned to those clusters.

In the current study, a buffer equivalent to 15 minutes of walking distance (1200 m) was created around the home location of each individual. Following that, buffers around the remaining visited destination clusters were created with a radius relative to the one of their home-cluster as per the following *Equation 2.9*:

$$r_{C_{j,i}} = \frac{nTrips_{C_{j,i}}}{nTrips_{C_{H,i}}} r_{C_{H,i}} \quad (2.9)$$

where $r_{C_{j,i}}$ is the buffer radius of familiarity cluster j for individual i , $nTrips_{C_{j,i}}$ and $nTrips_{C_{H,i}}$ are the trips to familiarity cluster j and to home-cluster H , respectively, and $r_{C_{H,i}}$ is the buffer radius of the home-cluster H which in the current study is fixed to 1200m.

It was assumed that the home cluster should have the majority of trips, therefore the largest buffer radius. As a result, in cases where other non-home clusters attracted more trips, those familiarity buffers were fixed to have the same radius as the buffer of the home cluster. The rationale for that, was that the home-cluster should always attract the highest number of trips and the cases where that was not observed could be attributed to the limited survey duration of 2 weeks and/or missing observations.

Contrary to Horni et al. (2011), in the current study the created FBs were subsequently merged with the previously defined SDEs, instead of the DE/PPA. That was decided since the FBs carry a notion of spatial awareness similar to the SDE and are not a result of trip-specific time-space constraints as the DE/PPA. The merged SDE/FB resulted in a common space of places, where the individual is likely to possess a better knowledge/awareness of the surrounding shopping opportunities compared to the rest of the study area. Furthermore, the addition of FBs into the previously created SDEs ensures that *outlier* locations outside of the SDE would still contribute to the spatial awareness of the individual. Those locations, even if they are not part of the usual movement patterns of the individual, they are still visited, hence the individual would likely possess some knowledge of their surrounding space.

3.4 Definition of sampling protocols

After the creation of DEs and SDEs/FBs, the different sampling strata, T , A and C , were defined. On average, 67% of the chosen shopping destinations are located within T , 28.2% are located within A and the remaining 4.8% within C . Not all alternatives within DEs are also within SDEs/FBs and vice versa, since there can be cases of trips performed outside the

usual movement spaces captured by SDEs/FBs. The aforementioned percentages were used to define the sampling probabilities for each stratum and they conform to our initial objective of having $\pi(T) > \pi(A) > \pi(C)$. That way, regardless of the total number of alternatives in the choice set, there will be more alternatives sampled from T , compared to the other 2 strata, provided there are enough alternatives within that space to sample from.

For the TAC protocol, on average there are 76 alternatives located within T , 403 within A and 846 within C per choice task/trip. Using the TAC protocol, if there are not enough alternatives in T to account for the 67% of the choice set, such as in the case of a long trip with a small estimated DF and resulting DE, then alternatives from A are sampled to reach that number, in addition to sampling the pre-specified number of alternatives from stratum A (i.e. 28.2%). The remaining number of alternatives required to reach the choice set size are always sampled from C .

The sampling probabilities for the TC protocol are 67% from T and 33% from C , since in that case C contains all alternatives outside T . On average, there are 76 alternatives located within T and 1249 within C per choice task/trip. Contrary to TAC , in cases of an insufficient number of alternatives in T , the remaining alternatives are sampled from C resulting in a higher probability of including alternatives in the choice set that are not relevant to the time-space constraints of the trip and to the individual's awareness, since the TC protocol lacks that notion of spatial awareness ingrained in TAC .

The sampling probabilities for the AC protocol are 91.5% from A and 8.5% from C . On average, there are 468 alternatives within A and 859 alternatives within C . That sampling protocol is used to illustrate the fact that by prioritising only the spatial awareness of the individual and neglecting the time-space constraints is still not as efficient as TAC that incorporates both. Finally, *Random sampling* is used for comparison reasons illustrating the evident limitations of that approach and the clear advantages of importance sampling protocols using AS concepts.

For each sampling protocol examined, a set of increasing choice set sizes was tested, between 10 and 250 alternatives, examining the rates of estimate improvements (*decreasing bias in the estimates and smaller standard errors*). Furthermore, for each choice set size per sampling protocol, five different choice set realisations were sampled and used for model estimation to assess model stability in terms of sampling standard deviation of estimated parameters and to eliminate the possibility of a lucky/unlucky draw. The estimated parameters, the standard errors and the fit statistics of the models estimated with sampled choice sets are compared with those of the full choice set model. It is expected that the sampled choice set models will produce unbiased estimates after a sufficient choice set size, meaning that parameters with only negligible differences from those of the full choice set model are obtained. The full choice set model, however, is expected to produce more efficient estimates (lower standard errors), but at the expense of higher estimation times, which in many application cases can be prohibitive. It may be noted that the *true* model used as a base for the evaluation of the sampling protocols refers to an MNL model using the full choice set. It should be stated, however, that the full choice set model should not be considered as the most accurate representation of individual shopping behaviour, but only as a *sufficient* one, since the true choice set per individual will always remain latent in the context of a spatial choice model.

4 Results

4.1 Full choice set model outputs

The MNL model using the full choice set in this case produced reasonable estimated parameters, VTT estimates and demand elasticities in accordance with official specifications as described in the following paragraphs.

4.1.1 Variable selection

The variables used in the subsequent modelling analysis can be categorised into level-of-service (LOS) and locational variables. The former capture the travel impedance to a specific destination with a specific mode of transport, while the latter aim to capture the attraction of certain characteristics of the shopping destinations. These are described in the following paragraphs.

Regarding LOS variables, travel time for car and PT and travel distance for walking were selected. For PT, travel time was segmented into in-vehicle time (IVT), first access time, last egress time and the remaining out-of-vehicle time (OVT) containing waiting time and time between transfers. The parameter for travel time was specified having the travel time for car for the shopping trip as the base and then having multipliers for the sensitivities of PT travel time components and for the travel time of the following trip in order to capture their difference with respect to the base (car time for shopping trip). A similar approach was implemented for walking distance, as well, by having the travel distance for the shopping trip as the base and then having a multiplier capturing the sensitivity difference for the following trip. For travel cost, a generic parameter was specified across modes (car/PT) and trip legs (shopping/following trip).

Characteristics of the shopping clusters and their respective surrounding areas were also defined, in buffer zones of 400m (immediate area), 400-1000m (small distances), 1000-2000m (medium distances) and 2000-5000m (large distances). Those characteristics, including parking areas and retail/commercial store areas extracted from OpenStreetMaps (OSM) and population and average residential price statistics during the years 2016-2017, were acquired from the Office for National Statistics (ONS). Specifically, the average residential prices were computed around shopping and home clusters (400m buffers - immediate area). Furthermore, the weighted price averages for home and shopping locations were discretised into quartiles to analyse whether e.g. people living in richer areas (fourth quartile of average residential prices) are willing to go shopping in poorer areas (first quartile of average residential prices) or vice versa. The rationale behind that variable specification is that the immediate environment around the home location will have an influence on the behaviour of the individual. The prior expectation was that individuals living in richer areas will have a lower probability of choosing shopping destinations located in poorer areas (Pellegrini et al., 1997).

Shopping store variability was captured using Shannon’s entropy (H_k) (Equation 2.10) (Shannon, 1948; Whittaker, 1949) measuring the percentage of the area covered by specific store type $t \in T$ inside a shopping cluster k . Shannon’s entropy has been widely used to quantify land-use variability mostly in studies related to walkability (Brown et al., 2009; Mavoia et al., 2018) and urban sprawl (Effat and Elshobaki, 2015). In the current study, it is used to see whether an increased variability in store types adds to the attraction of a shopping destination. A key thing to note here, is that n should refer to the total number of unique store types across all shopping clusters and not only in the cluster in question in order to ensure a proper comparison among different locations (Hajna et al., 2014). In total, 101 unique shopping store types were included in the shopping clusters based on the OSM data. The H_k calculated for each cluster k ranges from 0 to 1, with higher values denoting large store type variability and vice versa, while values around 0.5 indicate a more balanced distribution of store types within a shopping destination.

$$H_k = - \frac{\sum_{t=1}^T (p_t \ln(p_t))}{\ln n} \quad (2.10)$$

In addition to the above, the location of the most popular retailers in the UK market per shopping type, grocery-clothes-durables, was identified across the study area and matched with the shopping clusters. For grocery shopping, the focus was on the “Big Four” retailers, namely Tesco, Sainsbury, Asda and Morrisons, as referred to in Rhodes (2018) and also

reported in Kantar world panel (2020) website for the end of 2017, holding 70.7% of the total market share in the UK. For clothes shopping, the analysis was focused on the top 3 retailers for the year 2018/19 as reported in Retail Economics (2020) website, namely Marks & Spencer, Next and Primark. Finally, for durable shopping, the focus was on IKEA, as it is a well-established brand in that sector achieving a market share growth for the sixth consecutive year at 2017 and accounting for 8.1% market share according to their 2017 annual report (IKEA, 2017). A binary dummy variable was created for each one of the aforementioned stores based on whether they are located within a 400m buffer radius around a shopping cluster centroid.

4.1.2 Estimated parameters

The fit statistics of the full choice set model, together with the estimated parameters, their standard errors and the t-ratios are depicted in Table 2.3. Overall, the model achieves a high level of performance with an adjusted rho-square of 0.6162 and an average choice probability for correct predictions of 0.18 having a choice set of 1584 mode-destination alternatives. The main limitation that the sampling approach will aim to address is the high estimation time of more than 5 hours. Regarding the behavioural interpretation of the estimated parameters, it should be mentioned that, all else held equal, individuals with car ownership in their households have a positive inherent preference for car compared to PT and walking. Cost sensitivity, specified using a box-cox transformation, decreases as income increases with a sensitivity of -0.2435, which is close to the value (-0.3) proposed in Daly and Fox (2012) for non-work trips (cited in Sanko et al., 2014). Time (linear) and distance (box-cox) sensitivities of following trips are shown to be higher by 35.7% and 25.2%, respectively, than for the first shopping trip. Furthermore, time and distance sensitivities tend to decrease with the increase of shopping duration, as captured by the respective shopping duration elasticities.

Individuals living in areas of high residential prices are less likely to go shopping in areas with low residential prices, all else held equal, a finding also discussed in Pellegrini et al. (1997). Retail areas per store type (clothes shopping, groceries and other types of shopping) act as significant attractions for trips of their respective shopping types. Moreover, the presence of major retailers per shopping category, also has a positive impact on the utility function. Finally, shopping store diversity captured using the Shannon's entropy (Shannon, 1948; Whittaker, 1949) was found to be a significant attractor both in the immediate area of a shopping destination (400m buffer) and also in medium distances (1000-2000m buffer) for *O-S-D* trip chains with two consecutive shopping trips. It is acknowledged that there is an inherent uncertainty behind the reasons for making a subsequent shopping trip, since that could be a result of a pre-planned activity scheduling, of product unavailability in the first shopping destination, or simply a result of a random event (Kitamura, 1984). The final specification presented here shows that the attraction of neighbouring destinations, captured through shopping diversity, adds to the attraction of the visited destination only for cases where the individuals are going to make a subsequent shopping trip. The same was not true for cases where the following trip is for a different type of activity. That could serve as an additional indication that the choice of a daily activity plan generally precedes the mode-destination choice.

4.1.3 Value of Travel Time estimates and demand elasticities

Value of Travel Time (VTT) estimates and demand elasticities from the full choice set model were also computed to assess the performance of the sampling protocols. In Table 2.4, the VTT estimates of the full choice set model are presented in GBP/hour, namely the VTT for car, PT in-vehicle time, PT first access and last egress time and the remaining PT out-of-vehicle time, both for the first/shopping and the following trip. The VTTs were calculated as the ratio of the partial derivatives of the respective variable (i.e. car time, PT

Table 2.3: Modelling outputs of the full choice set model

Fit statistics	Value	
<i>Log-likelihood (0)</i>	-11045.05	
<i>Log-likelihood (model)</i>	-4184.126	
<i>Adjusted Rho-square</i>	0.6162	
<i>AIC</i>	8478.25	
<i>BIC</i>	8771.96	
<i>Number of individuals</i>	270	
<i>Number of observations</i>	1541	
<i>Estimation time (min)</i>	322	
<i>Average choice probability of correct prediction</i>	0.18	
Parameter	Estimates	Rob. t-ratios 0 (* t-ratios 1)
Locational constants		
<i>Constant rest Yorkshire</i>	0.5494	3.77
Households with car ownership		
<i>Constant Car-Other (PT/walking)</i>	-2.7299	-10.01
<i>Constant Other (PT/walking)-Car</i>	-0.8606	-3.69
<i>Constant PT-PT</i>	-1.0775	-2.63
<i>Constant PT-Walking</i>	-1.5518	-3.29
<i>Constant Walking-PT</i>	-1.2089	-2.51
<i>Constant Walking-Walking</i>	0.8418	2.32
Mode shifts for households with no car ownership		
<i>Constant Car-Other (PT/walking)</i>	2.3264	3.64
<i>Constant Other (PT/walking)-Car</i>	0.6329	1.06
<i>Constant PT-PT</i>	4.2697	8.70
<i>Constant PT-Walking</i>	3.3536	5.83
<i>Constant Walking-PT</i>	2.7945	5.94
<i>Constant Walking-Walking</i>	2.6604	6.54
Mode shifts for central area destinations		
<i>PT-PT</i>	1.7449	5.50
<i>PT-Walking</i>	1.8249	4.32
<i>Walking-PT</i>	2.6880	5.74
<i>Walking-Walking</i>	1.6469	6.33
Mode shifts for individuals with season ticket ownership		
<i>Walking-Walking</i>	-0.5606	-1.76
Mode shifts for trips with more than 1 passenger		
<i>PT first/shopping trip</i>	-1.8619	-5.46
<i>PT following trip</i>	-0.8646	-2.43
<i>Walking first/shopping trip</i>	-0.8007	-3.53
<i>Walking following trip</i>	-0.3679	-1.50
Mode shifts for students		
<i>Walking-Walking</i>	1.0751	2.84
Mode shifts for married individuals		
<i>Walking-Walking</i>	-0.7828	-2.73
Mode shifts for individuals living in 3-member households		
<i>Walking-Walking</i>	0.6899	1.86
LOS variables		
<i>Travel time for first trip (base)</i>	-0.0912	-10.10
<i>Travel time shift for clothes shopping</i>	0.0265	2.78

Continued on next page

Table 2.3 – continued from previous page

Parameter	Estimates	Rob. t-ratios 0 (* t-ratios 1)
<i>Travel time for O-S-O trip chains</i>	0.0152	2.49
<i>Travel time for HWH tours</i>	-0.0445	-4.77
<i>Travel time multiplier for car</i>	1.0000	–
<i>Travel time multiplier for PT IVT</i>	0.5859	-6.41
<i>Travel time multiplier for PT first access trip</i>	0.8196	-0.82
<i>Travel time multiplier for PT last egress trip</i>	0.6089	-2.37
<i>Travel time multiplier for PT remaining OVT</i>	0.3535	-4.02
<i>Travel time multiplier for following trip</i>	1.3574	3.71
<i>Travel time - Shopping duration elasticity</i>	-0.3157	-10.30
<i>Travel walking distance for first trip (base)</i>	-1.6259	-13.30
<i>Travel walking distance for O-S-O trip chains</i>	0.2691	2.41
<i>Travel walking distance multiplier for following trip</i>	1.2515	2.78
<i>Box-cox lambda for travel walking distance</i>	0.8051	-3.79
<i>Travel walking distance - Shopping duration elasticity</i>	-0.1396	-4.19
<i>Travel cost</i>	-0.6518	-8.20
<i>Box-cox lambda for travel cost</i>	0.5362	-9.27
<i>Travel cost - Personal income elasticity</i>	-0.2435	-2.53
Locational variables		
<i>Living in rich areas-shopping in poor areas</i>	-0.8037	-2.9534
<i>Parking areas (400m buffer)</i>	0.0930	3.5367
<i>Box-cox lambda for parking areas (400m buffer)</i>	0.4218	-7.3756
<i>Presence of major clothes shopping retailers (400m buffer)</i>	1.9623	9.5925
<i>Presence of major grocery retailers (400m buffer)</i>	0.5334	5.4901
<i>Presence of major durables retailers (400m buffer)</i>	2.0478	2.5363
Size variables		
<i>Natural logarithm multiplier ϕ</i>	0.7298	-2.71
<i>Population (400m buffer) (base)</i>	1.0000	–
<i>Exponent of retail areas for clothes shopping stores (400m buffer)</i>	0.2185	0.42
<i>Exponent of retail areas for grocery stores (400m buffer)</i>	0.6728	1.81
<i>Exponent of retail areas for durables/other stores (400m buffer)</i>	0.5873	0.80
<i>Exponent of shopping store variability (400m buffer)</i>	1.2847	1.71
<i>Exponent of shopping store variability when following trip purpose is shopping (1000-2000m buffer)</i>	2.7750	4.02

in-vehicle time etc.) over the partial derivative of travel cost including all of the specified parameters affecting them (i.e. shifts, elasticities etc.). Additionally, the standard errors of the VTT estimates, calculated using the *delta* method (Daly et al., 2012) are presented. All of the VTT estimates are significant at the 95% confidence level. Besides the fact that the purpose of the current study was not the estimation of VTT values representative of the UK population, a comparison of the estimated values can still be performed with the potential of yielding interesting insights. In general, it can be said that the VTT estimates are very close to the average value suggested by the Transport Appraisal Guidance in the UK (WEBTag) for an average vehicle, namely 13.87 GBP/hour (using 2010 prices) (Department for Transport, 2014). In addition, a closer assessment on the VTT estimates for the first shopping trip can also be performed by comparing them with the latest UK official VTT values based on an Stated Preference (SP) survey (Batley et al., 2019). The respective official VTT values for "Other" purpose trips, including shopping, for car, bus and rail are 5.12, 3.40 and 9.05 £/hour. Those values are lower than the respective GPS-based VTT values, which

conforms to the general finding in the literature suggesting that SP-based VTTs are generally lower than values based on Revealed Preference (RP) surveys, such as the GPS trip diary used in the current study (Wardman et al., 2016).

Table 2.4: Value of Travel Time estimates of full choice set model

VTT measure	Estimate (£/hour)	Robust st. errors
<i>Car for first/shopping trip</i>	10.7728	0.0349
<i>PT IVT for first/shopping trip</i>	9.4761	0.0331
<i>PT first access trip for first/shopping trip</i>	13.2542	0.0741
<i>PT last egress trip for first/shopping trip</i>	9.8467	0.0566
<i>PT OVT remaining for first/shopping trip</i>	5.7177	0.0460
<i>Car for following trip</i>	13.7762	0.0440
<i>PT IVT for following trip</i>	8.7583	0.0298
<i>PT first access trip for following trip</i>	12.2501	0.0687
<i>PT last egress trip for following trip</i>	9.1007	0.0525
<i>PT OVT remaining for following trip</i>	5.2846	0.0431

Demand elasticities were also calculated for the full choice set model with respect to a unit increase of travel cost and travel time, made separately for car and PT. It is assumed that the change of cost will affect both trips, i.e. shopping and following trip, since it will be an increase of fuel cost for car or a general increase on PT fare and season tickets. The increase of car travel time and PT in-vehicle time is assumed to affect the accessibility to the shopping destination, hence the change is applied only on the shopping trip. Choice forecasting was computed before and after the respective change using the estimated parameters and the demand elasticities per mode and mode combination were calculated as $\log \frac{demand_{after}}{demand_{base}} / (\log(1.01))$, which are presented in *Table 2.5*. The total elasticities for car, PT and walking were computed by aggregating the elasticities of all the mode combinations affecting each one of those three modes. A comparison similar to the previous one for the VTTs can also be conducted for the estimated cost and time elasticities presented here by comparing them with elasticities from previous meta-analyses reported in Wardman and Shires (2003), Wardman (2012) and Wardman (2022). The car cost elasticity of -0.135 is between the values presented in Wardman (2012) for leisure trips and urban-suburban trips of -0.10 and -0.20, respectively. The PT cost elasticity of -0.567 is between the values of bus cost elasticity for urban trips and rail cost elasticity for suburban trips, namely -0.5 and -0.6, respectively, reported in Wardman and Shires (2003). It is also fairly close to the bus cost elasticities for suburban leisure trips and urban-suburban trips of -0.57 and -0.55, respectively, reported in Wardman (2022). Larger discrepancies are observed, however, for time elasticities where the estimated values are half in size from the ones reported in previous studies. Specifically, the estimated car time elasticity is -0.134, while the respective value reported in Wardman (2012) is -0.30 and the estimated PT time elasticity is -0.315, while the reported bus and rail time elasticities in Wardman (2012) are -0.63 and -0.69, respectively. Nonetheless, those lower values can be partly justified as they refer mostly to shopping trips, while we could assume that individuals would be more sensitive for one unit of time change for commuting and business trips.

4.2 Sampling protocol evaluation/comparison

The evaluation of the sampling protocols is performed with regard to the fit statistics, the estimation times and the estimated parameters of the respective sampled choice set models, i.e. beta estimates, VTT estimates and demand elasticities, as described in the following paragraphs.

Table 2.5: Demand elasticities of full choice set model

Demand elasticities	Increase of car cost (both trips)	Increase of car time (shopping trip)	Increase of PT cost (both trips)	Increase of PT IVT (shopping trip)
<i>Car</i>	-0.135	-0.158	0.061	0.037
<i>PT</i>	0.386	0.518	-0.567	-0.316
<i>Walking</i>	0.203	0.239	-0.019	-0.008
<i>Car -Car</i>	-0.163	-0.194	0.065	0.039
<i>Car-PT</i>	0.174	-0.427	-0.609	0.203
<i>Car-Walking</i>	0.103	-0.719	0.137	0.158
<i>PT-Car</i>	0.415	0.963	-0.742	-0.928
<i>PT-PT</i>	0.370	0.467	-0.847	-0.538
<i>PT-Walking</i>	0.401	0.602	-0.394	-0.768
<i>Walking-Car</i>	0.179	0.839	0.111	0.034
<i>Walking-PT</i>	0.401	0.530	-0.446	0.100
<i>Walking-Walking</i>	0.166	0.170	0.054	0.022

4.2.1 Fit statistics comparison

At a first stage, the fit statistics, the estimation times of the sampled choice set models and the average choice probabilities of correct predictions are presented in *Table 2.6* are compared with those of the full choice set model. In that table, it is clearly shown how estimation times increase linearly as the size of the choice set increases. The models estimated using the largest choice set size examined of 250 alternatives, i.e. 15.8% of the global choice set of 1584 alternatives, on average need almost 12% of the estimation time of the full choice set model (38 minutes compared to 322 minutes), which highlights the practical advantages of the sampling approach.

Out of all the sampling protocols examined, *Random sampling* leads to generally more deterministic models compared to the importance sampling protocols, as shown by the comparison of log-likelihood, adjusted rho-square and the average choice probability of correct prediction among models of the same choice set size. The main reason behind that is the fact that with the *Random sampling* protocol the choice set of size J includes the chosen alternative and $J - 1$ alternatives that are randomly sampled from the remaining global choice set. That leads to inevitably including many alternatives located further away from the chosen alternative and the space around the O and D of the specific choice task/trip. As a result, these alternatives will have an increased travel time/distance/cost compared to the chosen alternative and will not provide meaningful trade-offs for the model to properly evaluate the trade-offs the individuals would consider during the decision making process. On the other hand, all of the importance sampling protocols examined provide much more balanced choice sets leading to less deterministic models with the *TAC* protocol being the most balanced approach. That is also evident from the average choice probability of correct prediction, where for the *TAC* protocol with 250 alternatives that value, 0.229, is closer to the one of the full choice set model, namely 0.18. In contrast, for the same choice set size, *TC* and *AC* achieve average choice probabilities of correct prediction of 0.266, 0.299, respectively, and the more deterministic *Random sampling* a much higher average choice probability of 0.464. Those findings serve as a first indication that importance sampling protocols and especially *TAC* will converge faster to the full choice set model compared to *Random sampling* that will require bigger choice sets.

Table 2.6: Fit statistics of sampling protocols

Fit statistics	Choice set sizes					
	10	50	100	150	200	250
<i>Log-likelihood (0)</i>	-3548.284	-6028.427	-7096.567	-7721.389	-8164.707	-8508.093
<i>Average estimation time (min)</i>	1.75	8.50	16.75	26.00	33.25	38.00
Random sampling						
<i>Average Log-likelihood (model)</i>	-194.5996	-799.467	-1268.742	-1608.966	-1877.833	-2082.2
<i>Average adjusted Rho-square</i>	0.9296	0.8583	0.8135	0.7845	0.7633	0.7488
<i>Average choice probability of correct prediction</i>	0.932	0.761	0.632	0.564	0.505	0.464
AC sampling						
<i>Average Log-likelihood (model)</i>	-435.7331	-1484.0916	-2091.9002	-2528.5710	-2860.0574	-3088.101
<i>Average adjusted Rho-square</i>	0.8617	0.7447	0.6975	0.6654	0.6475	0.6346
<i>Average choice probability of correct prediction</i>	0.851	0.582	0.456	0.378	0.333	0.299
TC sampling						
<i>Average Log-likelihood (model)</i>	-806.2441	-2021.0204	-2565.6798	-2906.7886	-3090.3342	-3236.4498
<i>Average adjusted Rho-square</i>	0.7573	0.6557	0.6307	0.6164	0.6148	0.6132
<i>Average choice probability of correct prediction</i>	0.739	0.468	0.369	0.311	0.282	0.266
TAC sampling						
<i>Average Log-likelihood (model)</i>	-929.5913	-2299.664	-2903.2052	-3219.2278	-3406.7728	-3555.7114
<i>Average adjusted Rho-square</i>	0.7225	0.6094	0.5831	0.5760	0.5759	0.5756
<i>Average choice probability of correct prediction</i>	0.698	0.402	0.307	0.265	0.245	0.229

4.2.2 Sampled estimate comparison

In *Table 2.7*, an assessment of the accuracy, stability and statistical efficiency of the estimated parameters of the sampled choice set models is depicted, together with the average distance of the sampled alternatives from the chosen one per sampling protocol. Furthermore, in *Table 2.8*, a comparison between the sampling protocols is presented with regard to how much better the performance on each evaluation measure is for the protocol in focus compared to the remaining three protocols. As an example, the numbers presented for TAC-TC comparison with regard to *AAPD* are calculated as $(AAPD_{TC} - AAPD_{TAC})/AAPD_{TAC}$. In the same Table, the number of parameters where each sampling protocol performs better is also included. The assessment and the comparison of the sampling protocols is performed based on the following evaluation measures:

- *Average Absolute Bias (AAB)*, measuring the absolute difference between the *true* and sampled estimates and taking the average across the r number of sampling realisations.
- *Average Absolute Percentage Difference (AAPD)*, measuring the absolute percentage difference between the *true* and the sampled estimates and taking the average across the r number of sampling realisations. *AAPD* offers a normalised equivalent to *AAB*, which can be important when there are significant scale differences among the estimates.
- *Absolute Coefficient of Variation (ACoV)*, offering a normalised measure for capturing the stability or the lack thereof of sampling realisations per choice set size. *ACoV* is defined as the absolute value of the ratio of the sampling standard deviation over the average sampled estimate across the r number of sampling realisations. A small *ACoV* would provide the analyst the certainty that a following sampling realisation would still result in similar estimates.

4. Results

- *Root Mean Square Error (RMSE)*, calculated for the standard errors across the r number of sampling realisations per parameter with the purpose of assessing the statistical efficiency of the sampling protocols. In general, a small *RMSE* would indicate a more accurate estimation per parameter.
- *Improvement rates*, calculated from linear regressions per parameter and for each of the four previously-defined evaluation measures across the six choice set sizes examined. A higher improvement rate (more negative) indicates that the sampling protocol will benefit more by further increasing the size of the choice set.

With regard to the average straight distance between the sampled and the chosen alternatives, *Random sampling* results in sampled alternatives with similar average distances from the chosen alternatives regardless of the choice set size, since the alternatives are sampled with a uniform probability from the global choice set. The sampled alternatives in the *AC* protocol have a smaller average distance from the chosen alternative compared to the *TC* protocol due to the bigger size of the SDEs/FBs offering a sufficient pool of alternatives to sample from without the need of further sampling from C . The higher average distance of alternatives in the *TC* protocol is in accordance with our initial hypotheses that this specific protocol will result in having an increased number of spatially irrelevant alternatives to the chosen one. On the other hand, the *TAC* protocol, with the addition of SDE/FB spaces, manages to provide choice sets with a smaller average distance between sampled and chosen alternatives leading to less deterministic models and to average probabilities for the chosen alternatives that are closer to those of the *true* model (0.18), as shown in *Table 2.6*. That finding supports the idea of the current study, that an additional space is required around the DEs in order to sample more spatially relevant alternatives for the respective choice task. The role of the additional stratum A in the *TAC* protocol is to provide a further structure of sampling for the remaining alternatives and to minimise the inclusion of spatially irrelevant alternatives that will not provide a meaningful trade-off comparison for the model.

In general, the three stratified importance sampling protocols, namely *AC*, *TC* and *TAC*, perform significantly better than *Random sampling* given the choice set size. The average rates of improvement for all evaluation measures for the *Random sampling* are higher compared to those of the importance sampling protocols meaning that the performance of *Random sampling* models would benefit more with increased choice set sizes. That is a further indication that using *Random sampling* would require a higher choice set size to achieve the same level of accuracy compared to an importance sampling approach. On average, *TAC* leads to 98.9%-242.6% lower *AAPD* and more than 51 out of 55 better estimated parameters than *Random sampling*. *TC* leads to slightly less improvements with 85.3%-206.9% lower *AAPD*, and 48-52 better estimated parameters. Finally, *AC* leads to 48.4%-120.1% lower *AAPD* and 41-51 better estimated parameters. Sampling stability, as captured by the *ACoV*, provides similar conclusions with *TAC* showing the most significant improvements compared to *Random sampling*, followed by *TC* and *AC*.

An interesting finding can be discerned by examining the *RMSE* across sampling protocols. Importance sampling protocols still achieve lower *RMSE* than *Random sampling*, but the improvements are much smaller, namely below 25% for choice sets of more than 50 alternatives. That means that parameters estimated with *Random sampling* will have narrow confidence intervals, i.e. high significance, but will still be highly biased compared to the true estimates of the full choice set model. In a practical setting, with the absence of a full choice set model, that can lead the analyst to make a false assessment of the behavioural model, which in turn can have severe policy implications both during interpretation and application.

Regarding the three importance sampling protocols, their differences are less stark, but clear trends can still be observed. Both *TAC* and *TC* outperform *AC* in all evaluation measures. On average, *TAC* is by 34%-111.3% and by 75.2%-106.6% better than *AC* in terms of *AAPD* and *ACoV*, respectively, for choice sets with more than 10 alternatives. In a similar notion, *TC* is by 24.9%-57.7% and by 29.6%-91.7% better for the same evaluation measures

and choice set sizes than *AC.TAC* models are generally more accurate and stable than their *TC* counterparts with an average 7.3%-33.9% lower *AAPD* and 0.6%-38.5% lower *ACoV* for choice sets with more than 10 alternatives. *TC* achieves its most comparable performance with *TAC* and significantly outperforms *AC* at a choice set size of 100 alternatives. A possible explanation is that, on average, there are 76 alternatives in stratum *T* meaning that at a choice set size of 100, there are enough alternatives in stratum *T* to sample from in order to reach the required number of alternatives, i.e. $0.67 * 100 = 67$ alternatives from that stratum, without replenishing them from *C*. After that choice set size, however, there is the need to sample further alternatives from *C* reducing the performance of the estimated sampled models. That is also evident from the performance of the evaluation measures of *TC*, where for a choice set of 100 alternatives, *TC* models perform only marginally worse than *TAC*. After that point, however, *TAC* models manage to increase their performance gap from *TC*, going from an average of 7.3% to a 33.9% lower *AAPD*, for 250 alternatives, and from 30 to 41 better estimated parameters. The increasing inclusion of worse alternatives in the choice set has an impact on stability, as well, with *TAC* models going from a mere 0.6% better *ACoV*, for 100 alternatives, to a much higher 38.5%, for 250 alternatives. Furthermore, that is captured in the average improvement rates of *AAPD* and *ACoV*, where *TAC* shows higher decreasing rates than *TC*, meaning that it can still benefit more by increasing the choice set despite being already more accurate and stable than *TC*. Based on that finding, a reverse-engineering approach can be implemented, where the analyst can get a rough approximation of the optimal choice set size per sampling protocol by examining the average number of alternatives within the stratum that she wants to prioritise.

Regarding the choice set size, there is not any guideline as to which percentage of the full choice set is required to estimate stable parameters with insignificant bias. Therefore, the required choice set size should be viewed as case-specific and be carefully examined by the analyst. *Figure 2.6* provides a graphical representation of *Table 2.6* and can be used to identify the minimum required choice set to achieve estimate accuracy and stability. In the current study, it seems that even after a choice set of 50 alternatives, there are significant improvements in estimate accuracy and stability for the importance sampling protocols. *Random sampling*, however, needs at least 150 alternatives to show more consistently accurate estimates. The improvements on the four evaluation measures tend to slow down after 150 alternatives and for each subsequent choice set size for all sampling protocols. In the same *Figure*, a clear verdict can be made about the benefits of the proposed importance sampling protocols using AS concepts compared to random sampling, which performs significantly worse across all four evaluation measures.

A visual representation of the sampled estimates and how they improve with the increase of the choice set is depicted in *Figures 2.7 and 2.8* focusing on two of the most important parameters from a policy perspective, namely β_{time}^{base} and β_{cost}^{base} , respectively. In those *Figures*, it can be seen how the sampled estimates across the five realisations tend to concentrate around the *true* value (red horizontal line) as the choice set size increases (green dashed lines represent the 95% confidence interval of the *true* value). Detailed tables depicting the average estimates and the evaluation measures per parameter across the five realisations per sampling protocol and choice set size can be found in the supplementary material provided in the *Appendix*.

4.2.3 Evaluation of sampled VTT estimates and demand elasticities

In *Table 2.9*, a comparison is performed with the VTT estimates of the full choice set model by calculating the *AAB*, *AAPD*, *ACoV* and *RMSE*, as defined earlier, while *Table 2.10* depicts a comparison between sampling protocols. The three importance sampling protocols, on average, have a less than 1£/hour difference from the *true* VTTs for choice sets with more than 100 alternatives, while VTTs derived from *Random sampling* are significantly more biased. *TC* manages to outperform the remaining protocols and achieves the best

4. Results

Table 2.7: Estimate evaluation of sampling protocols

Evaluation measure	Choice set sizes						Average rate of improvement
	10	50	100	150	200	250	
Random sampling							
<i>Average distance from chosen alternative (m)</i>	14908	14875.2	14888	14812.2	14819.8	14797.6	–
<i>Average AAB</i>	0.9691	0.3096	0.3593	0.1987	0.1910	0.1690	-0.1291
<i>Average AAPD</i>	1.0502	0.3658	0.3852	0.2328	0.2071	0.1888	-0.1401
<i>Average ACoV</i>	2.8367	0.3710	0.3384	0.2230	0.1660	0.1436	-0.4001
<i>Average RMSE</i>	1.1263	0.5058	0.3816	0.3460	0.3376	0.3168	-0.1311
AC sampling							
<i>Average distance from chosen alternative (m)</i>	8424.1	8457.4	9200.6	10014.6	10533.8	11023.2	–
<i>Average AAB</i>	0.4504	0.2035	0.1610	0.1231	0.1032	0.1000	-0.0598
<i>Average AAPD</i>	0.4984	0.2465	0.1750	0.1417	0.1187	0.1164	-0.0665
<i>Average ACoV</i>	0.5769	0.2001	0.1670	0.1337	0.1095	0.0879	-0.0767
<i>Average RMSE</i>	0.6522	0.3636	0.3428	0.3202	0.3116	0.3050	-0.0547
TC sampling							
<i>Average distance from chosen alternative (m)</i>	8495	11138.2	12642.2	13382	13842	14120.8	–
<i>Average AAB</i>	0.4058	0.1760	0.1183	0.0868	0.0774	0.0653	-0.0580
<i>Average AAPD</i>	0.4980	0.1974	0.1255	0.0996	0.0931	0.0738	-0.0703
<i>Average ACoV</i>	0.3491	0.1385	0.0871	0.0790	0.0845	0.0644	-0.0459
<i>Average RMSE</i>	0.5065	0.3406	0.3161	0.3062	0.2989	0.2919	-0.0345
TAC sampling							
<i>Average distance from chosen alternative (m)</i>	5124	7045.2	8164.6	8818.2	9527.8	10083	–
<i>Average AAB</i>	0.4012	0.1349	0.0955	0.0722	0.0597	0.0476	-0.0576
<i>Average AAPD</i>	0.5020	0.1839	0.1170	0.0874	0.0784	0.0551	-0.0740
<i>Average ACoV</i>	0.4399	0.1137	0.0876	0.0647	0.0625	0.0465	-0.0613
<i>Average RMSE</i>	0.4575	0.3275	0.3126	0.3064	0.3024	0.3021	-0.0245

The best-performing sampling protocol per choice set size and evaluation measure is highlighted

Table 2.8: Comparison of sampling protocols

Protocols compared	Choice set sizes					
	10	50	100	150	200	250
TAC-TC						
<i>Average AAB</i>	1.2% (31)	30.5% (35)	23.9% (30)	11.9% (35)	29.6% (37)	37.2% (41)
<i>Average AAPD</i>	-0.8% (31)	7.3% (35)	7.3% (30)	10.5% (35)	18.8% (37)	33.9% (41)
<i>Average ACoV</i>	-20.6% (27)	21.8% (35)	0.6% (33)	22.1% (27)	35.2% (30)	38.5% (33)
<i>Average RMSE</i>	10.7% (42)	4.0% (34)	1.1% (27)	0.07% (26)	-1.5% (22)	-3.4% (26)
TAC-AC						
<i>Average AAB</i>	12.3% (36)	50.8% (45)	68.6% (42)	70.5% (44)	72.9% (45)	110.1% (51)
<i>Average AAPD</i>	-0.7% (36)	34.0% (45)	49.6% (42)	62.1% (44)	51.4% (45)	111.3% (51)
<i>Average ACoV</i>	31.1% (27)	76.0% (38)	90.6% (39)	106.6% (36)	75.2% (32)	89.0% (35)
<i>Average RMSE</i>	42.6% (51)	11.0% (48)	9.7% (51)	4.5% (46)	3.0% (48)	1.0% (48)
TAC-Random						
<i>Average AAB</i>	141.6% (53)	129.5% (51)	276.2% (54)	175.2% (51)	219.9% (51)	255.0% (55)
<i>Average AAPD</i>	109.2% (53)	98.9% (51)	229.2% (54)	166.4% (51)	164.2% (51)	242.6% (55)
<i>Average ACoV</i>	544.9% (29)	226.3% (32)	286.3% (32)	244.7% (33)	165.6% (33)	208.8% (36)
<i>Average RMSE</i>	146.2% (53)	54.4% (51)	22.1% (49)	12.9% (49)	11.6% (47)	4.9% (44)
TC-AC						
<i>Average AAB</i>	11.0% (35)	15.6% (35)	36.1% (44)	41.8% (39)	33.3% (37)	53.1% (43)
<i>Average AAPD</i>	0.1% (35)	24.9% (35)	39.4% (44)	42.3% (39)	27.5% (37)	57.7% (43)
<i>Average ACoV</i>	65.3% (27)	44.5% (35)	91.7% (34)	69.2% (31)	29.6% (32)	36.5% (34)
<i>Average RMSE</i>	28.8% (51)	6.8% (47)	8.4% (48)	4.6% (46)	4.2% (46)	4.5% (45)
TC-Random						
<i>Average AAB</i>	138.8% (49)	75.9% (48)	203.7% (52)	128.9% (49)	146.8% (51)	158.8% (52)
<i>Average AAPD</i>	110.9% (49)	85.3% (48)	206.9% (52)	133.7% (49)	122.4% (51)	155.8% (52)
<i>Average ACoV</i>	712.6% (28)	167.9% (30)	288.5% (33)	182.3% (33)	96.4% (32)	123.0% (35)
<i>Average RMSE</i>	122.4% (54)	48.5% (53)	20.7% (49)	13.0% (50)	12.9% (49)	8.5% (45)
AC-Random						
<i>Average AAB</i>	115.2% (51)	52.1% (47)	123.2% (46)	61.4% (41)	85.1% (49)	69.0% (45)
<i>Average AAPD</i>	110.7% (51)	48.4% (47)	120.1% (46)	64.3% (41)	74.5% (49)	62.2% (45)
<i>Average ACoV</i>	391.7% (29)	85.4% (23)	102.6% (28)	66.8% (34)	51.6% (32)	63.4% (26)
<i>Average RMSE</i>	72.7% (51)	39.1% (50)	11.3% (46)	8.1% (46)	8.3% (44)	3.9% (39)

The number in parenthesis denotes the number of parameters with lower evaluation measure for the sampling protocol in focus out of a total of 55 parameters

4. Results

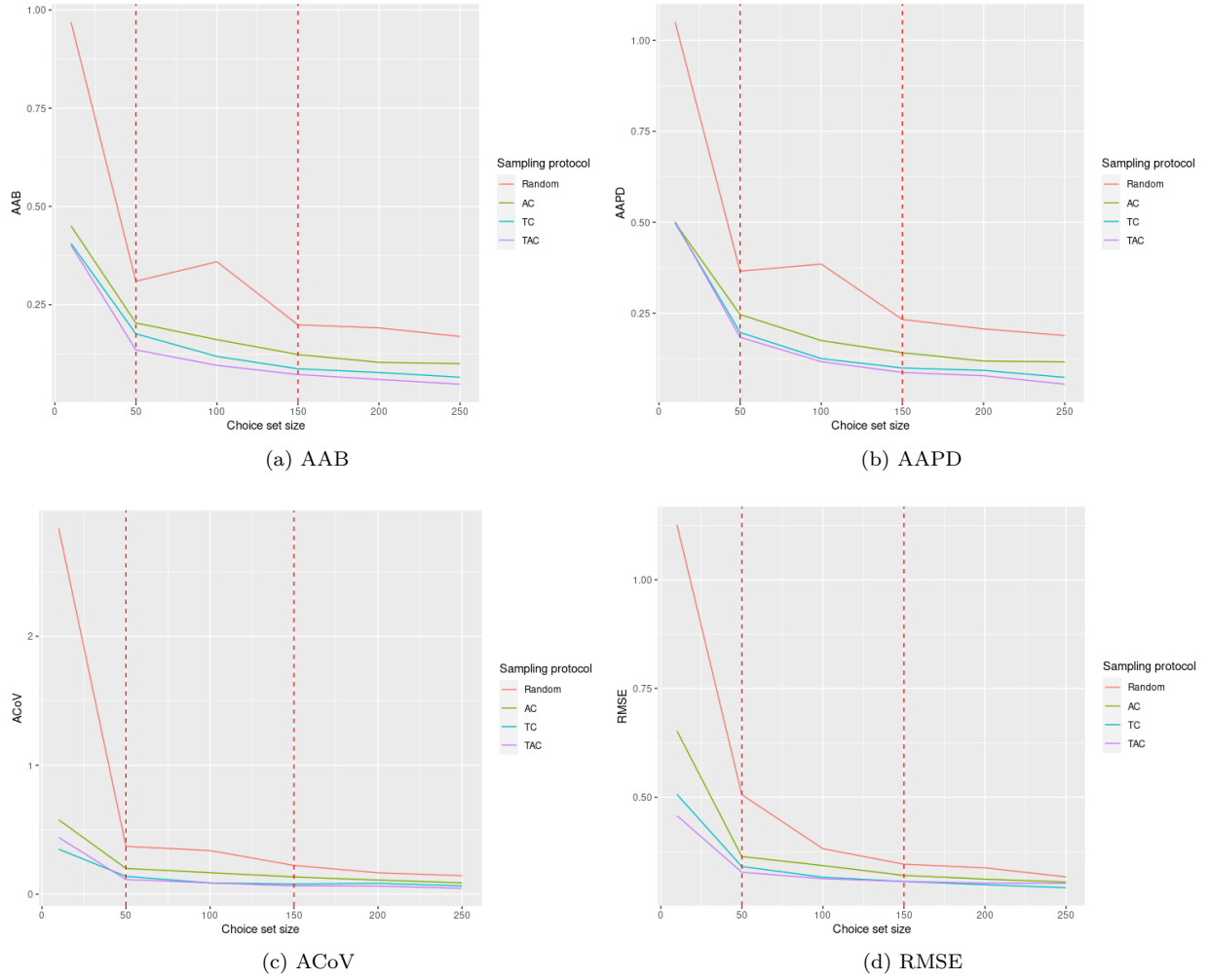


Figure 2.6: Improvements of evaluation measures across sampling protocols and choice set sizes

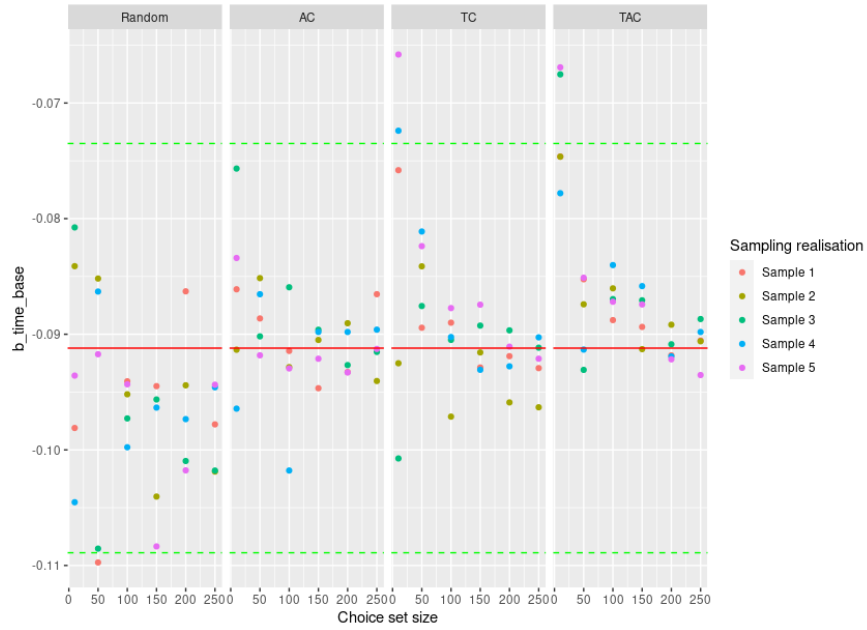


Figure 2.7: Plots for β_{time}^{base} estimates for each sampling realisation across sampling protocols

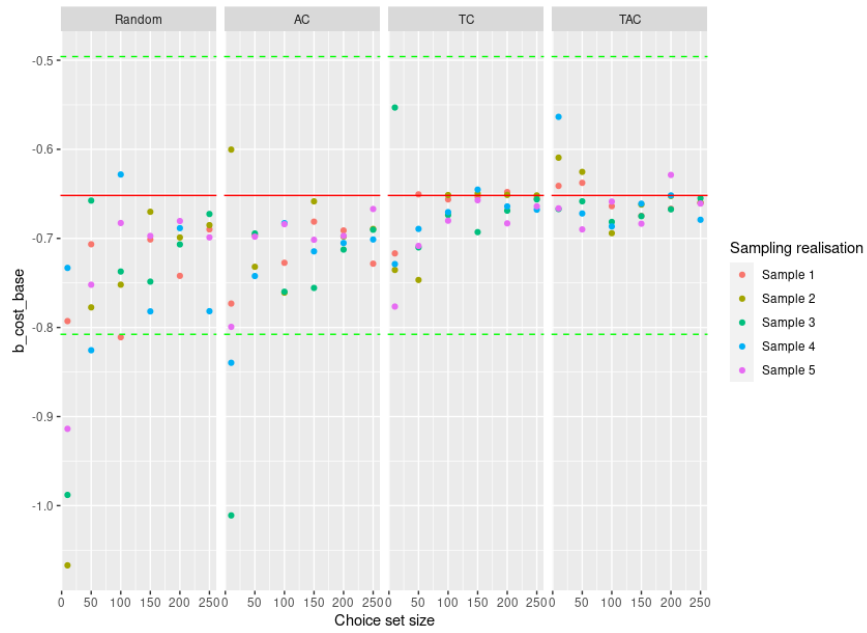


Figure 2.8: Plots for β_{cost}^{base} estimates for each sampling realisation across sampling protocols

4. Results

performance with 100 alternatives. For that choice set size, it performs significantly better even than *TAC* by having more than 30% lower *AAB* and *AAPD*, 28.5% lower *ACoV* and 9 out of 10 better estimated VTTs. The performance of *TC*, however, deteriorates as the choice set size increases and inevitably more spatially irrelevant alternatives are included, reaching the point of an almost equal performance with *TAC* for 250 alternatives. Time and cost-related parameters that influence the VTT estimation show an equal performance between *TAC* and *TC*, in contrast to the remaining parameters where *TAC* excels, and that is the reason behind the good overall performance of *TC* for VTTs.

Table 2.9: Evaluation of VTT estimates of sampling protocols

Evaluation measure	Choice set sizes					Average rate of improvement	
	10	50	100	150	200		250
Random sampling							
<i>Average AAB (£/hour)</i>	4.5384	2.0949	1.7056	1.2674	1.1843	1.0772	-0.5850
<i>Average AAPD</i>	0.5108	0.2318	0.1979	0.1498	0.1286	0.1222	-0.0657
<i>Average ACoV</i>	0.4905	0.2392	0.2490	0.1756	0.0929	0.1314	-0.0660
<i>Average RMSE</i>	0.1209	0.0702	0.0602	0.0538	0.0546	0.0494	-0.0117
AC sampling							
<i>Average AAB (£/hour)</i>	3.4104	1.4050	1.2356	0.9829	0.8192	0.8003	-0.4303
<i>Average AAPD</i>	0.3544	0.1728	0.1391	0.1048	0.0880	0.0878	-0.0463
<i>Average ACoV</i>	0.4004	0.2063	0.1536	0.1164	0.0840	0.0695	-0.0588
<i>Average RMSE</i>	0.0904	0.0561	0.0516	0.0507	0.0489	0.0480	-0.0067
TC sampling							
<i>Average AAB (£/hour)</i>	2.2496	1.1970	0.7061	0.5570	0.4921	0.3972	-0.3293
<i>Average AAPD</i>	0.2475	0.1261	0.0781	0.0623	0.0559	0.0435	-0.0356
<i>Average ACoV</i>	0.2224	0.0885	0.0862	0.0658	0.0697	0.0492	-0.0269
<i>Average RMSE</i>	0.0704	0.0520	0.0517	0.0523	0.0492	0.0489	-0.0033
TAC sampling							
<i>Average AAB (£/hour)</i>	1.5254	1.0395	1.0281	0.7506	0.5209	0.4458	-0.2066
<i>Average AAPD</i>	0.1754	0.1239	0.1267	0.0826	0.0650	0.0501	-0.0242
<i>Average ACoV</i>	0.2351	0.1381	0.1205	0.0882	0.0754	0.0386	-0.0344
<i>Average RMSE</i>	0.0724	0.0560	0.0497	0.0500	0.0570	0.0486	-0.0039

The best-performing sampling protocol per choice set size and evaluation measure is highlighted

Demand elasticities estimated from sampled models are assessed in [Table 2.11](#) and a performance comparison between sampling protocols is presented in [Table 2.12](#). Contrary to the VTT estimates, the estimation of demand elasticities with *TAC* is much more accurate than *TC*, since in that context all of the 55 parameters take part during their calculation and not just the time and cost-related parameters. As already mentioned, *TC* achieves its best performance for a choice set of 100 alternatives, but even in that case, *TAC* achieves a 16.8% lower *AAB*, a 20.3% lower *AAPD* and 33 out of 48 better estimated elasticities, but also less stable estimates with 4.5% higher *ACoV*. As the choice set size increases, however, the performance gap for *TAC* shows gradual improvements reaching a 47.3% lower *AAB*, a 64.2% lower *AAPD*, 39 out of 48 better estimated elasticities and a 18% lower *ACoV*, for a choice set of 250 alternatives. *AC* performs worse than the other two importance sampling protocols, but still better than *Random sampling*. *TAC* shows the largest performance improvements compared to *Random sampling*, almost 1.5 times more than *TC* and 2.5 times more than *AC*. The overall better forecasting ability of *TAC* is indicative of the less deterministic models derived from that sampling protocol (see [Table 2.6](#)). The impact that this might have in a practical application presents a clear verdict in favour of combining DEs and SDEs/FBs for importance sampling and not neglecting the latter.

Table 2.10: VTT comparison of sampling protocols

Protocols compared	Choice set sizes					
	10	50	100	150	200	250
TAC-TC						
<i>Average AAB</i>	47.5% (9)	15.2% (6)	-31.3% (1)	-25.8% (3)	-5.5% (7)	-10.9% (5)
<i>Average AAPD</i>	41.1% (9)	1.8% (6)	-38.4% (1)	-24.6% (3)	-14.0% (7)	-13.2% (5)
<i>Average ACoV</i>	-5.4% (5)	-35.9% (4)	-28.5% (3)	-25.4% (4)	-7.6% (3)	27.5% (6)
<i>Average RMSE</i>	-2.8% (3)	-7.1% (0)	4.0% (8)	4.6% (8)	-13.7% (2)	0.6% (7)
TAC-AC						
<i>Average AAB</i>	123.6% (10)	35.2% (8)	20.2% (5)	30.9% (7)	57.3% (8) (9)	79.5% (7)
<i>Average AAPD</i>	102.1% (10)	39.5% (8)	9.8% (5)	26.9% (7)	35.4% (8) (9)	75.2% (7)
<i>Average ACoV</i>	70.3% (9)	49.4% (8)	27.5% (7)	32.0% (9)	11.4% (7) (8)	80.1% (10)
<i>Average RMSE</i>	24.9% (10)	0.2% (4)	3.8% (5)	1.4% (5)	-14.2% (2) (6)	-1.2% (4)
TAC-Random						
<i>Average AAB</i>	197.5% (10)	101.5% (10)	65.9% (10)	68.9% (9)	127.4% (9)	141.6% (10)
<i>Average AAPD</i>	191.2% (10)	87.1% (10)	56.2% (10)	81.4% (9)	97.8% (9)	143.9% (10)
<i>Average ACoV</i>	108.6% (10)	73.2% (8)	106.6% (10)	99.1% (8)	23.2% (8)	240.4% (10)
<i>Average RMSE</i>	67.0% (10)	25.4% (9)	21.1% (10)	7.6% (6)	-4.2% (6)	1.6% (4)
TC-AC						
<i>Average AAB</i>	51.6% (8)	17.4% (6)	75.0% (8)	76.5% (9)	66.5% (9)	101.5% (9)
<i>Average AAPD</i>	43.2% (8)	37.0% (6)	78.1% (8)	68.2% (9)	57.4% (9)	101.8% (9)
<i>Average ACoV</i>	80.0% (8)	133.1% (7)	78.2% (6)	76.9% (8)	20.5% (7)	41.3% (9)
<i>Average RMSE</i>	28.4% (10)	7.9% (8)	-0.2% (4)	-3.1% (4)	-0.6% (4)	-1.8% (4)
TC-Random						
<i>Average AAB</i>	101.7% (9)	75.0% (9)	141.6% (10)	127.5% (9)	140.7% (9)	171.2% (10)
<i>Average AAPD</i>	106.4% (9)	83.8% (9)	153.4% (10)	140.4% (9)	130.1% (9)	180.9% (10)
<i>Average ACoV</i>	120.5% (10)	170.3% (10)	188.9% (10)	166.9% (10)	33.3% (8)	167.1% (9)
<i>Average RMSE</i>	71.7% (10)	35.0% (10)	16.4% (10)	2.9% (5)	11.0% (7)	1.0% (4)
AC-Random						
<i>Average AAB</i>	33.1% (9)	49.1% (8)	38.0% (10)	28.9% (8)	44.6% (6)	34.6% (8)
<i>Average AAPD</i>	44.1% (9)	34.1% (8)	42.3% (10)	42.9% (8)	46.1% (6)	39.2% (8)
<i>Average ACoV</i>	22.5% (9)	15.9% (6)	62.1% (10)	50.9% (8)	10.6% (6)	89.1% (9)
<i>Average RMSE</i>	33.7% (10)	25.1% (10)	16.7% (10)	6.1% (7)	11.7% (9)	2.9% (6)

The number in parenthesis denotes the number of estimated VTTs with lower evaluation measure for the sampling protocol in focus out of a total of 10 VTT estimates

4. Results

Table 2.11: Evaluation of demand elasticities of sampling protocols

Evaluation measure	Choice set sizes						Average rate of improvement
	10	50	100	150	200	250	
Random sampling							
<i>Average AAB</i>	0.2455	0.1589	0.1133	0.0885	0.0740	0.0615	-0.0343
<i>Average AAPD</i>	0.7593	0.5032	0.3911	0.2968	0.2647	0.2257	-0.0994
<i>Average ACoV</i>	0.5224	0.1962	0.1414	0.1055	0.1042	0.0936	-0.0702
AC sampling							
<i>Average AAB</i>	0.2208	0.1077	0.0703	0.0507	0.0367	0.0316	-0.0337
<i>Average AAPD</i>	0.6794	0.3386	0.2335	0.1607	0.1277	0.1028	-0.1025
<i>Average ACoV</i>	0.3542	0.1113	0.1190	0.0807	0.0589	0.0532	-0.0486
TC sampling							
<i>Average AAB</i>	0.1890	0.0888	0.0480	0.0367	0.0275	0.0249	-0.0290
<i>Average AAPD</i>	0.5716	0.2631	0.1530	0.1140	0.0914	0.0852	-0.0853
<i>Average ACoV</i>	0.2219	0.1003	0.0617	0.0606	0.0528	0.0406	-0.0300
TAC sampling							
<i>Average AAB</i>	0.1850	0.0716	0.0411	0.0280	0.0189	0.0169	-0.0289
<i>Average AAPD</i>	0.5614	0.2157	0.1272	0.0873	0.0651	0.0519	-0.0868
<i>Average ACoV</i>	0.2449	0.0732	0.0646	0.0398	0.0409	0.0344	-0.0335

The best-performing sampling protocol per choice set size and evaluation measure is highlighted

Table 2.12: Demand elasticity comparison of sampling protocols

Protocols compared	Choice set sizes					
	10	50	100	150	200	250
TAC-TC						
<i>Average AAB</i>	2.2% (33)	24.0% (35)	16.8% (33)	31.1% (38)	45.5% (36)	47.3% (39)
<i>Average AAPD</i>	1.8% (33)	22.0% (35)	20.3% (33)	30.6% (38)	40.4% (36)	64.2% (39)
<i>Average ACoV</i>	-9.4% (26)	37.0% (40)	-4.5% (18)	52.3% (37)	29.1% (37)	18.0% (30)
TAC-AC						
<i>Average AAB</i>	19.4% (42)	50.4% (44)	71.0% (40)	81.1% (43)	94.2% (44)	87.0% (42)
<i>Average AAPD</i>	21.0% (42)	57.0% (44)	83.6% (40)	84.1% (43)	96.2% (44)	98.1% (42)
<i>Average ACoV</i>	44.6% (34)	52.0% (38)	84.2% (42)	102.8% (43)	44.0% (38)	54.7% (37)
TAC-Random						
<i>Average AAB</i>	32.7% (42)	121.9% (46)	175.7% (46)	216.1% (47)	291.5% (45)	263.9% (46)
<i>Average AAPD</i>	35.3% (42)	133.3% (46)	207.5% (46)	240.0% (47)	306.6% (45)	334.9% (46)
<i>Average ACoV</i>	113.3% (39)	168.0% (44)	118.9% (45)	165.1% (46)	154.8% (42)	172.1% (42)
TC-AC						
<i>Average AAB</i>	16.8% (45)	21.3% (36)	46.5% (41)	38.1% (39)	33.5% (30)	26.9% (33)
<i>Average AAPD</i>	18.9% (45)	28.7% (36)	52.6% (41)	41.0% (39)	39.7% (30)	20.7% (33)
<i>Average ACoV</i>	59.6% (33)	11.0% (24)	92.9% (44)	33.2% (33)	11.6% (23)	31.0% (36)
TC-Random						
<i>Average AAB</i>	29.9% (46)	78.9% (45)	136.0% (48)	141.1% (47)	169.1% (44)	147.0% (47)
<i>Average AAPD</i>	32.8% (46)	91.3% (45)	155.6% (48)	160.4% (47)	189.6% (44)	164.9% (47)
<i>Average ACoV</i>	135.4% (43)	95.6% (39)	129.2% (42)	74.1% (45)	97.3% (38)	130.5% (43)
AC-Random						
<i>Average AAB</i>	11.2% (43)	47.5% (46)	61.2% (45)	74.6% (45)	101.6% (46)	94.6% (44)
<i>Average AAPD</i>	11.8% (43)	48.6% (46)	67.5% (45)	84.7% (45)	107.3% (46)	119.6% (44)
<i>Average ACoV</i>	47.5% (41)	76.3% (39)	18.8% (31)	30.7% (29)	76.9% (41)	75.9% (36)

The number in parenthesis denotes the number of demand elasticities with lower evaluation measure for the sampling protocol in focus out of a total of 48 estimates

5 Conclusions

The paper proposes a novel stratified importance sampling protocol based on concepts from the activity space literature to overcome the computational challenges associated with the estimation of a joint mode-destination choice model in a behaviourally realistic manner. The results indicate that the proposed importance sampling protocol, TAC, combining both DEs and SDEs/FBs, is capable of achieving a better balance between estimate accuracy, sampling stability and statistical efficiency compared to the other importance sampling protocols examined and especially compared to random sampling, also leading to improvements in VTT estimation and demand forecasting. Furthermore, TAC-derived models avoid overfitting by more closely matching the average choice probabilities for correct predictions of the *true* model. The results hint to the fact that *Random sampling* will benefit more by an increased choice set size compared to the importance sampling protocols, since more spatially relevant alternatives would be required to achieve the same level of accuracy and stability.

A general recommendation regarding the choice set size, relative to the full choice set, in order to achieve stable and sufficiently accurate estimates cannot be made, since this is generally case-specific, but also specific to the sampling protocol employed, as showed in the current study with the performance of *TC*. As a general rule of thumb, though, it could be suggested that having only gradual improvements in estimate accuracy and stability can serve as a sufficient indication of reaching the optimal choice set size. In a practical setting, however, with the absence of a full choice set model to properly assess sampled model accuracy, sampling stability can be considered as a more appropriate evaluation measure.

The current study does not claim that the proposed AS-based importance sampling protocols are the most effective ones, since the main focus was simply to address the limitations identified in the relevant literature. Several other approaches could have been proposed, such as sampling with replacement, but the *TAC* protocol was chosen for comparison purposes as a more behaviourally accurate extension of the *TC* protocol. In future research, the problem of finding the most effective sampling protocol for reducing the choice set size in a destination choice problem of discretionary activities can be formalised as an optimisation problem analysing to what extent the three importance sampling protocols might be more suitable for specific trips/choice tasks or for specific individuals based on their observed behaviour. Future studies should also acknowledge the intricate complications of destination choice of discretionary activities (time-space constraints and travel impedance) that differentiates it from a residential location problem.

Finally, the current study also showcases that emerging data sources, such as GPS, can be effectively used for the specification-estimation of behavioural models. The benefit of the “DECISIONS” dataset, used in the current study, is that it presents a combination of a traditional household survey and GPS tracking over a 2-week period, providing a wealth of observed behaviour to the researcher. The lack of level of service information for the non-chosen alternatives can be sufficiently tackled with the use of readily available APIs even in the absence of a regional transport model. Furthermore, the lack of official land use data, important for the specification of a destination choice model, can be addressed with the use of open source OSM data. Although it is important to consider the potential errors in all of the aforementioned data sources (GPS, API, OSM), the estimated parameters and their signs, as well as the values derived from them, such as VTT estimates and demand elasticities, are behaviourally reasonable and within acceptable ranges.

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Appendix

Table 2.15: Evaluation of AC sampling protocol for choice sets of 10, 50 and 100 alts

Parameter	10 alts				50 alts				100 alts			
	Av.est.	AAPD	ACoV	RMSE	Av.est.	AAPD	ACoV	RMSE	Av.est.	AAPD	ACoV	RMSE
Locational constants												
Constant rest Yorkshire	1.3580	1.4717	0.2369	0.3662	0.9906	0.8030	0.1524	0.2286	0.7494	0.3640	0.1829	0.2001
Households with car ownership												
Constant Car-Other (PT/walking)	-2.7630	0.1091	0.1415	0.5948	-2.8108	0.0475	0.0567	0.3709	-2.8736	0.0526	0.0484	0.3314
Constant Other (PT/walking)-Car	-0.8126	0.4196	0.5225	0.5337	-0.7615	0.1317	0.1643	0.3043	-0.8626	0.2360	0.3091	0.2770
Constant PT-PT	-0.9213	0.3800	0.5193	0.7282	-1.1338	0.1335	0.1614	0.4842	-1.2381	0.1490	0.0772	0.4651
Constant PT-Walking	-1.3146	0.3793	0.5855	1.0283	-1.4213	0.1740	0.2223	0.5959	-1.7795	0.1877	0.1661	0.6393
Constant Walking-PT	-0.5743	0.5250	0.2354	0.8980	-1.2640	0.0856	0.0934	0.5805	-1.1244	0.1713	0.2363	0.5108
Constant Walking-Walking	1.4737	0.7506	0.3232	0.8270	1.1590	0.3767	0.0690	0.4834	1.1199	0.3303	0.1703	0.4356
Mode shifts for households with no car ownership												
Constant Car-Other (PT/walking)	1.2589	0.4589	0.3962	1.0019	1.9530	0.1605	0.0744	0.6410	2.1790	0.1054	0.1471	0.6931
Constant Other (PT/walking)-Car	1.7809	1.8141	0.1583	0.8804	0.9967	0.5749	0.2037	0.6970	0.8680	0.3716	0.1420	0.6915
Constant PT-PT	5.5339	0.2961	0.1414	0.9011	4.6813	0.0964	0.0648	0.5697	4.7026	0.1014	0.0353	0.5493
Constant PT-Walking	3.9305	0.1720	0.1114	0.9700	3.4049	0.0974	0.1348	0.6691	3.8796	0.1569	0.0328	0.7109
Constant Walking-PT	2.9049	0.0643	0.0679	0.8192	3.1943	0.1431	0.0366	0.5765	3.0983	0.1087	0.0582	0.5350
Constant Walking-Walking	3.4497	0.2967	0.0934	0.6641	2.9998	0.1276	0.0532	0.4715	3.0482	0.1458	0.0853	0.4537
Mode shifts for central area destinations												
PT-PT	1.8072	0.1919	0.2364	0.6333	1.8418	0.1032	0.1217	0.4188	1.8431	0.0801	0.0926	0.3992
PT-Walking	1.7459	0.3341	0.4748	0.8208	2.0025	0.1367	0.1152	0.5392	1.8852	0.1251	0.1464	0.5531
Walking-PT	2.7491	0.1091	0.1449	0.7612	2.8434	0.0618	0.0695	0.5540	2.7293	0.0530	0.0724	0.4986
Walking-Walking	1.4996	0.1233	0.1382	0.3957	1.4513	0.1187	0.1020	0.3209	1.5539	0.0704	0.0606	0.3156
Mode shifts for individuals with season ticket ownership												
Walking-Walking	-0.5680	0.2232	0.2749	0.4942	-0.8398	0.4980	0.2730	0.3892	-0.6791	0.2289	0.2464	0.3687
Mode shifts for trips with more than 1 passenger												
PT first/shopping trip	-2.3933	0.3116	0.2372	0.5749	-2.2622	0.2150	0.0257	0.4225	-2.0000	0.0878	0.1128	0.3975
PT following trip	-1.0317	0.3903	0.3720	0.6143	-0.7952	0.1529	0.1796	0.4238	-0.8403	0.2126	0.2695	0.3909
Walking first/shopping trip	-0.7289	0.5103	0.6676	0.4939	-0.7906	0.0488	0.0625	0.3053	-0.8959	0.1912	0.1876	0.2741
Walking following trip	-0.5509	0.9468	0.8140	0.5395	-0.5608	0.5637	0.3092	0.3365	-0.4150	0.2852	0.2861	0.3009
Mode shifts for students												
Walking-Walking	1.5656	0.5310	0.4064	0.6175	1.0471	0.0500	0.0685	0.4449	1.0021	0.0743	0.0807	0.4220
Mode shifts for married individuals												
Walking-Walking	-0.5557	0.5215	0.8849	0.5689	-0.6452	0.2037	0.2273	0.3640	-0.7598	0.1377	0.1763	0.3349
Mode shifts for individuals living in 3-member households												
Walking-Walking	0.8155	0.1819	0.1457	0.6725	0.9943	0.4411	0.1207	0.4446	0.7435	0.2214	0.2640	0.4297
LOS variables												
Travel time for first trip (base level)	-0.0866	0.0741	0.0911	0.0183	-0.0885	0.0329	0.0304	0.0119	-0.0930	0.0425	0.0612	0.0105
Travel time shift for clothes shopping	0.0020	0.9253	6.8277	0.0218	0.0085	0.7061	1.6917	0.0141	0.0175	0.3420	0.2892	0.0124
Travel time for O-S-O trip chains	0.0147	0.3103	0.4398	0.0117	0.0175	0.2087	0.1737	0.0070	0.0175	0.2494	0.2651	0.0068
Travel time for HWH tours	-0.0340	0.2802	0.3418	0.0144	-0.0455	0.0676	0.0823	0.0113	-0.0493	0.1069	0.0314	0.0107
Travel time multiplier for car	1.0000	-	-	-	1.0000	-	-	-	1.0000	-	-	-
Travel time multiplier for PT IVT	0.5449	0.1598	0.2007	0.1187	0.5731	0.0354	0.0450	0.0807	0.5788	0.0251	0.0290	0.0718
Travel time multiplier for PT first access trip	1.2339	0.5056	0.1843	0.4763	0.8582	0.1113	0.1449	0.2883	0.7498	0.0952	0.0917	0.2679
Travel time multiplier for PT last egress trip	0.5858	0.2968	0.3961	0.3196	0.5444	0.1915	0.2231	0.1702	0.5451	0.1047	0.0704	0.1943
Travel time multiplier for PT remaining OVT	0.2416	0.4719	0.6751	0.3974	0.2262	0.4048	0.5520	0.2118	0.3244	0.2460	0.4603	0.2096
Travel time multiplier for following trip	1.4495	0.0679	0.0447	0.2278	1.3872	0.0499	0.0538	0.1379	1.3242	0.0393	0.0409	0.1118
Travel time - Shopping duration elasticity	-0.3399	0.1324	0.1654	0.0653	-0.3375	0.0691	0.0532	0.0392	-0.3219	0.0201	0.0277	0.0350
Travel walking distance (base)	-1.8748	0.1805	0.1445	0.2416	-1.7064	0.0589	0.0619	0.1652	-1.6516	0.0253	0.0228	0.1528
Travel walking distance for O-S-O trip chains	0.4892	1.0733	0.5400	0.2091	0.3763	0.3982	0.2705	0.1471	0.3188	0.2155	0.1446	0.1345
Travel walking distance multiplier for following trip	1.2206	0.0527	0.0633	0.1515	1.2036	0.0507	0.0575	0.1072	1.2510	0.0179	0.0217	0.1087
Box-cox lambda for travel walking distance	0.6855	0.1835	0.1802	0.0871	0.7604	0.0555	0.0476	0.0614	0.7975	0.0214	0.0314	0.0606
Travel walking distance - Shopping duration elasticity	-0.1568	0.1879	0.2303	0.0551	-0.1703	0.2198	0.0681	0.0387	-0.1565	0.1213	0.0557	0.0361
Travel cost	-0.8047	0.2661	0.1828	0.1469	-0.7125	0.0932	0.0319	0.0945	-0.7230	0.1092	0.0533	0.0860
Box-cox lambda for travel cost	0.3244	0.3950	0.3799	0.1253	0.4182	0.2200	0.0529	0.0758	0.4651	0.1326	0.0920	0.0639
Travel cost - Personal income elasticity	-0.2904	0.3000	0.3098	0.1269	-0.2419	0.1504	0.2141	0.0985	-0.2168	0.1097	0.0672	0.0926
Locational variables												
Living in rich areas-shopping in poor areas	-0.8565	0.4590	0.5836	0.5960	-1.0699	0.3312	0.0519	0.3819	-0.9716	0.2227	0.1246	0.3231
Parking areas (400m buffer)	0.0755	0.2917	0.3769	0.0424	0.0877	0.0731	0.0762	0.0298	0.0942	0.0731	0.0954	0.0288
Box-cox lambda for parking areas (400m buffer)	0.6697	0.5877	0.2224	0.1841	0.5103	0.2098	0.0453	0.0974	0.4678	0.1090	0.0848	0.0897
Presence of major clothes shopping retailers (400m buffer)	1.7913	0.1500	0.1994	0.6721	2.3460	0.1955	0.1017	0.3635	2.2923	0.1681	0.0626	0.2874
Presence of major grocery retailers (400m buffer)	0.6901	0.3942	0.2676	0.2025	0.6139	0.1510	0.1362	0.1229	0.5967	0.1187	0.0569	0.1113
Presence of major durables retailers (400m buffer)	3.3681	1.3595	1.1242	1.8473	1.6180	0.5389	0.7255	1.0724	2.1408	0.3428	0.4076	1.5504
Size variables												
Natural logarithm multiplier ϕ	1.0431	0.4293	0.1594	0.3272	0.7114	0.0535	0.0745	0.1572	0.7826	0.0979	0.0983	0.1368
Population (400m buffer)	1.0000	-	-	-	1.0000	-	-	-	1.0000	-	-	-
Exp. of retail areas for clothes stores (400m buffer)	0.3701	1.9494	1.2811	0.9859	0.3854	1.6010	1.1433	0.7524	0.2720	1.0427	1.2265	0.6435
Exp. of retail areas for grocery stores (400m buffer)	0.2170	0.9064	3.2420	1.0913	0.8034	0.3940	0.4298	0.6765	0.6636	0.2521	0.3352	0.4922
Exp. of retail areas for dur./other stores (400m buffer)	-0.5344	2.0462	2.9334	4.0112	0.7488	0.6850	0.8303	0.8945	0.4043	0.5342	0.7774	0.7733
Exp. of shopping store variability (400m buffer)	2.3098	0.7978	0.2051	0.7663	1.9304	0.5026	0.2025	0.6499	1.5502	0.2077	0.1408	0.6518
Exp. of shopping store variability when following trip purpose is shopping (1000-2000m buffer)	0.9303	0.6648	1.4059	4.9276	2.3578	0.1504	0.1733	1.4044	2.6676	0.1842	0.2350	0.9237

Table 2.20: Evaluation of TAC sampling protocol for choice sets of 150, 200 and 250 alts

Parameter	150 alts				200 alts				250 alts			
	Av.est.	AAPD	ACoV	RMSE	Av.est.	AAPD	ACoV	RMSE	Av.est.	AAPD	ACoV	RMSE
Locational constants												
<i>Constant rest Yorkshire</i>	0.7301	0.3290	0.1091	0.1708	0.6680	0.2159	0.0996	0.1668	0.6527	0.1880	0.0620	0.1582
Households with car ownership												
<i>Constant Car-Other (PT/walking)</i>	-2.8391	0.0419	0.0276	0.2919	-2.8645	0.0493	0.0130	0.2841	-2.7983	0.0251	0.0149	0.2813
<i>Constant Other (PT/walking)-Car</i>	-0.8208	0.0462	0.0159	0.2381	-0.8709	0.0622	0.0866	0.2402	-0.8622	0.0424	0.0545	0.2387
<i>Constant PT-PT</i>	-1.2350	0.1461	0.0511	0.4398	-1.2034	0.1533	0.1326	0.4214	-1.1201	0.0406	0.0395	0.4185
<i>Constant PT-Walking</i>	-1.6200	0.0472	0.0385	0.4912	-1.6316	0.0575	0.0492	0.4840	-1.5801	0.0376	0.0481	0.4822
<i>Constant Walking-PT</i>	-1.1634	0.0486	0.0426	0.4829	-1.2912	0.0845	0.0615	0.4850	-1.2025	0.0279	0.0452	0.4806
<i>Constant Walking-Walking</i>	0.8634	0.0768	0.0845	0.3737	0.7677	0.0881	0.0815	0.3714	0.8275	0.0287	0.0393	0.3673
Mode shifts for households with no car ownership												
<i>Constant Car-Other (PT/walking)</i>	2.4436	0.0504	0.0254	0.6725	2.4353	0.0468	0.0207	0.6471	2.3976	0.0306	0.0109	0.6518
<i>Constant Other (PT/walking)-Car</i>	0.5800	0.1676	0.2098	0.6108	0.6451	0.1034	0.1187	0.6103	0.6383	0.0407	0.0574	0.6171
<i>Constant PT-PT</i>	4.4777	0.0487	0.0138	0.5013	4.3713	0.0285	0.0273	0.4949	4.3784	0.0255	0.0130	0.5065
<i>Constant PT-Walking</i>	3.4181	0.0330	0.0322	0.6026	3.3968	0.0168	0.0218	0.5811	3.4530	0.0296	0.0242	0.5873
<i>Constant Walking-PT</i>	2.7217	0.0291	0.0338	0.4752	2.8306	0.0154	0.0131	0.4667	2.7867	0.0059	0.0073	0.4762
<i>Constant Walking-Walking</i>	2.6366	0.0158	0.0218	0.4066	2.6616	0.0072	0.0108	0.4026	2.6935	0.0198	0.0200	0.4112
Mode shifts for central area destinations												
<i>PT-PT</i>	1.8123	0.0466	0.0499	0.3381	1.7869	0.0351	0.0432	0.3370	1.7084	0.0472	0.0584	0.3282
<i>PT-Walking</i>	1.8937	0.0556	0.0537	0.4580	1.8765	0.0341	0.0360	0.4434	1.7769	0.0333	0.0306	0.4394
<i>Walking-PT</i>	2.8277	0.0520	0.0149	0.4769	2.7540	0.0246	0.0072	0.4754	2.7517	0.0269	0.0230	0.4727
<i>Walking-Walking</i>	1.7114	0.0392	0.0197	0.2812	1.6796	0.0199	0.0140	0.2738	1.6577	0.0247	0.0268	0.2705
Mode shifts for individuals with season ticket ownership												
<i>Walking-Walking</i>	-0.4440	0.2080	0.0696	0.3230	-0.5205	0.0894	0.1108	0.3246	-0.5130	0.0921	0.0728	0.3222
Mode shifts for trips with more than 1 passenger												
<i>PT first/shopping trip</i>	-1.8738	0.0124	0.0159	0.3567	-1.9288	0.0435	0.0345	0.3465	-1.9111	0.0391	0.0450	0.3493
<i>PT following trip</i>	-0.8106	0.1083	0.1375	0.3500	-0.7481	0.1347	0.1005	0.3522	-0.7952	0.0802	0.0803	0.3532
<i>Walking first/shopping trip</i>	-0.8712	0.0881	0.0558	0.2333	-0.8545	0.0753	0.0690	0.2345	-0.8460	0.0566	0.0408	0.2322
<i>Walking following trip</i>	-0.3314	0.1208	0.1591	0.2538	-0.3144	0.1454	0.0853	0.2539	-0.3134	0.1481	0.0707	0.2515
Mode shifts for students												
<i>Walking-Walking</i>	1.1118	0.0347	0.0487	0.3751	1.1027	0.0414	0.0578	0.3693	1.0831	0.0357	0.0507	0.3788
Mode shifts for married individuals												
<i>Walking-Walking</i>	-0.8603	0.0991	0.0420	0.2933	-0.8149	0.0411	0.0400	0.2917	-0.8355	0.0674	0.0271	0.2912
Mode shifts for individuals living in 3-member households												
<i>Walking-Walking</i>	0.6591	0.0447	0.0255	0.3874	0.7295	0.0573	0.0567	0.3846	0.7057	0.0627	0.0676	0.3854
LOS variables												
<i>Travel time for first trip (base level)</i>	-0.0882	0.0335	0.0243	0.0092	-0.0912	0.0102	0.0135	0.0092	-0.0906	0.0166	0.0198	0.0093
<i>Travel time shift for clothes shopping</i>	0.0248	0.1249	0.1372	0.0097	0.0249	0.0920	0.1824	0.0100	0.0248	0.1224	0.1382	0.0100
<i>Travel time for O-S-O trip chains</i>	0.0133	0.1270	0.0960	0.0061	0.0144	0.0893	0.1242	0.0061	0.0142	0.0763	0.0821	0.0061
<i>Travel time for HWH tours</i>	-0.0436	0.0462	0.0621	0.0092	-0.0449	0.0195	0.0331	0.0094	-0.0447	0.0238	0.0264	0.0093
<i>Travel time multiplier for car</i>	1.0000	-	-	-	1.0000	-	-	-	1.0000	-	-	-
<i>Travel time multiplier for PT IVT</i>	0.5952	0.0169	0.0250	0.0653	0.5817	0.0094	0.0085	0.0636	0.5843	0.0077	0.0100	0.0632
<i>Travel time multiplier for PT first access trip</i>	0.7945	0.0811	0.0965	0.2652	0.8096	0.0460	0.0554	0.2422	0.7909	0.0349	0.0141	0.2361
<i>Travel time multiplier for PT last egress trip</i>	0.5885	0.0569	0.0739	0.1747	0.5880	0.0487	0.0604	0.1768	0.5959	0.0320	0.0346	0.1699
<i>Travel time multiplier for PT remaining OVT</i>	0.3358	0.1364	0.1858	0.1939	0.2943	0.1786	0.2271	0.1815	0.3352	0.0780	0.0964	0.1819
<i>Travel time multiplier for following trip</i>	1.3847	0.0211	0.0188	0.1051	1.3744	0.0152	0.0134	0.0987	1.3647	0.0163	0.0186	0.1000
<i>Travel time - Shopping duration elasticity</i>	-0.3243	0.0274	0.0184	0.0328	-0.3192	0.0159	0.0148	0.0314	-0.3172	0.0124	0.0212	0.0316
<i>Travel walking distance (base)</i>	-1.5921	0.0208	0.0101	0.1227	-1.6070	0.0117	0.0092	0.1229	-1.6117	0.0088	0.0056	0.1227
<i>Travel walking distance for O-S-O trip chains</i>	0.2497	0.0744	0.0593	0.1150	0.2495	0.0731	0.0423	0.1143	0.2435	0.0951	0.0564	0.1143
<i>Travel walking distance multiplier for following trip</i>	1.2529	0.0065	0.0078	0.0952	1.2501	0.0084	0.0105	0.0932	1.2497	0.0083	0.0119	0.0933
<i>Box-cox lambda for travel walking distance</i>	0.8105	0.0118	0.0133	0.0530	0.8067	0.0031	0.0053	0.0525	0.8072	0.0030	0.0037	0.0519
<i>Travel walking distance - Shopping duration elasticity</i>	-0.1470	0.0585	0.0485	0.0329	-0.1441	0.0330	0.0265	0.0332	-0.1400	0.0250	0.0312	0.0329
<i>Travel cost</i>	-0.6713	0.0298	0.0143	0.0796	-0.6534	0.0166	0.0240	0.0784	-0.6630	0.0171	0.0141	0.0784
<i>Box-cox lambda for travel cost</i>	0.5798	0.0814	0.0349	0.0539	0.5722	0.0671	0.0222	0.0538	0.5697	0.0625	0.0172	0.0518
<i>Travel cost - Personal income elasticity</i>	-0.2364	0.0426	0.0412	0.0979	-0.2403	0.0826	0.1153	0.0964	-0.2522	0.0483	0.0468	0.0961
Locational variables												
<i>Living in rich areas-shopping in poor areas</i>	-0.8054	0.1039	0.1421	0.3179	-0.8504	0.0701	0.0779	0.3181	-0.8184	0.0655	0.0804	0.3023
<i>Parking areas (400m buffer)</i>	0.0961	0.0372	0.0436	0.0273	0.0948	0.0448	0.0585	0.0277	0.0978	0.0509	0.0112	0.0278
<i>Box-cox lambda for parking areas (400m buffer)</i>	0.4278	0.0374	0.0426	0.0796	0.4331	0.0410	0.0475	0.0836	0.4147	0.0168	0.0125	0.0811
<i>Presence of major clothes shopping retailers (400m buffer)</i>	2.0760	0.0650	0.0575	0.2340	2.0318	0.0354	0.0131	0.2234	2.0139	0.0263	0.0046	0.2165
<i>Presence of major grocery retailers (400m buffer)</i>	0.5491	0.0323	0.0270	0.1008	0.5631	0.0556	0.0286	0.0990	0.5498	0.0416	0.0352	0.0992
<i>Presence of major groceries retailers (400m buffer)</i>	2.1292	0.1872	0.2127	1.3590	2.0369	0.1396	0.1979	1.3145	1.6899	0.1977	0.1719	1.4160
Size variables												
<i>Natural logarithm multiplier ϕ</i>	0.7276	0.0112	0.0138	0.1056	0.7220	0.0279	0.0340	0.1025	0.7467	0.0240	0.0247	0.1040
<i>Population (400m buffer)</i>	1.0000	-	-	-	1.0000	-	-	-	1.0000	-	-	-
<i>Exp. of retail areas for clothes stores (400m buffer)</i>	0.3792	0.7351	0.2813	0.5620	0.4392	1.0099	0.2900	0.5631	0.2789	0.3235	0.2595	0.5547
<i>Exp. of retail areas for grocery stores (400m buffer)</i>	0.7512	0.1311	0.1220	0.4037	0.7687	0.1605	0.1275	0.4057	0.6600	0.0758	0.0924	0.3813
<i>Exp. of retail areas for dur./other stores (400m buffer)</i>	0.7906	0.3462	0.1223	0.7541	0.6542	0.1139	0.0529	0.7570	0.6826	0.1623	0.0791	0.7250
<i>Exp. of shopping store variability (400m buffer)</i>	1.2536	0.0606	0.0748	0.7984	1.2522	0.0555	0.0837	0.8261	1.2250	0.0589	0.0605	0.7881
<i>Exp. of shopping store variability when following trip purpose is shopping (1000-2000m buffer)</i>	2.9791	0.0736	0.0534	0.7054	2.9645	0.0683	0.0435	0.6959	2.7594	0.0406	0.0487	0.7086

Chapter 3

Deriving Values of Travel Time estimates using emerging Revealed Preference data

Panagiotis Tsoleridis¹, Charisma F. Choudhury¹ and Stephane Hess¹

Abstract

Transport demand models are widely used to inform policy making and produce forecasts of future demand. A core output derived from demand models is the Value of Travel Time (VTT), which provides insights on the trade-offs that travellers are willing to make in terms of travel time and travel cost. VTT estimates are a critical input to cost-benefit analyses and feasibility assessments of potential projects, while they can also be used in forecasting demand models. Therefore, they play a crucial role in transport planning and policy decisions. While much of the early work on VTT made use of revealed preference (RP) data, their use decreased due to growing concerns about reporting errors that may result in omitted observations and measurement errors in the model inputs. As a consequence, VTT measures have, for the last two decades, primarily been estimated using state-preference (SP) surveys. While SP methods can assess the individual trade-offs in a controlled manner, they are prone to behavioural incongruence. More recently, RP data from passively-collected data sources have raised the promise of accounting for some of the limitations of traditional RP surveys due to the minimal (or even no) active input from the respondent. The present study utilises such a dataset that combined a 2-week trip diary captured through smartphone GPS tracking with a household survey containing individual socio-demographic information. A mixed Logit model for mode choice was specified and the estimated parameters were then applied on the National Travel Survey to calculate the VTT estimates. Those estimates were further adjusted based on trip distances to get more representative national VTT values. This process resulted in estimates similar to the official UK guidelines used in transport appraisal that were obtained from SP data, where our results are not affected by concerns about response quality or survey artefacts. The findings hence strengthen the case for shifting towards passively generated RP data sources and are important for transport practitioners.

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1 Introduction

Transport projects and schemes can substantially impact our day-to-day lives, as well as mid-term decisions like whether or not to buy a car or long-term decisions like where to live. They also have a profound impact on the economic growth of the country, its productivity and people's well-being. Cost-benefit analyses (CBA) and feasibility assessment of potential transport projects are primarily based on the monetary savings from travel time reductions. It is estimated that savings on travel time are responsible for around 80% of the predicted benefits of a new transport project in the UK (Mackie et al., 2001; Fosgerau and Jensen, 2003; Daly et al., 2014). The Values of Travel Time (VTT) estimates, which are used to quantify the trade-offs that decision-makers are willing to make in terms of travel time and travel cost, are hence critical components of CBA. An accurate estimation of VTTs is thus important in order to properly evaluate the costs and the benefits of a new transport project and sufficiently forecast future demand for specific services, e.g. a new public transport route, leading to better informed decisions during the planning phase.

Estimates of the trade-offs that travellers would be willing to make in terms of travel time and cost were first produced in the 1960s. For a long period of time, VTT estimates were derived as relative values to the average wage cost or as a percentage of it (wage cost method or cost savings approach - CSA) and that method is still in use in several countries (Daly et al., 2014). Another approach involved Contingent Valuation, where VTTs were derived from direct questions about how much a participant would be willing to spend for a particular service or an improvement of a current one. In recent decades, most types of VTT analysis are based on the work of Daly and Zachary (1975), who first estimated VTT values from behavioural models (Daly et al., 2014) based on theoretical frameworks of time allocation (Becker, 1965; DeSerpa, 1971) and the Random Utility framework (Marschak, 1960; McFadden, 1973; Domencich and McFadden, 1975; Williams, 1977; Ben-Akiva and Lerman, 1985; Train, 2009).

Revealed Preference (RP) data, usually coming from travel diaries, would at face value provide the natural data source for estimating VTTs, and indeed were used in early studies (Beesley, 1965; Daly and Zachary, 1975). Nonetheless, while RP data provide the ability to capture real-world choices, most of the parameters influencing them are outside of the analyst's control. Furthermore, traditional RP data sources include recalled/reported data that are prone to issues like omitted trips (particularly short ones), perception and rounding errors, etc. - often leading to large measurement errors. During the 1980s, there was also an increasing desire to capture VTTs for non-work trips –largely ignored up to that point– in addition to commuting VTTs. RP data, however, were proved to be unsuitable for providing useful real-world observed choices on non-work trips with the available data collection methods of that era. The aforementioned limitations of RP data led to the growing popularity, over the last two to three decades, of Stated Preference (SP) data as the main input to models, with RP data often being used only in limited scale for verification of the SP results (Mackie et al., 2003). SP surveys present respondents with a number of hypothetical scenarios, where they are asked to choose among a set of alternatives. This approach has a long tradition for example in the United Kingdom (UK) with the first major SP survey conducted in 1984 (MVA et al., 1987) and follow-up studies in 1994 (Accent and Hague Consulting Group 1996) with the same data then re-analysed by Mackie et al. (2003) before the most recent study involving primary data collection taking place in 2014-2015 (Batley et al., 2019; Department for Transport, 2015; Hess et al., 2017).

SP surveys are generally seen to have the advantage of providing the analysts with an environment where they have control over a large number of parameters that could influence VTT estimates, such as the attributes of the alternatives. On the other hand, SP surveys are prone to behavioural incongruence and hypothetical bias and are often criticised for being too sensitive to the experimental design and the representation of the SP scenarios (Brownstone and Small, 2005; Daly et al., 2014; Haghani et al., 2021). Concern in a VTT context has also

been raised in relation to the use of overly simplistic settings in some countries (Hess et al., 2020).

In a recent study examining the impact of hypothetical bias in SP surveys within several domains including transport (Haghani et al., 2021), the authors concluded that although it is more sensible to assume that individuals would likely overstate their Willingness-to-pay (WTP) in a hypothetical scenario (Li et al., 2020), there are a number of transport studies showing the opposite (Nielsen, 2004; Brownstone and Small, 2005; Shires and de Jong, 2009; Krcal et al., 2019). That downward bias of SP has also been proven in two meta-analyses on VTT values across countries and time of Shires and de Jong (2009) and Wardman et al. (2016).

Evidence from neuro-imaging studies also suggests that individuals would often react differently in a stressful situation compared to the lab setting of an SP survey, e.g. be willing to pay more in order to avoid an unpleasant outcome (Loewenstein, 2005; Kang and Camerer, 2013; Haghani et al., 2021). In addition to that, Kang and Camerer (2013) showed that a certain part of the brain was more strongly activated when participants had to make a real choice compared to a hypothetical one. Other psychological effects can also come into play during an SP survey influencing participants' responses, such as the desirability to appear more socially acceptable to the analyst (*social desirability bias*) (Champ and Welsh, 2006), the feeling that their choices will lack of any real-world consequences (*lack of consequentiality*) (Krcal et al., 2019), or the opposite with respondents deliberately giving misleading answers to avoid a potentially harmful outcome resulting from that study, e.g. a road pricing scheme (*strategic bias*) (Lu et al., 2008; Meginnis et al., 2018).

With that evidence in mind and considering that VTT estimates are to be used for the purpose of project evaluation during a CBA, it is only sensible to assume that policy makers would be mostly interested in the trade-offs individuals are willing to make under real-life conditions, sometimes stressful, while taking into account real distributions of travel time and cost and not the ones imposed by the analyst (Louviere and Hensher, 2001; Brownstone and Small, 2005). This thus motivates an increased interest in revealed preference (RP) data for VTT studies. For example, in a review of transport appraisal studies performed in various countries, Daly et al. (2014) concluded that despite SP data being the standard approach so far, researchers and practitioners should reconsider the use of RP data due to the benefits they can provide, while also taking advantage of the new emerging and more robust data collection methods. In addition to that, several studies using traditional RP data sources, such as national travel surveys, have showcased that VTT estimates can still be derived, which are consistent with the official SP-based values (Varela et al., 2018). Nonetheless, there is still a lack of similar studies utilising emerging data sources for VTT estimation purposes.

Emerging data sources, primarily from sensors, such as GPS and mobile phone data, have provided new breakthroughs and challenges to researchers. Travel diaries captured through GPS tracking are able to produce large panels of RP data per participant at a very high spatial and temporal resolution. Compared to traditional pen-and-paper diaries, GPS-based surveys offer the advantage of capturing an increased number of daily trips giving a more representative depiction of individual mobility behaviour without resulting in user fatigue. Though there have been limited efforts to infer VTTs from anonymous RP data sources (e.g. Bwambale et al. (2019)), the absence of socio-demographic information of the travellers and trip characteristics (e.g. trip purpose) have meant that it is not possible to capture the heterogeneity in the VTTs among different socio-demographic groups of users or due to the differences in trip purpose (e.g. commute, business, leisure) from such data.

A passively collected GPS trip diary without any additional mode or trip purpose information could require significant pre-processing efforts (Schuessler and Axhausen, 2009), which could still might not be sufficient enough to avoid biased estimates (Vij and Shankari, 2015). Contrary to that, a semi-passive GPS travel diary with minimum input from the participants and linked to a background household survey can help to account for those limitations. Several studies have used GPS datasets complimented with a background survey,

but most of them have limited their analysis on descriptive statistics of individual mobility behaviour based on the observed choices (Arifin and Axhausen, 2012) or estimated models of mode choice, but without reporting VTT estimates (Montini et al., 2017; Huang et al., 2021). An exception is the study of Calastri et al. (2018), who estimated mode choice models based on GPS data for the purpose of uncovering latent mode availability and consideration constraints of the individuals during their decision-making process. Their study also reported VTTs based on the estimated parameters, however, this was purely as a means of validating their proposed approach, with no emphasis on extrapolating the findings to a representative sample, as required for official VTT values.

The focus of GPS studies so far in the literature has thus not been on the estimation of behaviourally accurate VTTs, representative of the country’s population, which are derived from GPS tracking, and more importantly they have not been compared with national official estimated SP-based VTTs before. That limitation in the current literature and the lack of empirical evidence could partly explain the reluctance of policy makers to accept the use of new emerging GPS data for VTT estimation for appraisal purposes, a task that is still heavily reliant on SP surveys. Aiming to address that limitation, the current study utilises such an emerging data source, namely a 2-week GPS trip diary including 540 participants and 12524 trips, collected as part of the European Research Council funded “DECISIONS” project, for the purpose of estimating a behavioural model of mode choice. The estimated parameters are then applied to the National Travel Survey (NTS) data and VTT estimates are derived, which are further adjusted by distance band to ensure proper representativeness of the UK’s population. The main aim of the study is to compare the final distance-weighted VTT estimates with the latest official SP-based VTTs currently used in appraisal in the UK.

The remainder of the paper is as follows. In the following section, a review of the literature concerning previous VTT studies and their findings and the use of GPS data for transport-related research is performed. In the third section, the datasets used in the current study are described, while in the fourth section, the modelling framework is outlined. Following that, the modelling outputs and the derived VTT estimates are analysed in the fifth and sixth sections, respectively. A discussion regarding the policy implications of the study is performed in the following section, while in the final one the conclusions and limitations of the current study are summarised and the scope for future studies is outlined.

2 Literature review

2.1 Studies on Values of Travel Time estimates

Originating from the studies of Becker (1965) and DeSerpa (1971), the idea of optimal time allocation and the monetisation of non-work activity participation led to the first formulations of the Value of Time. Besides the importance of VTT estimates for CBA and transport project appraisal, they also provide important insights on individual transport behaviour that can lead to better informed policy measures. The willingness-to-pay for a reduction of travel time is closely related to the overall scheduling and time allocation of the individual during the day. As a result, individuals will tend to value higher their time in contexts that would lead to more significant time restrictions (or more potential time savings) in their overall daily schedules. Such contexts can be longer distance trips, which will leave the individuals with significantly less time to accomplish other activities. That is largely empirically proven in the literature, with VTTs increasing by distance (Small, 2012). Another context can be types of activities for which individuals are required to arrive in time, such as commuting trips, or times of day which provide the individuals with greater time restrictions, such as trips during the am peak period. The aforementioned rationale is closely related to the prospect theory (Tversky and Kahneman, 1991) postulating that individuals will put a higher value to avoid a negative outcome than achieving a positive one.

According to empirical evidence from the literature, SP-based VTTs tend to be lower compared to their RP-based counterparts and that can be attributed to several biases arising in the hypothetical setting of an SP design (Shires and de Jong, 2009; Wardman et al., 2016). As an example, we refer to the context of deriving WTP for toll pricing and specifically to the studies of Vrtic et al. (2010) and Brownstone and Small (2005). Vrtic et al. (2010) using SP data found that individuals have lower VTTs in the presence of tolls, compared to untolled roads, as they are willing to take longer routes in order to bypass the tolls. That finding, however, might be subject to *strategic bias* (Lu et al., 2008; Meginnis et al., 2018) from individuals who purposefully overstate their cost sensitivities to dissuade policy makers from such a measure, which will in turn decrease their WTP. Their behaviour in reality might in fact be significantly different as stated in Brownstone and Small (2005), who examined and compared SP and RP WTP for toll pricing among a range of road corridors in the United States. The authors of that second study found that the estimates obtained from hypothetical SP surveys systematically underestimated the VTTs compared to RP-based estimates. A potential cause could be that VTT estimates will depend to a large extent on the travel time and cost range values of the SP scenarios, which could differ substantially in a real-life scenario, such as the case of severe congestion during the morning peak, forcing individuals to place higher valuations of time so as to avoid arriving late at work, although that could also be the case of a higher Value of Travel Time Reliability (VTTR). In any case, such a situation in a real-life context might force the individuals to act differently if they do not leave enough time to take the longer route to avoid the tolls (a case of *lack of consequentiality* (Krcal et al., 2019)). That demonstrates that the hypothetical setting of an SP survey might not be sufficient to capture real-life behaviour, which would adapt according to the time restrictions arising in the daily activity schedules, resulting in biased estimates.

Another reason for the higher RP-based VTTs, however, could also be attributed to choice set misspecification for the case of choice tasks including only one alternative actually under consideration (i.e. captive users), as mentioned in Shires and de Jong (2009). It is generally acknowledged that lack of any explicit information on availability/consideration of alternatives is an important limitation of RP datasets that has hindered their wider adoption for VTT estimation. The analyst observes only the chosen alternatives and has no control over the alternatives actually considered by the individual during her decision making process and thus included in her choice set. Li et al. (2015) have stated that this problem is not exclusive to RP, however, since choices on SP experiments can also be subject to latent choice set formation mechanisms. The presence of those types of behavioural mechanisms on SP data has been proved empirically, as well, in the study of Thiene et al. (2017) examining destination choices for recreational activities.

It is clear then that the derivation of unbiased VTT estimates relies to a large extent on the SP survey design (Bliemer and Rose, 2009). Several techniques have been developed to accomplish that, such as the inclusion of an opt-out alternative, which guarantees that respondents are not forced to choose an alternative. That, however, might also have the adverse effect of choosing the opt-out more often if the attributes of the SP scenario are not reasonable or the SP design is not meaningful to the respondents. As a result, significant effort has been put for making the SP survey more comprehensive and relatable to the respondents by including images and graphics to better describe the attributes of the choice setting. Several sources of the aforementioned biases could also be influenced by the type of SP survey, with higher chances of *social desirability bias*, for example, occurring from face-to-face interviews (Champ and Welsh, 2006).

RP data of limited scale have also been used in VTT studies to provide realistic attribute levels for the SP design to pivot around them. That has been established as the usual approach in SP survey design for VTT estimation, where respondents are asked to provide information of a small number of recently completed trips (Li et al., 2020). Those reference trips are then being used as anchor points to pivot the attributes of travel time and cost for the SP choice scenario around them using reasonable variations of the observed times and costs. Nonetheless, in all those studies the limited use of RP data is evident and it is

reasonable to assume that significant variation in attributes is still left uncaptured and hence not used in the SP design, such as different attribute levels for different times of day, different trip purposes and before or after certain activities (e.g. work), among others.

In addition to the above, there is a constant debate about SP survey complexity and whether to include more attributes per choice task or to have more choice tasks with a limited number of attributes per alternative. The reason for that is to avoid causing too much cognitive fatigue to the respondent, whose choices would become more random as she becomes more fatigued (Bradley and Daly, 1994). The opposite might also be true, however, with choices becoming more deterministic as respondents learn how to respond to choice tasks as they go along (Hess et al., 2012). Instances of both fatigue and learning can occur for the same individual with evidence suggesting the presence of better quality responses at first (learning) followed by a quality decrease in further choice tasks (fatigue) (Hess et al., 2012). Furthermore, empirical evidence suggests that respondents, after a while, will tend to put more emphasis on certain attributes, such as cost, and neglect others, a behavioural process known as attribute-non-attendance (Hensher and Greene, 2010).

All of the aforementioned sources of hypothetical biases can have adverse impacts to the overall survey. It is true to say that the need to account for them has provided a strong motivation for developing state-of-the-art methodological frameworks, most of which having been implemented in the latest official UK VTT study and in other similar studies across Europe. Nonetheless, their mere existence poses significant limitations considering the importance of deriving national VTT estimates to be used in project appraisal, which would be driving future investments for at least the following decade, given their slow update rate documented so far. Even if the analyst is able to successfully account for the majority of those biases in the estimated VTTs, it requires significant effort to do so, which increases the cost and the time required to design an appropriate survey that would minimise any source of hypothetical bias, which is still never guaranteed.

Despite those limitations and potential pitfalls, SP surveys are currently the state-of-the-art approach for VTT estimation, with RP data being used only as auxiliary data to inform the attributes in the SP survey (Small, 2012; Ehreke et al., 2015). Studies have also proposed a combination of RP-SP choices during estimation for forecasting purposes acknowledging the hypothetical nature of SP data and the limitations that could arise in forecasting future demand (Cherchi and Ortuzar, 2006). Nonetheless, even in those cases, the VTT estimation primarily relies on SP data to avoid the limitations of RP data to capture non-linearities in the sensitivities, a notion that is still relevant among the research community due to the data limitations of the past. The dominance of SP data on VTT estimation can be clearly seen by examining the latest reported studies on national VTT values. The Danish (Fosgerau, 2006), Swiss (Axhausen et al., 2006), Norwegian (Halse et al., 2022), Swedish (Börjesson and Eliasson, 2014), Dutch (Kouwenhoven et al., 2014), German (Ehreke et al., 2015) and the UK (Batley et al., 2019) national VTT studies have based their analysis on SP data using only a limited number of RP trips as reference points for the SP attributes.

2.2 GPS data for transport research

Various forms of new emerging data sources are increasingly being used for transport-related research during the past decade (Grant-Muller et al., 2021). Mobile phone data have been one of the first emerging data sources, which gained popularity among researchers and practitioners due to their ubiquitous nature and their ability to capture a wide spectrum of daily urban mobility patterns (Bwambale et al., 2019; Essadeq and Janik, 2021). Similar to mobile phone data, social media data (e.g. Twitter, Foursquare, Weibo etc.) have also been used for the purpose of understanding individual mobility behaviour and are capable of providing interesting insights of aggregate mobility patterns (Yan and Zhou, 2019; Ebrahimpour et al., 2020).

Contrary to the aforementioned emerging passively collected data sources, GPS data

offer the advantage of providing large panels of real-world observed behaviour at a high spatio-temporal resolution. GPS data have been extensively used for transport research during the past twenty years (Wolf, 2004) for studies of understanding daily travel time budgets (Gallotti et al., 2015), destination (Huang and Levinson, 2015; Huang and Levinson, 2017), mode and destination (Tsoleridis et al., 2021), mode (Montini et al., 2017; Calastri et al., 2018), trip chaining and mode (Huang et al., 2021) and route choice behaviour (Li et al., 2005; Hess et al., 2015).

Traditional pen-and-paper trip diaries are likely to result in misreporting of trips, where shorter trips might be omitted by the individuals, while also time spend on travelling tends to be overstated compared to the actual one leading directly to biased (lower) VTT estimates (Kelly et al., 2013). GPS data, on the other hand, due to their passively collected nature, do not require individuals to recall their daily trips (Hess et al., 2015) resulting on average in a larger number of trips per day (Forrest and Pearson, 2005). The type of the GPS device can also have an impact on the quality of the reporting trips, with studies based on GPS loggers noting that many individuals tend to forget them (Bohte and Maat, 2009). Contrary to that, it is much less likely for individuals to forget their smartphone making it a more suitable GPS device for capturing their trips (Calastri et al., 2020).

Despite those advantages, however, there are instances of missing trips in those datasets, as well, due to signal issues or due to individuals turning off the GPS tracking from their devices either for battery or privacy preservation (Calastri et al., 2020). GPS data provide values at a very high resolution, however that characteristic is also one of their most important limitations since significant pre-processing efforts are required to make the data useful for analysis and for deriving insights on mobility behaviour (Stopher et al., 2005; Marchal et al., 2011).

Coupled with minimum input from the participants, such as mode and trip purpose, and an additional background household survey, GPS data have the potential of providing significant advantages over traditional RP data. Despite their extensive use in transport research over the past years, however, no study so far has tried to utilise such a dataset for the estimation of nation-wide VTT estimates and for their comparison with the official SP-based values.

3 Data

3.1 DECISIONS data

Several datasets are utilised in the current study. A behavioural model of mode choice is estimated using the labelled GPS dataset, which was collected between November 2016-March 2017, as part of the “DECISIONS” research project aiming to understand individual transport and energy choices. A detailed description of the dataset (referred to as DECISIONS dataset in the remainder of this paper) is presented in Calastri et al. (2020). That survey consists of several submodules including a trip diary captured through GPS tracking using a smartphone application and a household survey capturing important sociodemographic information of the participants. The GPS trip diary includes the participants’ trips during a 2-week period, in which additional information on the purpose and the chosen mode had to be provided at the end of each trip (semi-passively collected) as depicted in *Figure 3.1* showing the interface of the smartphone application.

The GPS diaries initially included 721 unique individuals and 56,693 observed trips around the UK (5.7 daily trips per individual) with the vast majority of those being around the region of Yorkshire and the Humber, and predominantly around the city of Leeds. As a result, only trips within the region of Yorkshire were selected for the subsequent analysis to avoid larger estimation errors for less represented areas, such as London. The spatial distribution of trips initially included in the dataset, represented as interzonal flows between

3. Data

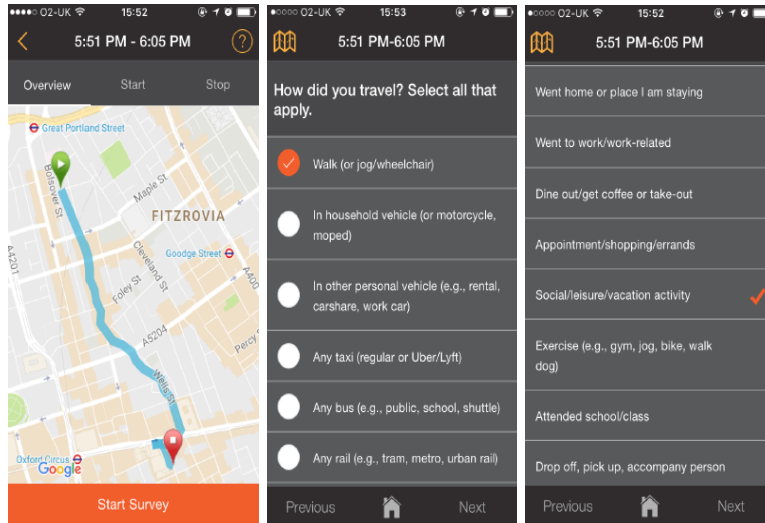


Figure 3.1: User interface of smartphone application used for the GPS trip diary (Calastri et al., 2020)

MSOA zones across the UK, is depicted in *Figure 3.2*, while *Figure 3.3* shows only the trips starting and finishing within the region of Yorkshire. The observed modes of transport included car, bus, rail, taxi, cycling and walking.

A significant effort was undertaken during the cleaning phase with an emphasis on detecting inconsistencies between consecutive trips, in terms of time (following trip starting before the end of the previous trip) and space (space gaps between two consecutive trips). Furthermore, a large number of trips were left *untagged*, meaning that participants did not provide mode and purpose information, and these thus had to be removed from the analysis. No pattern was identified for the erroneous observations or untagged trips that were removed and those were considered as missing at random for the subsequent analysis. Unique activity locations were defined by clustering the observed latitude/longitude coordinate pairs. Hierarchical Agglomerative Clustering (HAC) was used for that purpose, since it does not require the analyst to predetermine the number of clusters. A distance threshold of 200m was selected for the observed destinations to be considered in the same cluster, which resulted in the most plausible clusters for the sample after testing thresholds between 50-500m. As a result from that process, home and work locations were identified based on the tagged purposes for those locations, the time of the day that those locations were visited and the time spent there. Trips were then assigned into tours, starting from and finishing at the home location, per individual and for each day of the survey.

The aforementioned process allowed us to adopt a tour-based approach in terms of mode availability per individual and choice task. In that sense, if an individual chooses car for the first trip of the tour, then only car will be available for the remaining trips of the tour, since it has to be returned back home. Therefore, in such a choice task only the first trip is relevant in a mode choice context, which will include all alternatives in the choice set. The remaining trips of the tour where car would be the only available option in the choice set were removed from the analysis. Conversely, if any other of the available modes was chosen for the first trip, i.e. bus, rail, taxi, cycling or walking, then car would be available for the first trip of the tour and it would become unavailable for the remaining trips of the tour. In such cases, car would be included as an alternative only in the choice set of the first trip. Therefore, the utilised approach despite still being trip-based, it utilises some tour-based feasibility constraints in an attempt to increase the behavioural realism of the model.

A significant problem inherent to RP data and especially to those derived from new emerging data sources, such as GPS, is the lack of any information on the non-chosen alternatives. To overcome that obstacle, the “Directions” Google API was implemented



Figure 3.2: Spatial distribution of interzonal flows between MSOAs across the UK



Figure 3.3: Spatial distribution of interzonal flows between MSOAs across the region of Yorkshire

providing travel times and distances for a range of modes². Travel times/distances for both chosen and unchosen mode alternatives were re-calculated using the API for consistency reasons and to ensure that all values would come from the same data generation process (Calastri et al., 2018). The requests passed on to the API were for two weeks in the future from the date of analysis and for the same day of the week and time of day as in the initial dataset. Two weeks in the future were chosen, so as to avoid the short-term negative impacts of a recent traffic disruption and because the API cannot be used for past dates.

The API provided travel times for car/taxi based on traffic information for the specific time of day when the observed trip was performed. Travel times on the shortest distance routes are calculated for walking and cycling trips. For bus and rail trips, a timetable approach is used and a detailed breakdown of the whole route is provided including walking segments, waiting times and transfers between different services. That level of detail was essential in order to quantify in-vehicle and out-of-vehicle travel times and to be in line with the official VTT estimates. The travel times for the observed modes acquired from the API were compared with the stated travel times for validation purposes. The mean absolute difference across modes was very small, namely 8 mins, indicating that, on average, Google API is capable of providing travel times comparable with the actual ones.

Travel cost was also missing for all alternatives. Car costs were calculated using the official WebTAG specifications regarding fuel³ and operating costs (Department for Transport, 2014). Parking costs were also calculated based on the location of the observed destination (central areas, local high streets etc.) and the activity duration there. Information on hourly and fixed parking costs was obtained from the local authorities in the region of Yorkshire. Fuel, operating and parking costs were added together to form the total car travel cost used for estimation. Bus and rail costs were calculated based on a distance-based fare of the most popular bus and rail operators in the region and a discount was applied for season ticket holders. Finally, taxi cost was calculated using fixed, hourly and distance-based average costs for different cities around Yorkshire.

The final dataset used for model estimation contained 12,524 trips and 540 unique individuals, which is significantly smaller than the SP sample used for analysis in the official study consisting of 7,692 individuals and 15 choice tasks per individual (Hess et al., 2017). Regarding the observed/chosen modes, 47.6% were car trips, 14.6% bus, 5.2% rail, 3.2% taxi, 3.3% cycling and 26.1% walking trips. Commuting and business trips were observed for 19.1% and 9.7% of the sample, respectively. The majority of respondents were female (59.6%) of an average of 40 years old, 75.4% had at least one car in their household and finally 20.7% and 13.3% had a bus and rail season ticket, respectively. The average trip distance across modes per choice task is 2.4 miles (3.9km) with a maximum of 61.1 miles (98.4km) depicting the urban nature of the trips captured in this survey and the absence of longer-distance interurban trips.

In addition to the aforementioned tour-based approach for defining mode availability, a further step was taken to define mode consideration in order to form the final set of alternatives actually considered during the decision making process. Several approaches have been proposed to account for consideration of alternatives, which differ in their level of complexity ranging from fully probabilistic choice set formation approaches (Manski, 1977; Swait and Ben-Akiva, 1987; Calastri et al., 2018) to captivity models (Gaudry and Dagenais, 1979; Swait and Ben-Akiva, 1986) to the incorporation of penalties in the utility function for alternatives exceeding certain attribute thresholds (Cascetta and Papola, 2001; Martinez et al., 2009) and finally to defining consideration of alternatives in a deterministic manner with exogenous thresholds. In the current study, the latter approach was utilised taking into account the observed behaviour in the sample and the results obtained from the API. In that regard, car and taxi trips were excluded for short trips below 5 mins, which was the

²More details can be found here: <https://developers.google.com/maps/documentation/directions/overview>

³Historical petrol and diesel prices for the survey period (November 2016-March 2017) were obtained from <https://www.racfoundation.org/data/uk-pump-prices-over-time>

minimum observed time for those modes in the sample. Bus and rail were excluded for trips in which the API returned only walking segments due to short distances or lack of service. Finally, regarding cycling and walking, which are modes that require physical effort, they were excluded for long distance trips, namely 20km and 3km respectively, which were the maximum observed cycling and walking distances in the sample. Having said that, however, we do acknowledge that there are more behaviourally accurate ways to model alternative consideration, e.g. using a probabilistic choice set formation approach, which could form the basis of future research on that topic in order to assess the impact of uncovering such behavioural mechanisms on the estimated VTTs.

3.2 NTS dataset

The estimates derived from the best-performing model estimated on the DECISIONS were applied on the NTS dataset. The NTS is the official annual survey in the UK providing invaluable long-term information on travel behaviour and mobility trends⁴. Three consecutive years of the NTS data were used, namely 2015-2016-2017, to ensure a representative sample, while also providing an overlap with the period of the DECISIONS survey. A non-sensitive version of the NTS dataset was acquired⁵, where information on personal income was missing. Furthermore, household income was not reported for more than 65% of participants for each year rendering it practically unusable. In addition, since the parameters were estimated on a dataset containing trips mostly around the region of Yorkshire (DECISIONS), it was decided to exclude trips in London from the NTS data, due to the individuals there generally having a different set of available modes, e.g. underground. Contrary to London, the remaining areas around the UK have similar mode availability with regard to public transport, i.e. bus and rail. Furthermore, an important assumption made at this point is that individuals in Yorkshire exhibit a mobility behaviour, which is transferable to the rest of the UK.

The NTS dataset did not provide any information on travel cost for car trips and for a large number of bus and rail trips. For the former, only information on parking cost was provided and fuel and operating costs were imputed using the same approach as in the DECISIONS dataset (Department for Transport, 2014). Fare cost for bus and rail was missing or reported as zero for 49% and 13.4% of bus and rail trips, respectively, which were performed by season ticket holders. Since it is not reasonable to assume a zero VTT for season ticket holders, an average daily cost of a season ticket was applied for bus and rail, based on the cost calculations performed for the DECISIONS data.

The final NTS dataset used for the analysis, excluding London-based trips, included 453,438 trips performed by 29,127 unique individuals (3.1 daily trips per individual), with 52.6% of those being female and with an average age of 50 years old. The average trip distance is 7.9 miles (12.7km) with a maximum of 719 miles (1,157.1 km) showing a more accurate depiction of mobility behaviour including both urban and interurban trips. Regarding the observed modes, 80.4% were car trips, 5.1% bus, 1.2% rail, 1.2% taxi, 1.9% cycling and 10.1% walking trips. Finally, commuting and business trips account for 17.4% and 4.0% of NTS trips, respectively. Detailed descriptive statistics of DECISIONS and NTS trips per mode and purpose are presented in *Table 3.1*.

4 Modelling framework

The VTT estimates presented in the current study are derived from a behavioural model based on the Discrete Choice Modelling (DCM) framework (Ben-Akiva and Lerman, 1985; Train, 2009). A DCM framework based on Random Utility Maximisation assumes that each individual n has a preference for a specific alternative i among a set of J alternatives in a

⁴Details can be found here: <https://www.gov.uk/government/collections/national-travel-survey-statistics>

⁵The NTS dataset was acquired from <https://beta.ukdataservice.ac.uk>

Table 3.1: Number of DECISIONS and NTS trips per mode and purpose

Mode	Commuting	Business	Other (non-work)	Total
DECISIONS trips				
<i>Car</i>	1,015 (8.1%)	693 (5.5%)	4,253 (34.0%)	5,961 (47.6%)
<i>Bus</i>	510 (4.1%)	201 (1.6%)	1,117 (8.9%)	1,828 (14.6%)
<i>Rail</i>	243 (1.9%)	55 (0.4%)	350 (2.8%)	648 (5.2%)
<i>Taxi</i>	23 (0.2%)	30 (0.2%)	352 (2.8%)	405 (3.2%)
<i>Cycling</i>	121 (1.0%)	19 (0.2%)	269 (2.1%)	409 (3.3%)
<i>Walking</i>	477 (3.8%)	214 (1.7%)	2,582 (20.6%)	3,273 (26.1%)
<i>Total</i>	2,389 (19.1%)	1,212 (9.7%)	8,923 (71.2%)	12,524 (100%)
NTS trips				
<i>Car</i>	62,750 (13.8%)	16,199 (3.6%)	285,594 (63.0%)	364,543 (80.4%)
<i>Bus</i>	5,054 (1.1%)	406 (0.09%)	17,580 (3.9%)	23,040 (5.1%)
<i>Rail</i>	2,133 (0.5%)	488 (0.1%)	2,916 (0.6%)	5,537 (1.2%)
<i>Taxi</i>	725 (0.2%)	143 (0.03%)	4,786 (1.0%)	5,654 (1.2%)
<i>Cycling</i>	3,475 (0.8%)	254 (0.1%)	4,927 (1.1%)	8,656 (1.9%)
<i>Walking</i>	4,729 (1.0%)	487 (0.1%)	40,792 (9.0%)	46,008 (10.1%)
<i>Total</i>	78,866 (17.4%)	17,977 (4.0%)	356,595 (78.6%)	453,438 (100%)

choice task t represented as a latent utility U_{int} consisting of a deterministic part V_{int} and a disturbance term ϵ_{int} . Different distributional assumptions about the disturbance term would yield a different specification form. The most commonly used specification is the Multinomial Logit model (MNL) assuming a type-I (Gumbel) Extreme Value distributed disturbance term (McFadden, 1973). The deterministic part V_{int} consists of alternative- and individual-specific attributes, x_{int} and z_n , respectively, as shown in Equation 3.1. The choice probabilities of an MNL model are derived from Equation 3.2.

$$U_{int} = V_{int} + \epsilon_{int} = f(\beta, x_{int}, z_n) + \epsilon_{int} \quad (3.1)$$

$$P_{int}(\beta) = \frac{e^{V_{int}}}{\sum_{j=1}^J e^{V_{jnt}}} \quad (3.2)$$

where β is a vector of parameters to be estimated.

The basic MNL specification assumes that individuals will have the same sensitivity to the specified parameters. Deterministic taste variation in response to specific attributes can be captured as shifts from their base level for specific types of individuals or choice tasks. In the present study, deterministic heterogeneity was captured by specifying shifts from the base level of the alternative specific constants (ASCs) for specific sociodemographic attributes. Furthermore, shifts were also included for the base time and cost parameters of level-of-service (LOS) variables for business and commuting trips. An elasticity specification was used for interactions with continuous sociodemographic attributes, such as age and income, with a separate beta being specified for respondents who did not provide any income information.

Even in the case of accounting for deterministic heterogeneity, however, it is reasonable to assume that some degree of heterogeneity would still remain uncaptured among and/or within individuals leading to biased estimates. Mixed Logit models (McFadden and Train, 2000) can be used to account for that, offering a more flexible specification, where parameters are allowed to vary randomly across individuals. Mixed Logit models are considered as the most general form of a Logit, since they are able to approximate any other specification

(McFadden and Train, 2000). The results, however, will largely depend on the distributional assumptions for each random parameter, a task bestowed on the analyst.

The choice probabilities in a mixed MNL model are now given by an integral over the distribution of individuals' sensitivities (which follow a density function $\phi(\beta|\Omega)$), where this integral does not offer a closed form solution. Simulated log-likelihood estimation is an alternative way of calculating the integral of choice probabilities, based on drawing random numbers from a pre-specified distribution. From that process, the choice probabilities can be calculated as the average over the draws (Equation 3.3) and the simulated log-likelihood can be computed as shown in Equation 3.4.

$$\widehat{P}_{int}(\Omega) = \frac{1}{R} \sum_{r=1}^R P_{int}(\beta^r) \quad (3.3)$$

$$SSL(\Phi) = \sum_{n=1}^N \ln(\widehat{P}_{int}(\Phi)) \quad (3.4)$$

where β^r is a random draw from a distribution with $\phi(\beta|\Omega)$.

It is reasonable to assume that the impact of LOS parameters should be strictly negative, indicating that an additional minute spent travelling or an additional unit of cost spent for a trip will decrease the utility and therefore the choice probability for a certain mode alternative. The specified distribution for the random LOS parameters should be able to account for that, with the negative log-normal distribution being the most applied one for that purpose. In the current study, the long tails of the log-normal distribution resulted in numerical issues during estimation, prompting us to take a different approach. As a consequence, the negative log-uniform distribution was chosen instead, with its shorter tails ensuring no problems during estimation, similarly to the official UK study, which provided the first large scale application of that distribution (Hess et al., 2017). Under that distribution, a variable x is log-uniformly distributed, if $y = \log(x)$ is uniformly distributed. The log-uniform distribution is defined by two additional parameters, a and b denoting its lower bound and spread, respectively. The mean and the variance of the log-uniform distribution are calculated as following (Hess et al., 2017):

$$E(\beta_0) = \frac{e^{a+b} - e^a}{b} \quad (3.5)$$

$$Var(\beta_0) = e^{2a} \left[\frac{e^{2b} - 1}{2b} - \frac{(e^b - 1)^2}{b^2} \right] \quad (3.6)$$

In total, nine parameters were specified as random, namely travel time for car, taxi, walking and cycling, in-vehicle (IVT) and out-of-vehicle (OVT) travel times for bus and rail and finally travel cost. Due to the multidimensionality of the integral, Modified Latin Hypercube Sampling (MLHS) draws were chosen over Halton draws to avoid the multicollinearity issues identified with multidimensional Halton sequences (Hess et al., 2006). For the simulated log-likelihood estimation, 1,000 MLHS numbers r_{UV} were drawn from a uniform distribution for each randomly distributed β , which was specified as $\beta_{LU(a,b)} = e^{a+b*r_{UV}}$. At that number of draws, a sufficient level of stability was observed among the estimates and model fit, hence it was decided not to increase the number of draws any further.

Finally, another issue worth addressing is the presence of heteroscedasticity in the choices occurring from the variance differences across the choice tasks. In the official SP-based VTT study, a multiplicative error term was used instead of the additive one in

Equation 3.1 following the proposed specification in Fosgerau and Bierlaire, (2009), such as $U_{int} = V_{int}\epsilon_{int}$. That specification can be simplified by taking a logarithmic transformation as $\log(U_{int}) = \log(V_{int}) + \log(\epsilon_{int})$ (Fosgerau and Bierlaire, 2009), which requires a strictly positive V_{int} . Instead of that specification, we tried to capture heteroscedasticity by assuming that more uncertainty, hence variance, will exist for choice tasks/trips of longer distances. Therefore, for those trips, the systematic part of the utility, V_{int} , will be smaller compared to trips of shorter distances. In order to capture that, additional scale parameters ϕ_l are specified for different distance bands l and multiplied with the utility function with one scale parameter ϕ_{l_0} being fixed to 1.0. If the base ϕ_{l_0} refers to trips in the shortest distance band then the remaining estimated ϕ_l should be smaller and ideally decreasing as distance increases.

5 Modelling results

The outputs of the behavioural models estimated on the DECISIONS dataset, base MNL, scaled MNL and scaled mixed MNL, are presented in Table 3.2. The scaled MNL model showed significant model fit improvements over the base MNL of 15.5 LL units with 2 additional parameters, namely the scaling parameters ϕ . Those scaling parameters are significantly lower than 1.0 and are decreasing as the distance band increases. Therefore they are able to uncover significant heteroscedasticity among the choices based on distance, hence conforming to our initial hypothesis.

The scaled MNL model was used as the initial point of departure for the mixed MNL specification with the purpose of capturing unobserved heterogeneity. The mixed MNL model with 9 additional parameters provided significant improvements in model fit reducing the LL by 1166.5 units from the scaled MNL model. The adjusted ρ^2 of 0.7723 also signifies that the model is able to explain a significant portion of the variation in the dataset. The Alternative Specific Constants (ASCs) reveal that, all else held equal, individuals of higher income or those who are employed have a negative inherent preference for bus, while also bus is less preferred for trips over the weekend. Interestingly, individuals have an inherent positive attitude for rail compared to car signifying the perceived quality superiority of rail over bus, despite both being public transport modes. Individuals have a negative preference for taxi, although that is not the case for younger individuals below 30 years old. Individuals of lower education (with no undergraduate degree), which can be considered a proxy of income, have a significantly higher dispreference for taxi. Furthermore, there is a negative preference for cycling and an even higher higher dispreference from unemployed individuals, but less so from male individuals and students. Cycling is also more preferred by both the lowest and the highest personal income bands. Finally, all else held equal, individuals and specifically those of younger ages and students have a positive inherent preference for walking.

The importance of capturing non-linear sensitivities with a Box-Cox transformation (Box and Cox, 1964) of travel time and cost attributes for a more accurate VTT estimation has been stated before in the literature (Koppelman, 1981; Gaudry et al., 1989). A common approach is to have either linear or logarithmic specifications of time and cost attributes in the utility function assuming a linear increase of sensitivities or a decreasing one, respectively, as the attribute values increase. Such a specification can be limiting as it assumes that one of those two extreme cases exist in the sample. On the other hand, a Box-Cox transformation provides a more generalised specification as it allows the analyst to capture non-linearities across the whole spectrum of possible values. Using a Box-Cox transformation, an attribute x is specified as $\frac{x^\lambda - 1}{\lambda}$ with λ being an estimable parameter capturing the degree of non-linearity. If λ is not statistically different than 1.0, then the sensitivities for that particular attribute are indeed increasing linearly. If λ is not statistically different than 0, then the sensitivities take a logarithmic form leading to a steep increase at first for small values followed by a decreasing rate for high attribute values (decreasing marginal disutilities). In most cases, the

estimated λ will be between 0 and 1.0, however empirical evidence shows that it can also take values above 1.0 capturing a slow increase in sensitivities for small values and followed by a steeper increase for higher values (increasing marginal disutilities) as shown in Gaudry et al. (1989).

In the current study, a Box-Cox transformation was specified for all LOS attributes in order to assess the estimated λ parameters and their behavioural meaning. For the final model, it was decided to keep a Box-Cox transformation for car, bus, taxi, cycling, walking, OVT bus and OVT rail, which resulted in $\lambda = 0.4581$ significantly different than 1.0 and 0 capturing significant decreasing marginal disutilities, but still not at the extreme of a logarithmic specification. Contrary to the above travel times, a linear specification was used for rail IVT. A behavioural meaning of those specifications and the respective uncovered sensitivities could be that individuals are more sensitive for higher in-vehicle travel times when travelling by rail compared to travelling by car, for example. That can be attributed to an increased discomfort caused by longer distance rail trips or to an increased time restriction for the rest of the daily schedule imposed by the longer distance trip, which prompts the individuals to choose faster and more expensive services. Commuters and business car travellers have also increased time sensitivities due to the importance of arriving on time for those activities compared to non-work trips. Increased car time sensitivities were found for trips during the am peak period (7.00-10.00), while the opposite was true for the pm period (16.00-19.00), relative to all other time periods of the day. That denotes the increased time restrictions of morning trips and the need to arrive on time to the various destinations (mostly work locations), compared to evening trips, most of which are either leisure, shopping or returning trips to home. The decreased time sensitivity for car in the pm period could also denote the individuals' desire to take that extra time to diffuse themselves from the stress of work in the privacy of their car. That difference in time sensitivities between am-pm periods, however, was not evident for public transport and taxi trips. More specifically, individuals showed the same increased sensitivities in both periods for bus and rail trips possibly due to similar crowding levels in those modes from people going to and returning from work resulting in similar unpleasant conditions. For taxi trips, individuals had a lower sensitivity for pm compared to am period, but still higher relative to all other periods of the day.

A Box-Cox λ not statistically different than 0 was found for travel cost, which led us to keep a logarithmic specification of travel cost for the final models presented here signifying the presence of cost damping effects in the sample (Daly, 2010). That also signifies that cost sensitivity decreases at a faster rate than the time sensitivities, which will result in higher valuations for larger potential time savings, i.e. in longer distance trips (De Borger and Fosgerau, 2008; Small, 2012). Different combinations of personal and household income were specified as elasticities for the LOS parameters, with only the elasticity of personal income and OVT for bus and rail resulting in statistically significant estimates for the MNL models, at least. The sign of the parameter is positive, meaning that as income increases, the sensitivity to OVT also increases, which is behaviourally sensible. That OVT-income elasticity, however, became statistically insignificant in the mixed MNL model. Finally, all of the β parameters of the log-uniform distributions, i.e. the spread, were found to be statistically significant capturing significant inter-individual heterogeneity.

Table 3.2: Outputs of base MNL and mixed MNL models

Fit statistics	Base MNL	Scaled MNL	Scaled Mixed MNL
<i>Log-likelihood (0)</i>	-14,974.45		
<i>Log-likelihood (model)</i>	-4,535.41	-4,519.92	-3,353.41
<i>Adjusted ρ^2</i>	0.6941	0.6950	0.7723
<i>AIC</i>	9,162.81	9,135.83	6,820.82
<i>BIC</i>	9,504.84	9,492.73	7,244.64
<i>Number of parameters</i>	46	48	57

Continued on next page

5. Modelling results

Table 3.2 – continued from previous page

Parameter	Estimate (Rob. t-rat. 0) [Rob. t-rat. 1]		
	Base MNL	Scaled MNL	Scaled Mixed MNL
<i>Number of individuals</i>	540		
<i>Number of observations</i>	12,524		
Parameter	Estimate (Rob. t-rat. 0) [Rob. t-rat. 1]		
	Base MNL	Scaled MNL	Scaled Mixed MNL
Alternative-specific constants			
<i>Constant Bus</i>	-0.0929 -0.26	0.3195 (0.80)	-0.0905 (-0.20)
<i>Constant Bus shift for personal income >50k</i>	-1.1902 -1.44	-1.4445 (-1.46)	-4.4972 (-5.77)
<i>Constant Bus shift for weekend</i>	-0.7165 (-4.05)	-0.8230 (-3.99)	-1.1573 (-4.19)
<i>Constant Bus shift for unemployed individuals</i>	0.7378 (1.08)	0.7066 (0.94)	0.7765 (1.43)
<i>Constant Rail</i>	2.4421 (2.21)	3.1648 (2.58)	2.3179 (2.23)
<i>Constant Taxi</i>	-1.8075 (-4.09)	-1.3129 (-2.37)	-1.8398 (-2.91)
<i>Constant Taxi shift for male</i>	-0.6434 (-2.10)	-0.7479 (-2.19)	-0.5739 (-1.32)
<i>Constant Taxi shift for age 18-24</i>	1.5014 (4.67)	1.8120 (4.66)	2.8605 (6.74)
<i>Constant Taxi shift for age 25-29</i>	0.9324 (2.64)	1.1385 (2.79)	2.0238 (3.86)
<i>Constant Taxi shift for lower education levels</i>	-1.3979 (-2.46)	-1.5940 (-2.44)	-2.4137 (-2.66)
<i>Constant Taxi shift for personal income 40k-50k</i>	-0.7975 (-2.18)	-0.9311 (-2.26)	-1.3510 (-2.35)
<i>Constant Cycling</i>	-4.0728 (-7.85)	-4.1352 (-7.21)	-4.3336 (-6.71)
<i>Constant Cycling shift for male</i>	1.1047 (2.69)	1.2663 (2.80)	2.0747 (4.89)
<i>Constant Cycling shift for personal income 10k-20k</i>	0.8020 (1.93)	0.9510 (2.08)	2.0946 (4.97)
<i>Constant Cycling shift for personal income 75k-100k</i>	3.5150 (3.49)	4.0077 (3.61)	5.7908 (4.96)
<i>Constant Cycling shift for not reported income</i>	-2.4544 (-1.69)	-2.9037 (-1.72)	-2.9202 (-2.89)
<i>Constant Cycling shift for weekend</i>	-0.6604 (-2.01)	-0.7803 (-2.06)	-1.5423 (-2.51)
<i>Constant Cycling shift for student</i>	1.1559 (2.23)	1.4223 (2.49)	2.8486 (5.57)
<i>Constant Cycling shift for unemployed individuals</i>	-1.1964 (-2.22)	-1.5084 (-2.59)	-5.5566 (-10.02)
<i>Constant Walking</i>	3.0294 (5.73)	3.1564 (5.34)	3.4426 (4.95)
<i>Constant Walking shift for age 18-29</i>	0.6964 (2.62)	0.6948 (2.55)	0.8225 (2.82)
<i>Constant Walking shift for lower education levels</i>	-0.7563 (-3.47)	-0.7843 (-3.43)	-1.1039 (-4.09)
<i>Constant Walking shift for weekend</i>	-0.5704 (-2.87)	-0.6310 (-2.90)	-0.8050 (-3.11)
<i>Constant Walking shift for student</i>	0.7277 (2.37)	0.8039 (2.53)	1.1111 (2.92)
LOS parameters			
<i>Travel time Car (Box-Cox)</i>	-0.2426 (-3.02)	-0.1680 (-2.33)	–
<i>Travel time Car shift for commuting</i>	-0.1478 (-2.92)	-0.1709 (-2.95)	-0.2347 (-3.37)*
<i>Travel time Car shift for business</i>	-0.0408 (-0.97)	-0.0308 (-0.65)	-0.1180 (-1.79)*
<i>Travel time Car shift for am peak</i>	-0.1637 (-3.08)	-0.1817 (-3.07)	-0.2315 (-3.48)*
<i>Travel time Car shift for pm peak</i>	0.1282 (2.47)	0.1279 (2.43)	0.1720 (2.41)*
<i>IVT Bus (Box-Cox)</i>	-0.1281 (-3.19)	-0.1363 (-3.32)	–
<i>IVT Bus shift for am-pm peak</i>	-0.0998 (-3.33)	-0.1010 (-3.29)	-0.0902 (-2.51)*
<i>IVT Rail (linear)</i>	-0.0080 (-0.66)	-0.0105 (-0.71)	–
<i>IVT Rail shift for am-pm peak</i>	-0.0327 (-2.91)	-0.0366 (-2.65)	-0.0472 (-2.54)*
<i>Travel time Taxi (Box-Cox)</i>	-0.4525 (-3.22)	-0.5299 (-3.40)	–
<i>Travel time Taxi shift for am peak</i>	-0.1709 (-2.71)	-0.1918 (-2.85)	-0.2877 (-3.70)
<i>Travel time Taxi shift for pm peak</i>	-0.1423 (-3.24)	-0.1346 (-2.96)	-0.1305 (-2.31)
<i>Travel time Cycling (Box-Cox)</i>	-0.3343 (-3.15)	-0.3478 (-3.22)	–
<i>Travel time Walking (Box-Cox)</i>	-0.6774 (-3.26)	-0.6116 (-3.32)	–
<i>Box-Cox lambda for Travel time for Car, Bus, Taxi, Cycling, Walking</i>	0.5424 (5.25) [-4.43]	0.5942 (5.91) [-4.03]	0.5932 (5.57) [-3.82]*
<i>OVT Bus (Box-Cox)</i>	-1.1484 (-5.59)	-1.2007 (-5.57)	–
<i>OVT Bus for income non respondents</i>	-1.1920 (-5.14)	-1.2663 (-5.05)	-1.4745 (-6.62)
<i>OVT Rail (Box-Cox)</i>	-1.7365 (-3.50)	-1.8308 (-3.44)	–

Continued on next page

Table 3.2 – continued from previous page

Parameter	Estimate (Rob. t-rat. 0) [Rob. t-rat. 1]		
	Base MNL	Scaled MNL	Scaled Mixed MNL
<i>OVT Rail for income non respondents</i>	-1.4853 (-3.04)	-1.5539 (-2.93)	-1.4900 (-4.48)
<i>Box-Cox lambda for OVT Bus, OVT Rail</i>	0.1452 (1.59) [-9.35]	0.1884 (1.97) [-9.59]	0.3131 (4.67) [-10.25]
<i>Income elasticity for OVT Bus, OVT Rail</i>	0.0880 (2.26)	0.0962 (2.36)	0.0572 (1.11)
<i>Travel cost (log)</i>	-0.8362 (-10.73))	-0.9428 (-10.43)	–
Random LOS parameters			
<i>a of Travel time Car (Box-Cox)</i>	–	–	-0.1553 (-0.60)*
<i>b of Travel time Car (Box-Cox)</i>	–	–	-3.0508 (-5.60)*
<i>a of IVT Bus (Box-Cox)</i>	–	–	-0.2598 (-0.97)*
<i>b of IVT Bus (Box-Cox)</i>	–	–	-2.9434 (-5.64)*
<i>a of IVT Rail (linear)</i>	–	–	-0.9137 (-7.59)*
<i>b of IVT Rail (linear)</i>	–	–	-7.4859 (-4.01)*
<i>a of Travel time Taxi (Box-Cox)</i>	–	–	0.9373 (4.86)
<i>b of Travel time Taxi (Box-Cox)</i>	–	–	-1.7604 (-8.33)
<i>a of Travel time Cycling (Box-Cox)</i>	–	–	2.2121 (8.32)
<i>b of Travel time Cycling (Box-Cox)</i>	–	–	-3.6775 (-8.09)
<i>a of Travel time Walking (Box-Cox)</i>	–	–	-0.6679 (-1.81)
<i>b of Travel time Walking (Box-Cox)</i>	–	–	0.8886 (6.97)
<i>a of OVT Bus (Box-Cox)</i>	–	–	1.3095 (6.15)
<i>b of OVT Bus (Box-Cox)</i>	–	–	-1.8183 (-7.20)
<i>a of OVT Rail (Box-Cox)</i>	–	–	0.0579 (0.22)
<i>b of OVT Rail (Box-Cox)</i>	–	–	1.1181 (7.41)
<i>a of Travel cost (log)</i>	–	–	-1.8271 (-4.53)*
<i>b of Travel cost (log)</i>	–	–	3.0789 (5.83)*
Scale parameters			
<i>Scale ϕ_1 for trip distances <3km</i>	–	1.0000 (–)	1.0000 (–)
<i>Scale ϕ_2 for trip distances 3km-20km</i>	–	0.8313 (16.50) [-3.35]	0.8031 (14.84) [-3.64]
<i>Scale ϕ_3 for trip distances >20km</i>	–	0.6805 (8.54) [-4.01]	0.6560 (7.09) [-3.72]

6 Values of Travel Time estimates

The estimated parameters of the mixed MNL model (see *Table 3.2*) were applied to the NTS dataset, which provides mobility-related information on a sample of the UK population. Acknowledging the fact that the NTS dataset is still a sample of the UK population, we further adjusted the resulting VTTs using appropriate distance-based factors in order to calculate VTT values representative for the population of the UK (with the exclusion of London). Distance correction was performed using mode-specific information on travel distances for work trips obtained from the Census of 2011. The process is detailed below and also depicted in *Figure 3.4*.

Sample level VTT calculation

VTTs were computed using sample enumeration over the car, bus and rail trips of the NTS sample. VTTs are calculated as the relative importance of one unit of change in time relative to one unit of change in cost. In mathematical terms, that is represented as the ratio of the partial derivatives of travel time over travel cost, as shown in *Equation 3.7*.

*Estimated parameters used for the VTT calculations

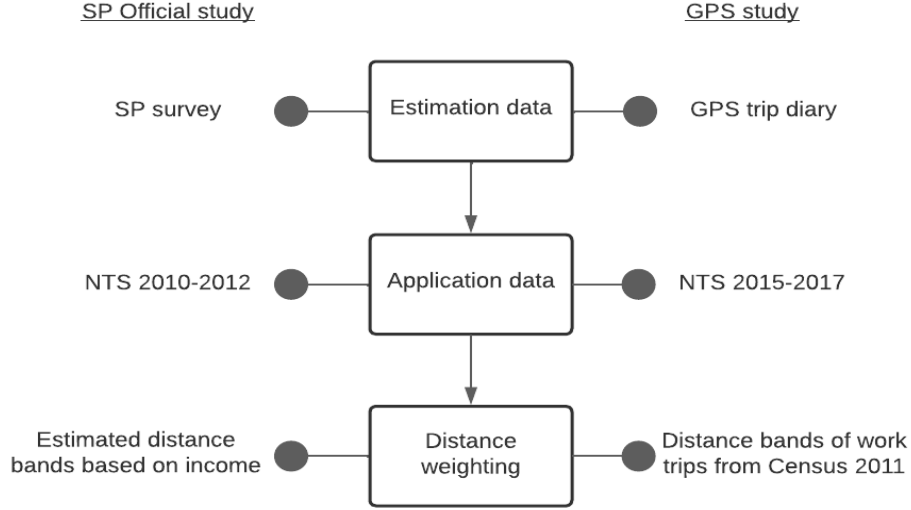


Figure 3.4: Comparison approach between SP and GPS-based VTTs

$$VTT = \frac{\frac{\partial V_i}{\partial tt_i}}{\frac{\partial V_i}{\partial tc_i}} = \frac{\partial V_i}{\partial tt_i} \frac{\partial tc_i}{\partial V_i} \quad (3.7)$$

Sample enumeration is required because the attributes of travel time for car and bus and travel cost for all three modes enter the VTT calculation due to their specification in the respective utility functions. Taking car travel time as an example, its specification using a Box-Cox transformation leads to a partial derivative of $\beta_{tt}^{car} tt_{car}^{(\lambda-1)}$. Furthermore, travel cost, specified using a logarithmic transformation, leads to a partial derivative of $\beta_{tc} \frac{1}{tc}$. Therefore, the VTTs are computed for each choice task of the sample taking into account their respective trip attributes of travel time and cost for the chosen mode.

Deriving representative VTT for different distance-bands

In the guidance provided by DfT, the VTT values were both adjusted based on covariates included in the NTS data and were further weighted based on trip distances of different synthetic household income bands acknowledging the impact of distance on the VTT (Zhang and Laird, 2014; Batley et al., 2019). In the current study, due to the absence of any information relating to the distance weighting per income band, only the first correction was performed. According to that, distance-based factors were derived based on the relative importance of the mode-specific distance bands from the Census 2011 (excluding London) over the NTS distance bands and applied on the sample level VTTs (Equation 3.8). For that purpose, the NTS car, bus and rail trips were allocated to the same eight distance bands as the ones in the Census, namely 0-2km, 2-5km, 5-10km, 10-20km, 20-30km, 30-40km, 40-60km and over 60km, and the trip distributions over those distance bands were calculated for both datasets. The distance-based correction factor w_t for trip t was computed as $w_t = \frac{perc_{d_t,i,p,m}^C}{perc_{d_t,i,p,m}^{NTS}}$, where $perc_{d_t,i,p,m}^C$ and $perc_{d_t,i,p,m}^{NTS}$ are the Census and the NTS distributions of distance band i

Table 3.3: Distance band distributions and distance-based correction factors per mode

Distance band	Census 2011 (%)	NTS (%)	correction factor
Car			
0-2 km	13.52	7.65	1.77
2-5 km	21.83	20.57	1.06
5-10 km	22.67	21.48	1.06
10-20 km	21.97	23.31	0.94
20-30 km	9.04	11.19	0.81
30-40 km	3.93	5.03	0.78
40-60 km	3.18	5.89	0.54
Over 60 km	3.87	4.88	0.79
Bus			
0-2 km	12.39	3.91	3.17
2-5 km	40.22	30.13	1.34
5-10 km	28.18	37.17	0.76
10-20 km	11.91	23.32	0.51
20-30 km	2.67	4.08	0.65
30-40 km	1.00	0.91	1.11
40-60 km	1.05	0.34	3.08
Over 60 km	2.57	0.15	16.74
Rail			
0-2 km	3.55	–	–
2-5 km	5.74	2.97	1.93
5-10 km	10.84	9.09	1.19
10-20 km	17.62	22.64	0.78
20-30 km	15.75	18.63	0.85
30-40 km	12.10	17.28	0.70
40-60 km	16.77	10.08	1.66
Over 60 km	17.65	19.31	0.91

for trip t of purpose p and mode m , respectively ⁶. Due to the lack of any additional explicit information regarding distances for non-work trips, the same correction factors were applied in those cases, as well. The distance band distributions of the NTS and the Census 2011 per mode and purpose, as well as the respective correction factors applied are presented in *Table 3.3*.

$$\overline{VTT}_{p,m} = \frac{\sum_t (w_t VTT_{t,p,m})}{\sum_t w_t} \quad (3.8)$$

where $VTT_{t,p,m}$ and $\overline{VTT}_{p,m}$ are the VTT for choice task t , purpose p and mode m and the weighted average VTT, respectively.

Due to the complex specification of the utility function and the resulting VTT calculation, we rely on simulation for the calculation of standard errors for the different VTTs and not on the most commonly used approach of the Delta method (Daly et al., 2012). Confidence intervals and standard errors for the estimated VTTs were calculated using multivariate normal draws based on the estimated parameters and the covariance matrix of the behavioural model (Train, 2009). Specifically, 3,000 draws for the estimated parameters were drawn and

⁶Details can be found here: <https://www.nomisweb.co.uk/census/2011/dc7701ewla>

simulated VTTs were calculated for each of the 3,000 samples. At that number of draws the distance-adjusted means of the simulated VTTs per mode and purpose had only small discrepancies from $\overline{VTT_{p,m}}$, so no further draws were deemed necessary for the analysis. The 95% confidence interval was then calculated for the resulting simulated VTT distribution per mode and purpose using the percentile interval method and the standard errors were calculated as the standard deviations of the simulated VTT distributions. Finally, the t-stat of the difference between the estimated VTT means were calculated based on *Equation 3.9*.

$$t - stat_{diff} = \frac{\overline{VTT_{GPS}} - \overline{VTT_{SP}}}{\sqrt{s.e.^2_{GPS} + s.e.^2_{SP}}} \quad (3.9)$$

VTTs in the official study were segmented into distance bands of 0-20 miles, 20-100 miles and over 100 miles, however, those were later revised by the DfT to 0-50 miles, 50-100 miles, 100-200 miles and over 200 miles (Batley et al., 2019). The behavioural model in the current study was estimated on a dataset where the maximum trip distance was 61.1 miles. Despite that, we decided to apply the estimates on NTS trips of longer distances, as well, to present a more complete comparison across the different distance bands with the official VTT study. As a result, the same distance bands of <20 miles, 20-100 miles and over 100 miles have been used. In addition to not having long distance trips in the estimation data, the application data of NTS also includes only a small number of medium and long distance trips, namely 8.09% of trips are above 20 miles, 2.16% above 50 miles and 0.78% above 100 miles. The same issue of a small number of long distance NTS trips was tackled in the official SP study by conducting additional intercept sampling favouring trips of longer distance and specifically business trips (Batley et al., 2019), however that was not possible in our case. Therefore, we should acknowledge the fact that calculated VTTs for medium (20-100 miles) and longer distances (above 100 miles) might contain higher estimation errors. Furthermore, when comparing the derived VTTs of the current study with the official ones, the exclusion of London is an important factor to be taken under consideration, as well. As a consequence, in the current study there is no ‘‘Other PT’’ as a mode alternative, which was included in the official VTTs and mainly referred to London-specific mode alternatives, such as light rail and the underground. The exclusion of London-based trips from the NTS data, also has an impact on the total sample size for our GPS-based VTTs, which is much smaller than the NTS sample size used in the official SP study.

The official VTT estimates based on the latest nationwide UK SP survey (adjusted for 2016 prices) are presented in *Table 3.4*, both overall and distance segmented values, and are compared with the respective GPS-based VTT estimates of the current study. In the official VTT study, bus was not included as an alternative for business trips, hence we decided to follow the same approach here, as well, for consistency reasons. The overall VTT values, which are to be used for appraisal, show only negligible differences with the official ones, despite that only a limited number of longer distance trips was used in the calculation of the GPS-based VTTs. The distance segmented values are mainly used for reporting purposes (Daly et al., 2014), however, interesting findings can be extracted by their examination. Firstly, there are very small differences between the GPS-based and SP-based VTTs for the shortest distance band below 20 miles, and there is a higher estimation accuracy on the VTTs of that distance band due to the larger sample size in the NTS data. Another reason for these small discrepancies could be the that the SP surveys were able to sufficiently capture individual mobility behaviour in such hypothetical scenarios of small trip distances. On the contrary, starker differences are observed across the remaining VTTs for medium to long distance trips, which to a large extent can be attributed to the small number of trips in those bands. Nonetheless, those significant differences could also be attributed to the inherently more unpredictable nature of longer trips that is more challenging to be sufficiently accounted for in the hypothetical setting of an SP survey. As it is evident from *Table 3.4*, the GPS-based values might be able to capture a more behaviourally accurate depiction of

Table 3.4: Official VTT estimates per mode, purpose and distance band based on the latest SP survey (Batley et al., 2019) and the respective derived GPS-based VTT estimates (£/hour) (2016 prices)

Distance band	Commute trips	Other trips	Business trips			
	All modes	All modes	All modes	Car	Other PT	Rail
Official SP values						
<i>All distances</i>	11.69	5.34	19.01	17.46	8.69	28.80
<i><20 miles</i>	8.63	3.78	8.67	8.56	8.69	10.54
<i>20-100 miles</i>	12.67	6.77	16.74	16.53	8.69	30.23
<i>>=100 miles</i>	12.67	9.67	29.85	26.84	8.69	30.23
GPS-based values						
<i>All distances</i>	12.90	5.40	17.13	16.60	–	33.43
<i><20 miles</i>	11.24	4.68	11.16	11.20	–	9.78
<i>20-100 miles</i>	30.52	15.67	36.59	36.21	–	43.78
<i>>=100 miles</i>	75.57	24.29	82.25	70.12	–	187.96

the VTTs, which increase significantly for longer distance trips capturing the individuals' increased time restrictions during their daily activity schedule, as it is also supported by the literature. Having said that, however, it is important to note that a more balanced sample would be required in terms of trip distances in order to draw more robust conclusions about that.

The standard errors of the estimated mode- and purpose-specific VTT means (across all distances) and their 95% confidence intervals are presented in *Table 3.5* along with the t-statistic of the difference of the means between the GPS-based and the official SP-based VTTs. Overall, standard errors of the GPS-based VTTs are higher and that can be attributed to a higher degree of heterogeneity captured in our study compared to the SP survey or it could also simply be due to the smaller sample size. For all VTTs presented in *Table 3.5*, we cannot reject the null hypothesis of difference from the official valuations, at the 95% confidence level. Furthermore, the GPS-based VTTs follow the general trends of the SP values. Values for rail are higher than car and bus, with the latter has the lowest values overall. Furthermore, business VTTs are higher than commuting and other non-work trips. Commuting values are in general higher than non-work trips, however, the opposite was found for SP bus and GPS rail VTTs for non-work trips. Bus VTT for commuting trips show the largest difference compared to the rest, followed by other non-work rail VTTs, but those are still not statistically significant differences. Finally, in most cases, the GPS-based VTTs are higher than the SP-based ones conforming with previous evidence in the literature (Wardman et al., 2016), however the downward hypothetical bias for SP is less significant in that case.

The distributions of the simulated VTTs are also presented in the box plots in *Figures 3.5-3.7*. In those plots, the impact of the smaller sample size for rail trips becomes evident as it leads to wider distributions highlighting the uncertainty around the estimation of those VTTs, contrary to the more compact distributions of commuting and non-work VTTs.

7 Discussion

The results of this study clearly demonstrate that the argument of RP data collection limitations of the past does not hold anymore in the current age of data revolution. Semi-passively collected emerging data sources have the ability to provide the analysts with large panels of observed mobility behaviour at a high spatio-temporal resolution and at a relatively low cost. Those types of datasets, in that case a GPS trip diary coupled with a background household survey, have the ability of providing robust behavioural models and VTT estimates statistically equal with official national values derived from traditional SP surveys.

Table 3.5: Confidence intervals and standard errors of the mean estimates for the overall official VTT estimates per mode and purpose (Batley et al., 2019; Hess et al., 2017) and the respective derived GPS-based VTT estimates (£/hour) (2016 prices)

Mode-Purpose	VTT (St.error) [95% C.I.]		t-stat diff
	SP-based values	GPS-based values	
Car			
<i>Commuting</i>	12.20 (2.05) [8.18-16.23]	13.52 (2.68) [9.17-19.78]	0.39
<i>Business</i>	17.46 (2.04) [13.47-21.45]	16.60 (4.60) [9.94-27.40]	-0.17
<i>Other</i>	5.12 (1.84) [1.53-8.72]	5.45 (1.28) [3.50-8.32]	0.15
Bus			
<i>Commuting</i>	3.29 (0.48) [2.34-4.23]	5.46 (1.14) [3.59-7.97]	1.75
<i>Other</i>	3.40 (0.43) [2.56-4.24]	3.99 (0.88) [2.60-5.94]	0.60
Rail			
<i>Commuting</i>	12.95 (0.91) [11.17-14.73]	12.41 (3.28) [7.26-20.00]	-0.16
<i>Business</i>	28.80 (2.49) [23.91-33.68]	33.43 (9.11) [19.82-55.09]	0.49
<i>Other</i>	9.05 (0.64) [7.80-10.30]	14.26 (3.94) [7.32-23.39]	1.31

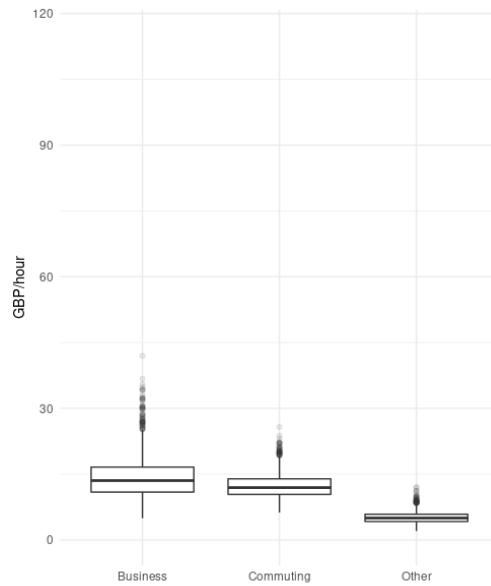


Figure 3.5: Box plots of GPS-based Car VTTs per purpose

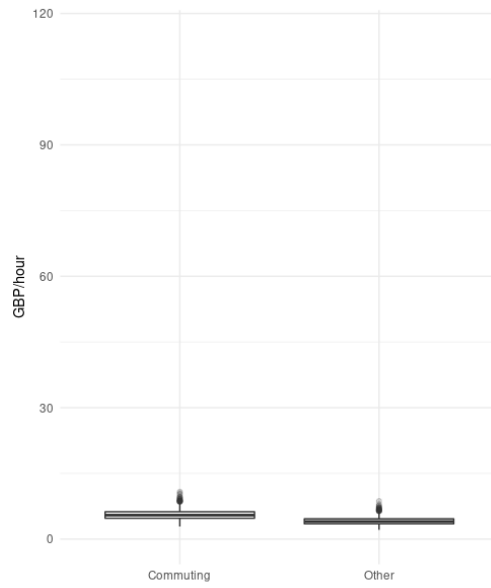


Figure 3.6: Box plots of GPS-based Bus VTTs per purpose

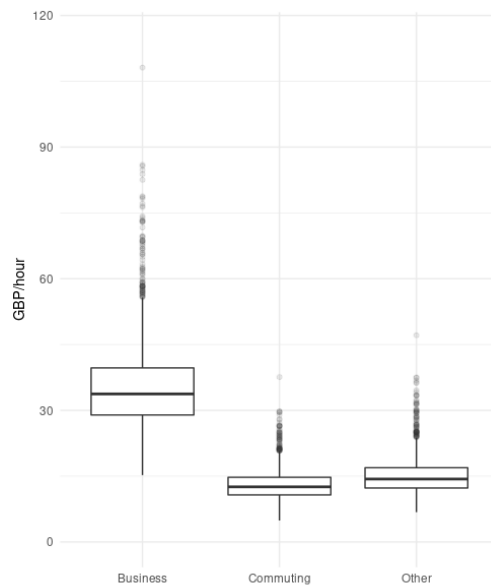


Figure 3.7: Box plots of GPS-based Rail VTTs per purpose

It may be noted though that the overall sample size of the finally utilised estimation dataset was smaller compared to the SP survey, as a large share of trips had to be removed from the original DECISIONS data during the cleaning phase in order to exclude inconsistent, incomplete and untagged trips. Furthermore, the trips recorded in the DECISIONS dataset were mostly urban trips, while the official SP survey included longer distance trips, as well. The aforementioned limitations, however, can be easily overcome in nationally important studies by designing a more comprehensive data collection process. Those limitations can be partly justified since the DECISIONS dataset was not collected with the purpose of estimating nation-wide VTT values in mind. Despite those limitations, the study has two key findings which are of importance to transport planners and policy makers:

1. The study demonstrates that the overall VTT estimates were similar to the official SP-based values used for appraisal, even with a smaller sample size. As a result, there is a smaller hypothetical bias in the official SP study compared to the usual RP/SP documented in the literature across a range of studies (Wardman et al., 2016).
2. Segmenting the VTTs by distance bands, larger discrepancies start to become evident among longer distance bands with the SP-based VTTs being smaller in most cases. That hints to a downward bias for SP surveys potentially originating from the hypothetical nature of the longer trips, which made them difficult to comprehend. In contrast, the smaller differences of VTTs for shorter distance bands could mean that the design of the SP survey was sufficient enough to capture realistic mobility behaviour.

The results hence demonstrate that by harnessing recent technological advances in data collection, transport planners and policy-makers can make a successful shift to RP data sources, which have more behavioural validity compared to SP. Furthermore, the findings of the current study also demonstrate that smaller sample sizes derived from GPS smartphone data could be sufficient for the estimation of behaviourally accurate VTTs for the whole population. That finding could lead to a more frequent data collection process for the purpose of updating the national VTT estimates, compared to the so far slower update rate of traditional SP-derived VTTs (approximately every 10-20 years for most countries with some exceptions, e.g. in Sweden and Norway).

GPS-derived VTTs could also be used by policy-makers to complement the official SP-derived VTTs, since the more frequent GPS studies could help to detect any significant deviations from the previously SP-based estimated VTTs due to income increase or other unforeseen circumstances that could occur in the meantime, such as economic recession or the introduction of new disruptive modes/technologies into the transport market. Technologies like online shopping and its ever-increasing popularity especially in a post-Covid world, electric vehicles, shared ride modes (Uber, Lyft etc.) and policy initiatives like Mobility as a Service are constantly changing the transport sector, which has become more volatile than ever before. Transport is rapidly changing and the usual update rate of nation-wide official VTTs might be too slow nowadays to provide insights into the current trade-offs or even capture the sensitivities on new technologies in hypothetical scenarios and in a behaviourally realistic manner. As a result, new transport projects might not be properly evaluated if the appraisal is based on individual trade-offs that no longer represent the current behaviour of the target population.

8 Conclusions

The current paper presents a study of deriving VTT estimates in a manner comparable to the official values currently used in appraisal. Though the level of detail included in the initial GPS trip diaries provided challenges during the data cleaning phase, there were significant advantages in terms of accuracy. For example, the time-stamped geo-locations provided the ability to better capture individual mobility behaviour by making it possible to

get precise travel times for the chosen modes and to extract travel times between specific latitude/longitude pairs (opposed to between TAZ centroids as done in traditional RP survey data). It also enabled the estimation of more behaviourally rich models by offering a more comprehensive representation of tours, where even very short stops and/or trips have been included.

Despite those advantages, it is worth noting that limitations do exist in the utilised dataset, as well. Information on trip attributes were obtained several years after the initial data collection period from an API that does not provide historical network information, hence the actual traffic conditions for each trip can not be retrieved. Furthermore, additional information on weather conditions and other intrinsic information that would influence both the formation of the consideration set and the choice itself are not accounted for in the present study. Future studies using GPS data for VTT estimation should aim to incorporate a probabilistic choice set formation framework to account for the inherent latent choice sets in RP datasets. An immediate extension of the current study is to analyse the impact of such a framework on the estimated VTTs and assess their discrepancies from the official SP-based VTTs. Further trip-specific attributes can be incorporated in the analysis to enrich the estimation dataset regarding historical weather conditions, hilliness/slope and the type of land uses both around home locations and also along the route to the destination of each choice task.

The findings in the current study can provide practitioners and policy makers with additional confidence when it comes to using new emerging data sources for future nationwide VTT studies. The small differences across the overall VTT estimates, regardless of distance bands, showcase that RP data captured through new emerging data collection methods –GPS in this case– can provide behaviourally reasonable VTT estimates that are in line with the official SP-based values currently used in appraisal. Of course, a reader may ask why RP data should be used if the results are no different from SP data. The simple answer to this question is that RP data provides the truth, and the fact that the findings in this case are in line with the SP results thus arguably also serves as a validation of SP rather than RP and a result of the rigorous work of the researchers involved in the official study. Furthermore, our results are achieved using a much smaller sample size during estimation, compared to the SP study, which can lead to a reduced cost or more frequently performed surveys in general. Performing a large scale GPS-based RP study at the country level will result in a significantly more accurate representation of individual mobility behaviour, capturing choices over a large number of real-life scenarios, independent of the researcher’s assumptions, while also resulting in less fatigue for the respondents.

This study comes at a time where ubiquitous sensing data sources are steadily gaining ground in transport research and provides empirical evidence for their further adoption into the field of practice. Nonetheless, more studies are required offering similar practical applications, even in small sample sizes, before we can see a departure from the current state of practice that has been dominant over the last several decades.

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Chapter 4

Accounting for distance-based correlations among alternatives in the context of spatial choice modelling using high resolution mobility data

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Abstract

Accounting for similarity among alternatives is of paramount importance for having unbiased estimates and for ensuring behaviourally accurate substitution patterns when making demand forecasts. Capturing similarity in a spatial context is a challenging task and the literature has failed to provide a clear answer as to how the presence of similar alternatives would influence the demand for a specific destination, i.e. acting as complements or competitors. The basic approach of relying on Nested Logit models that discretise space into a number of disjoint nests containing alternatives of the same geographical area ignores the influence of alternatives belonging in other areas/nests. We argue that such an approach will lead to uncaptured correlations in a spatial context, since as according to Tobler's First law of Geography "everything is related to everything else". On the other hand, relying on more complex error structures quickly leads to computational issues, while also relying on non-trivial analyst assumptions. In the present paper, we propose an alternative approach, where a Cross-Nested Logit (CNL) modelling framework with a flexible correlation structure is used, where space is treated as continuous and the allocation parameters are distance-based. The proposed structure is applied in the context of stand-alone destination choice models, as well as joint models of mode and destination choices of shopping trips. A smart-phone panel survey dataset with high resolution location traces from Leeds, UK, is used to benchmark the improvements of the proposed model against traditional ones. Results indicate that in addition to the improvements in model fit, the proposed CNL specification is able to uncover interesting findings about individual mobility behaviour which can be leveraged to make better planning decisions.

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1 Introduction

Individuals produce trips in order to participate in activities and fulfil their everyday needs (Bhat and Koppelman, 2003). The location and accessibility of those activities play an important role in the trips that are produced. For example, individuals with car availability in their household could be more likely to choose a major suburban shopping centre with an abundance of parking spaces to cover their grocery shopping needs. On the other hand, individuals with no available car might choose a nearby shopping destination or a shopping destination in the city centre with good public transport accessibility. The activity locations and the modes available to access them could thus have important environmental, social and economic implications (Brundtland Commission, 1987). Understanding the relative impacts of different factors on the mode and destination choices is therefore an important first step for formulating sustainable planning and policy measures - for instance devising targeted measures to improve accessibility and reduce car dependency.

Destination choice models are of paramount importance for demand forecasting, as they provide insights on individual preferences for certain locations depending on the time of day, activity purpose, and mode availability, amongst others. Much of the work in destination choice modelling focuses on discretionary activities (shopping, leisure, etc.), since those activities give the individual the freedom to choose from a range of possible locations on a day-to-day basis. However, given the large numbers of available alternatives and high level of heterogeneity associated with choices, modelling the choice of destinations for discretionary activities presents a number of significant challenges for the transport system. The choice of transportation mode is also considered to play an important role in the choice of destination and vice versa. Transportation models used in practice often consider destination choice to precede mode choice, commonly referred to as steps 2 and 3 in a traditional 4-step demand model (Ortuzar and Willumsen, 2011). There is empirical evidence, however, suggesting that the direction of causality between the two choice dimensions is less than clear and it could depend on trip characteristics, level of service variables and individual socio-demographics (Chakour and Eluru, 2014; Keya et al., 2021). Since there is not a general consensus as to which choice dimension comes first, it would be safer to examine the two decision processes in a joint fashion acknowledging the complex interrelations between them (Ben-Akiva, 1973; Ozonder and Miller, 2019).

Mathematical travel behaviour models relating to questions of where (destination choice models) and how (mode choice models) individuals travel have been the primary tool for quantifying the relative impact of factors affecting individual behaviour and forecasting future demand for the transport system and related services. Early modelling applications in spatial contexts focused on the use of spatial interaction models, mainly aggregate Gravity models (Haynes and Fotheringham, 1985), which draw analogies from Newton's law of gravity, assuming that, all else held equal, larger (in terms of population, employment opportunities, etc.) and closer (in terms of distance, travel time or cost) areas are going to attract more trips. Since its inception, the Gravity model has been extensively used in aggregate transport models (Ortuzar and Willumsen, 2011) and studies of Regional/Urban Economics (Duranton et al., 2015), in general. A non-parametric extension of the gravity model, called the radiation model, was proposed by Simini et al. (2012).

Daly (1982) formally extended the specification of the Gravity model by re-formulating it as a Multinomial Logit (MNL) model (McFadden, 1973) and making it applicable for disaggregate analysis. In that specification, the utility function is split into variables of travel impedance and variables measuring the attraction of a destination, called size variables. Due to the vast number of elemental locations, e.g. specific stores in the context of shopping destinations, some form of aggregation usually needs to take place, such as at the level of traffic analysis zones. Size variables are used in order to best represent the utility of elemental alternatives within the aggregated destination alternatives (Kristoffersson et al., 2018). Since then, most studies focusing on destination choice have relied on structures belonging to the

family of random utility maximisation (RUM) models, such as MNL, and have relied on Daly’s specification with the inclusion of size variables.

One of the main principles governing the behaviour explained by an MNL model is the *IIA* (independent and irrelevant alternatives) principle. This postulates that no unobserved correlation exists among alternatives in the choice set, hence a change in the attributes of one alternative will proportionately affect the demand for the other alternatives in the choice set. As in many other areas of application, this assumption is unlikely to be valid in the context of destination choice, or indeed joint mode and destination choice. The key issue then relates to how to capture the correlation among alternatives.

Capturing unobserved correlation among alternatives requires the use of further extensions of the MNL model. One approach involves the addition of the same multivariate random term in the utility function of alternatives that are assumed to share common unobserved characteristics. That model, known as the Error Components (EC) model, has the limitation of requiring simulation during estimation, thus significantly increasing the computational cost, while also often being subject to identification issues (Walker et al., 2007). A different approach that has the advantage of having a closed form solution and not requiring simulation is the GEV family of models (McFadden, 1978), which includes a wide range of models, such as the Nested Logit (NL) and the Cross Nested Logit (CNL) models (Small, 1987; Vovsha, 1997). The NL model (Williams, 1977; Daly et al., 1978) has arguably been the most prominent GEV specification utilising a *tree* structure in which the choice set is partitioned into a finite set of *nests*, where each nest consists of similar/substitute alternatives.

Similarity among alternatives is highly dependent on the choice context itself, and this affects the decision on how to treat it. In a mode choice context, similarity among alternatives such as car, public transport and walking, can depend on the level of comfort, privacy and flexibility that each mode alternative can provide to the decision maker. In many cases, the use of a simple Nested Logit structure (McFadden, 1973; Williams, 1977; Daly et al., 1978) is then appropriate. A more complex topic of study when it comes to correlation between alternatives has been that of route choice, where similarity can occur with overlapping links between two different route alternatives with prominent examples including the C-Logit (Cascetta et al., 1996) and Path Size (Ben-Akiva and Bierlaire, 1999) models. Similarities in a destination choice context, however, can be much more complex, since they can depend on public transport accessibility, availability of parking spots or other specific amenities, the existence of other competing neighbouring locations, etc. and a range of characteristics that the analyst might not be in a position to measure explicitly. Furthermore, there is not a clear consensus in the literature whether similar nearby locations would increase the utility of a destination, due to agglomeration effects, or decrease its utility due to spatial competition (Bhat et al., 1998; Schüssler and Axhausen, 2007; Bernandin Jr. et al., 2009).

A simple NL model can still be used of course, in the context of shopping store choice, Suarez et al. (2004) utilised an NL specification grouping location alternatives into nests of hypermarkets that resulted in a better model fit than a base MNL model and in significant substitution patterns among alternatives belonging within the same nest. Nonetheless, the required division of destinations into mutually exclusive nests is arbitrary, and can be counter-intuitive, with for example heightened correlation between two destinations at opposite sides of a hypermarket cluster and with no correlation between two adjacent destinations that are in different clusters. Ideally, an analyst would thus want to capture the correlation between each pair of destinations, as in a Paired Combinatorial Logit (PCL) model (Chu, 1989), which is a specification of a CNL model in which the unobserved correlation among alternatives is captured by specifying nests for each pair of alternatives in the choice set. An alternative i can belong to every nest by a certain percentage to be estimated, called the allocation parameter $\alpha_{i,ij}$, measuring the allocation probability of alternative i into the nest with alternative j . The α s should be between 0 and 1 and they should add up to 1.0 for every target alternative i . The Spatially Correlated Logit (SCL) model of Bhat and Guo (2004) adapts the allocation parameters of the PCL specification to account for similarities

among adjacent traffic analysis zones (zones sharing a common boundary) in a residential location choice context. A similar SCL-based specification was also proposed in Bekhor and Prashker (2008) in the context of shopping destination choice. An important limitation of those approaches is that the spatial correlations among non-adjacent zones are assumed to be zero. The alternative of working with each possible pair of alternatives of course quickly becomes difficult in terms of the number of parameters to estimate.

All of the aforementioned specifications share a common characteristic; they present some form of space discretisation either in the form of hypermarkets or based on adjacency. Discretising space, however, can quickly lead to a wide range of different potential nesting structures to be examined, such as nests based on administrative area or geographical location relative to the city centre etc. More importantly, it fails to treat space as continuous, which would be more behaviourally plausible, since setting arbitrary borders on a map would hardly have any real behavioural meaning, especially in the context of discretionary activity location choice. In fact, *Tobler's first law of geography* (Tobler, 1970) postulates that in a spatial context “*everything relates to everything else, but near things are more related than distant things*”. The study of Sener et al. (2011) based their proposed methodology around that principle by addressing the main limitation of Bhat and Guo (2004) and relaxing the allocation parameters to account for spatial correlation across all alternatives in the choice set. Their proposed SCL specification, however, failed to provide any significant improvements in terms of model fit compared to a base MNL model in their empirical application. In addition to that, the main limitation of the specification in Sener et al. (2011) is the large number of nests that had to be specified, which has to be equal to the number of all possible combinations of two alternatives in the same nest, hence $\frac{J!}{(J-2)!(2)!}$, where J is the total number of alternatives in the choice set. In a more recent study, Weiss and Habib (2017), moving away from GEV models, proposed an EC model to account for spatial unobserved correlation among alternatives in a park & ride location choice model. They based their methodology on Tobler's principle, however, due to the high computational cost, the choice set was constrained to include only the five closest alternatives from the origin of each trip, a simplification that is fair to assume in the context of park & ride location choice, but not behaviourally reasonable in the context of shopping destination choice. Therefore, the first limitation that the current study will aim to address is to propose a more efficient nesting structure suitable for uncovering unobserved correlations among destinations without imposing an analyst-specified grouping of alternatives, while being flexible enough to treat space as continuous.

Our discussion so far has focused on the treatment of correlation between destinations alone. However, as discussed earlier, destination choices are often made jointly with mode choices, and the simultaneous modelling of the two raises additional issues in the treatment of the correlation between alternatives. In the context of a joint mode and destination choice modelling, while most of the early applications revolved around the use of MNL models (Richards and Ben-Akiva, 1974; Adler and Ben-Akiva, M., 1976; Southworth, 1981), in recent years more advanced modelling specifications have been put forward, mainly NL models. Two main approaches have been used for the specification of the nesting tree, one with mode at the upper level and destination at the lower, known as *Mode-over-Destination (MoD)*, and another structure where destination is at the upper level and mode at the lower level, known as *Destination-over-Mode (DoM)* (Figure 4.1). An *MoD* nesting structure implies that the errors in destination choice are smaller than in mode choice, hence the choice of destination is more deterministic than the choice of mode, while the opposite is true for *DoM*. Those NL specifications are simply a way of representing the error distribution across the choice dimensions and do not imply a sequential decision making process, as was emphasised in Daly et al. (1978). Each one of the two aforementioned nesting structures has to be tested for a specific application context (Ozonder and Miller, 2019) and there is empirical evidence suggesting that it could be influenced by the socio-cultural characteristics of the sample (Newman and Bernandin Jr., 2010; Kristoffersson et al., 2018), while it could also change

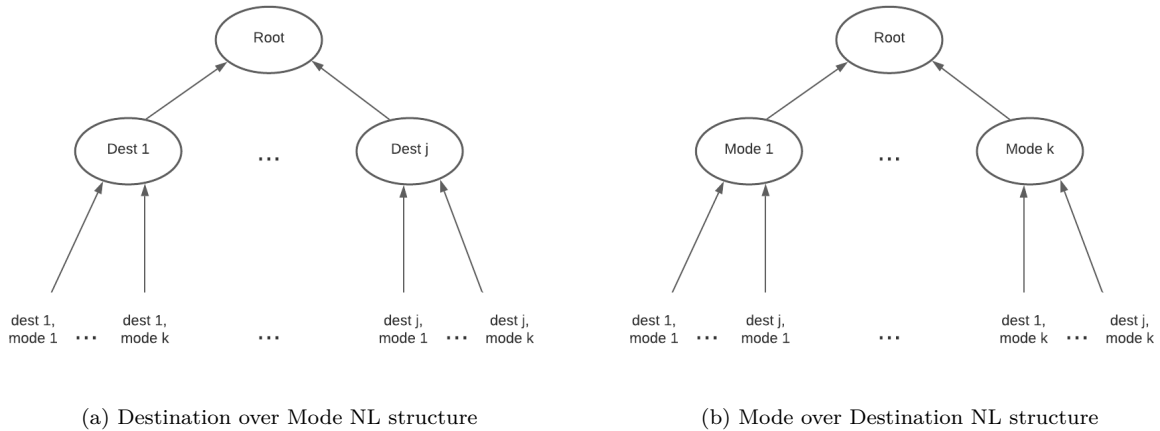


Figure 4.1: NL structures for joint mode and destination choice model

through the years due to network and administration changes (Fox et al., 2014; Fox, 2015).

Independent of whether mode is nested above destination or destination above mode, additional levels of nesting could be introduced to capture differential levels of correlation between different groups of destinations, just as in a NL model for destination choice alone. The limitations of this have already been made clear in our discussion of destination choice models. A further limitation arises in NL models of multiple choice dimensions, such as a joint mode and destination model. In such models, the NL nesting structure imposes constraints on the captured correlation. For example, in a *MoD* NL specification, full correlation is only explained along the mode dimension and two alternatives sharing similar unobserved characteristics based on their location will not be nested together leading to uncaptured correlation and hence to biased estimates. Similarly, in a *DoM* NL specification, only correlation among alternatives sharing the same location can be explained. Hess and Polak (2006) demonstrated the benefits of a CNL structure for such multi-dimensional choice processes in a joint model of airport, airline and access mode choice, where a joint alternative is allowed to belong to all three nests of the different choice dimensions at the same time. The $\alpha_{j,m}$ s in that study were fixed to 1/3 assuming an equal proportion of each alternative falling within each nest. A CNL specification allows for a simultaneous capturing of correlation across all choice dimensions and for all alternatives, where, as in a PCL model, the degree of membership of an alternative j to a specific nest m in CNL is captured by specifying an additional allocation parameter $\alpha_{j,m}$, with $0 \leq \alpha_{j,m} \leq 1$ and $\sum_{m=1}^M \alpha_{j,m} = 1$. The advantage of CNL over PCL is that it provides a much simpler nesting structure without the need of specifying nests for each pair combination of alternatives. CNL models have, however, not gained much attention in destination and joint mode and destination choice modelling, with Schüssler and Axhausen (2009) going as far as arguing that CNL models are not suitable to be used in spatial choice modelling that usually includes a large number of alternatives, mainly due to the increased estimation time forcing the analyst to work with only a subset of the initial dataset. To the best of the authors' knowledge, the study of Ding et al. (2014) and more recently the study of Fox et al. (2019) are the only examples presenting a CNL application for joint mode and destination choices, with a nesting structure inspired by the study of Hess and Polak (2006), where an alternative is allowed to belong to one destination and one mode nest at the same time with α_{dest} and α_{mode} , respectively (Figure 4.2). In the study of Ding et al. (2014), the authors followed an approach similar to the study of Hess and Polak (2006) keeping the $\alpha_{j,m}$ s fixed to 0.5 to avoid numerical issues during estimation. Nonetheless, their proposed CNL specification failed to outperform a base MNL and a *DoM* NL model in terms of model fit. In the study of Fox et al. (2019), a grid search approach

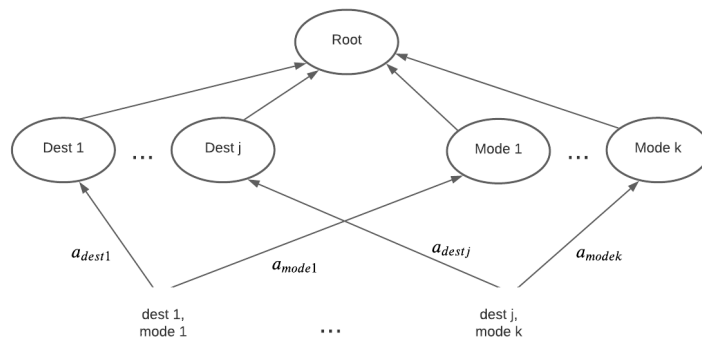


Figure 4.2: Existing CNL nesting structure for a joint mode and destination choice model (Ding et al., 2014)

was employed for finding the best combination of $\alpha_{j,ms}$, but still their CNL model was not able to outperform a simpler NL model.

The aforementioned CNL specifications are still susceptible to behavioural limitations that could be a potential cause for their low performance. Specifically, they do not take into account how the existence of neighbouring destinations might affect the allocation parameter to a specific destination nest. Therefore, the second limitation that the current study will aim to address is to propose a CNL structure in which a joint mode and destination alternative, instead of belonging to a mode nest and a single destination nest, belongs with a non-zero probability to every destination nest, but still with a higher probability to its *own* nest. Spatial proximity, measured as the distance among destinations, can be utilised as a means of understanding if and how the remaining destination nests might impact the allocation parameters.

The current study aims to propose a novel, efficient and operational CNL structure for a destination and a joint mode and destination choice model of shopping trips. That is achieved by proposing a distance-based parameterisation of the allocation parameters and by treating space as continuous, which is a novel addition to spatial CNL models. The proposed specifications are empirically tested on trips captured through smartphone GPS tracking and performed across the region of Yorkshire, UK. More specifically, the purpose of the destination model is to analyse the individual behaviour for choosing an intermediate shopping destination S between a previous origin O and a next destination D , while the joint model aims to capture both the location of that intermediate shopping destination, as well as the modes used to travel to that and to the following location.

The remainder of the paper is as follows. In the second section, the methodological frameworks of the proposed model specifications are thoroughly explained, while in the following section, the data used in the practical application is described. In the fourth section, the modelling outputs and their interpretations are highlighted. Finally, in the last section the conclusions of the study are summarised and recommendations for future research are suggested.

2 Methodology

We start our model description by looking at the destination choice scenario alone, i.e. without mode choice. Let us consider a situation where an individual faces a finite set of D independent and mutually exclusive destinations with specific attributes x_d for destination d in a specific journey. The utility for a destination is a latent construct comprised by a deterministic utility V_d and a disturbance term ϵ_d . The deterministic part of the utility is a

combination of individual- and alternative-specific attributes as shown in *Equation 4.1*.

$$U_d = V_d + \epsilon_d = f(\beta, x_d) + \epsilon_d \quad (4.1)$$

Assumptions regarding the disturbance term can yield different specifications. In a CNL model, we make use of a Generalised Extreme Value (GEV) distribution for the error term, allowing us to capture flexible correlation structures between the errors. Specifically, an alternative can now belong to multiple nests, and the unconditional choice probability for alternative d is given by a sum over all S nests, each time using the product of the probability of choosing an alternative within nest s and the conditional probability of choosing alternative d within nest s as shown in *Equation 4.2*. The choice probability of nest s and the choice probability of alternative d conditional on choosing nest s are shown in *Equations 4.3* and *4.4* (Train, 2009):

$$P(d) = \sum_{s=1}^S P(s) P(d | s) \quad (4.2)$$

$$P(s) = \frac{(\sum_{j \in A_s} (\alpha_{sj} e^{V_j})^{\frac{1}{\lambda_s}})^{\lambda_s}}{\sum_{k=1}^S (\sum_{j \in A_k} (\alpha_{kj} e^{V_j})^{\frac{1}{\lambda_k}})^{\lambda_k}} \quad (4.3)$$

$$P(d | s) = \frac{(\alpha_{sd} e^{V_d})^{\frac{1}{\lambda_s}}}{\sum_{j \in A_s} (\alpha_{sj} e^{V_j})^{\frac{1}{\lambda_s}}} \quad (4.4)$$

where A_s is the set of alternatives in nest s , $P(d)$ is the unconditional choice probability of alternative d , $P(s)$ is the probability of choosing nest s , $P(d | s)$ is the conditional probability of choosing destination d in nest s , λ_s is the structure parameter for nest s , and α_{sd} is the allocation parameter of alternative d for nest s . We have that $0 < \lambda_s \leq 1 \forall s$, $0 \leq \alpha_{sd} \leq 1 \forall d, s$, and $\sum_{s=1}^S \alpha_{sd} = 1 \forall d$.

In our proposed CNL specification for the destination choice model, we define as many nests as there are destinations, such that $S = D$. The key question now relates to the specification of the allocation parameters. Rather than freely estimating these parameters, or fixing them to a specific value, we define the allocation parameters to be a function of distance. Specifically, let the $X - Y$ coordinates for destination d be defined by the projected latitude and longitude X_d and Y_d . We then impose a one-to-one mapping between destinations and nests, such that nest s uses the coordinates of the s^{th} destination. This then allows us to calculate a straight-line distance between the geographic location of a specific destination d and the *location* of a given nest s as $dist_{ds} = \sqrt{(X_d - X_s)^2 + (Y_d - Y_s)^2}$, where we thus have that $dist_{ds} = 0$ when $d = s$.

Using this notation, we then specify the allocation parameters as:

$$\alpha_{sd} = \frac{e^{\gamma_{dist} dist_{ds}}}{\sum_{k=1}^S e^{\gamma_{dist} dist_{dk}}} \quad (4.5)$$

where the additional γ_{dist} parameter captures the impact of distance. If $\gamma_{dist} = 0$, each alternative falls into each nest with the same proportion, while the expectation is that $\gamma_{dist} < 0$, such that an alternative falls more into nests closer to its own location, with the highest allocation into its *home nests*.

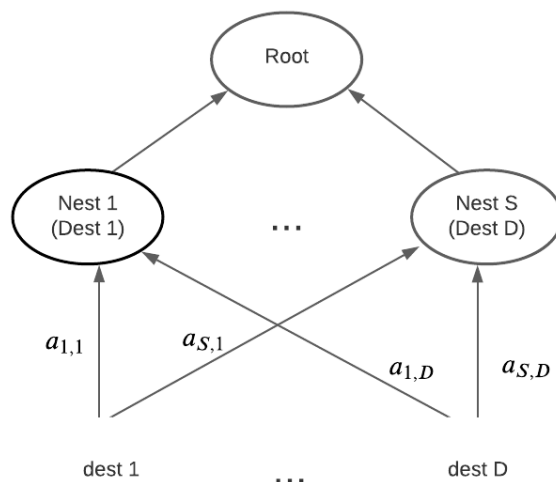


Figure 4.3: Proposed CNL nesting structure for destination choice model

The allocation is thus a function of the straight line distance, but where each destination alternative can belong to every nest with a non-zero probability, captured by the estimated $\alpha_{sd} \in \mathbf{A}$, where \mathbf{A} is the matrix of allocation parameters (Figure 4.3). The diagonal elements in \mathbf{A} refer to the allocation parameters of the alternative to its own nest, labelled here as the *home nest*. In order to achieve that, the product of $d_{sd} \in \mathbf{D}$, where \mathbf{D} is the symmetrical distance matrix of all destinations, and the respective γ_{dist} parameter was normalised using a logit transformation as defined in Equation 4.5.

A simplified example is presented in the following where a distance matrix \mathbf{D} of five destinations is computed, where d_{sd} are measured in km. The distance matrix \mathbf{D} is then multiplied by the γ_{dist} parameter. Assuming that $\gamma_{dist} = -1$, the logit transformation of the product yields the matrix \mathbf{A} of the allocation probabilities α_{sd} . In \mathbf{A} , the columns represent the destination alternatives d , while the rows represent the nests s . The sum of each column is equal to 1.0 and the diagonal elements have the highest α_{sd} per column. Furthermore, the most isolated destination, namely alternative 3, which has a mean distance of 4 km from the remaining destinations, has the highest diagonal element, $\alpha_{3,3}$, in \mathbf{A} . In contrast, alternative 5 has the lowest mean distance from the remaining destinations of 2.1 km and $\alpha_{5,5}$ is the lowest diagonal element in \mathbf{A} .

$$\mathbf{D}\gamma_{dist} = \begin{pmatrix} 0 & 2 & 6 & 3 & 0.5 \\ 2 & 0 & 7 & 5 & 2 \\ 6 & 7 & 0 & 2 & 5 \\ 3 & 5 & 2 & 0 & 3 \\ 0.5 & 2 & 5 & 3 & 0 \end{pmatrix} \xrightarrow[\text{trans.}]{\text{logit}} \mathbf{A} = \begin{pmatrix} 0.5574 & 0.1059 & 0.0022 & 0.0401 & 0.3373 \\ 0.0754 & 0.7823 & 0.0008 & 0.0054 & 0.0753 \\ 0.0014 & 0.0007 & 0.8730 & 0.1090 & 0.0037 \\ 0.0277 & 0.0053 & 0.1181 & 0.8054 & 0.0277 \\ 0.3381 & 0.1059 & 0.0059 & 0.0401 & 0.5561 \end{pmatrix}$$

The role of γ_{dist} is to dictate what percentage of the alternative will be allocated to the home nest and what percentage to the neighbouring ones. If $\gamma_{dist} < -1$, then the logit transformation will result in larger diagonal elements in \mathbf{A} meaning that alternatives will

2. Methodology

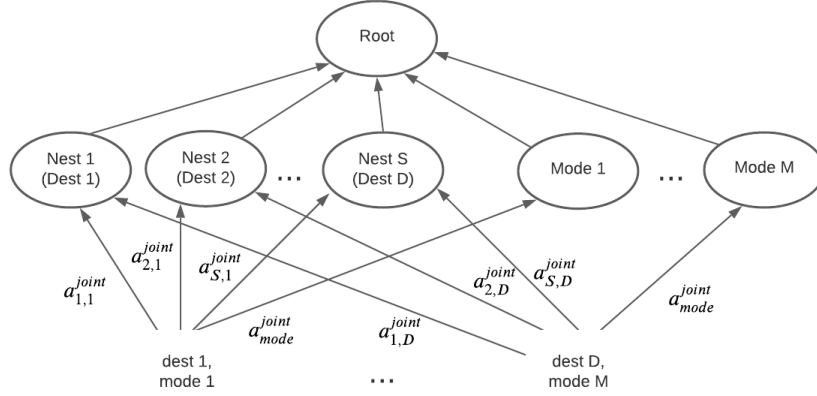


Figure 4.4: Proposed CNL nesting structure for the joint choice model

belong more to their own nest compared to the neighbouring ones. On the contrary, if $-1 < \gamma_{dist} < 0$ then the alternatives will be more evenly distributed across the neighbouring nests and their own nest and if $\gamma_{dist} = 0$, the alternatives would be equally allocated across all nests. Finally if $\gamma_{dist} > 0$, the alternatives would be allocated with a higher probability to the nests that are located at the largest distance, which is not behaviourally sensible. In order to guarantee their positive sign and avoid the latter case, the γ_{dist} parameters were specified using a negative exponential transform, as $\gamma_{dist} = -e^{\gamma_{dist}^*}$.

Although the above specification on its own might be sufficient enough to capture distance-based correlation among alternatives in the destination choice model, the joint mode and destination model would require further adjustments to simultaneously capture correlations among all choice dimensions. In that context, each alternative represents a joint choice of a destination d and a mode m . To adapt the previously described formulation in that joint choice context, the nesting structure is defined as depicted in *Figure 4.4* including nests for the destination as well as the mode choice component. Each joint mode-destination alternative is allocated into all of the destination nests, as previously described, and into one mode nest. The new combined allocation parameters still need to add up to 1.0, such that $\sum_{s=1}^S \alpha_{sd}^{joint} + \alpha_{mode}^{joint} = 1 \forall d$. This is achieved by scaling down the distance-based allocation parameters to each destination nest (see *Equation 4.5*), with

$$\alpha_{sd}^{joint} = \alpha_{dest}^{joint} \alpha_{sd} \quad (4.6)$$

and

$$\alpha_{mode}^{joint} = 1 - \alpha_{dest}^{joint} \quad (4.7)$$

We only require the additional constraint that $0 \leq \alpha_{dest}^{joint} \leq 1$, which can be achieved via a logistic transform, thus estimating α_{dest}^{joint*} and using the transform

$$\alpha_{dest}^{joint} = \frac{e^{\alpha_{dest}^{joint*}}}{e^{\alpha_{dest}^{joint*}} + 1} \quad (4.8)$$

We now turn to the specification of the utility functions themselves. In order to account for shopping destination attraction and to combine that with mode preferences, the specification used in Kristoffersson et al. (2018) based on the size variable specification in Daly (1982) was utilised. According to this, the systematic utility V_{md} for mode m and destination d , presented

in Equation 4.9 (linear-in-the-parameters in that case), has three components: a component capturing the sensitivities related to the level of service (LOS) variables depending on the mode and destination, a component capturing the destination’s quality, and a component capturing the destination’s attraction.

$$V_{md} = \sum_{r \in R} b_r x_{rmd} + \sum_{q \in Q} b_q y_{qd} + \phi \log(S_d) \quad (4.9)$$

The first component includes mode- and destination-specific variables that best describe the trip to destination d with mode m , such as travel time and cost for motorised modes and distance for active travel, as well as ASCs capturing inherent preferences for specific modes/destinations and sociodemographic interactions. With this, x_{rmd} is the r -th LOS variable for mode m and destination d . The second component captures the impact (positive or negative) that certain characteristics could have on the utility of a specific destination, such as available parking space for car users, where y_{qd} is the q -th quality variable for destination d .

The final component in Equation 4.9 is considered independent from the rest of the utility function and aims to capture the attraction or the “size” of a destination irrespective of the LOS variables to that place or the decision maker’s socio-demographic characteristics. The log-size parameter ϕ is usually fixed to 1.0 assuming that utilities and subsequently the choice probabilities are not affected by the zoning discretisation that usually forms the destination alternatives. Kristoffersson et al. (2018), however, showed that allowing the ϕ to be freely estimated can result in estimated values different than 1.0, leading to a behavioural interpretation on the formation of destination alternatives. Specifically, if $\phi < 1$, the model captures significant correlation among the utilities of the elemental alternatives within each aggregate destination alternative. Therefore, in that sense the ϕ has a similar role as the nesting parameter λ (Kristoffersson et al., 2018). Finally, in addition to capturing unobserved correlations among the alternatives with the proposed CNL structure, observed correlations can also be captured with the inclusion of attraction attributes of neighbouring destinations in the size variable of destination d .

The size variable S_d is a composite measure of the size of destination d and b_r , b_q and ϕ are the respective parameters to be estimated. The composite size measure S_d is defined as:

$$S_d = a_{1d} + \sum_{r>1} \exp(\gamma_r) a_{rd} \quad (4.10)$$

where a_{1d} is the attraction attribute used as a base with a γ parameter normalised to 1.0, a_{rd} are the additional attraction attributes of destination d relative to the base attribute, and γ_r are the parameters to be estimated capturing the effect of those attributes on the attraction of the target destination. The γ_r parameters are constrained to be positive by using an exponential transform.

3 Data

3.1 Background

The data used in the current study was collected as part of the research project “DECISIONS” carried out by the Choice Modelling Centre at the University of Leeds, between November 2016 and March 2017. The project aimed at observing individual decisions over a range of in-home and out-of-home activities with an emphasis on travel over a 2-week period. A detailed description of the survey is presented in Calastri et al. (2020). The trips were

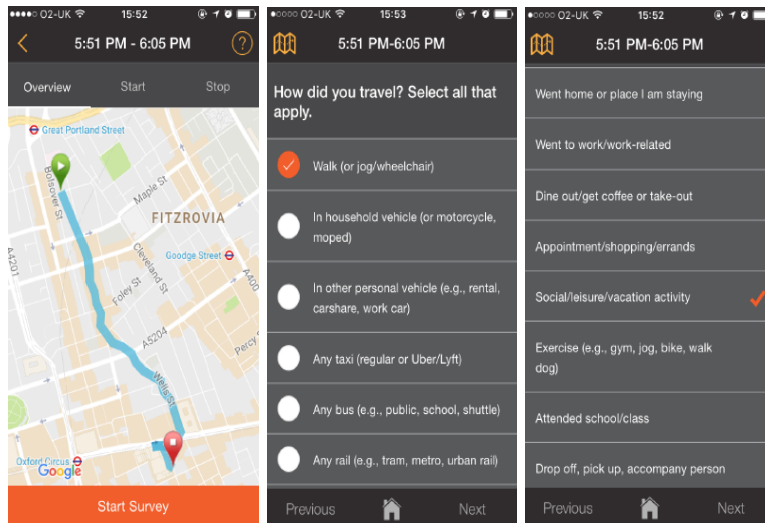


Figure 4.5: User interface of smartphone application used for the trip diary (Calastri et al., 2020)

captured through GPS tracking using a smartphone application at a high spatial and temporal resolution. The chosen mode and purpose of the trip were provided by the participants at the end of each trip (Figure 4.5). Important socio-demographic information was captured from an additional household survey, giving the advantage of combining high resolution mobility data with participant characteristics, such as income, car ownership etc.

3.2 Initial data processing

The empirical analysis in the present paper focuses on shopping trips and the study area was defined as the region of Yorkshire. Only residents of the city of Leeds were selected, assuming they will have a similar knowledge of their surrounding shopping destinations (Thill, 1992). The purpose of the analysis is to understand where the individuals are more likely to go for shopping with respect to the previous and the following activity locations. The locations of the previous origin O and the following destination D were considered fixed and the modelling analysis focused on the intermediate shopping destination S . Therefore, from the initial dataset, the shopping trips and their following trips were chosen for the subsequent analysis. The final dataset used in the analysis contained 1,541 shopping trips and an equal number of following trips performed by 270 unique individuals.

The shopping and their following trips were combined to create trip chains, which formed the basis of the analysis performed. Most trip chains, 66%, were from the origin O to the intermediate shopping destination S and then to the following destination D , which will be referred to as $O-S-D$ trip chain. The remaining trip chains, 34%, were from the origin O to S and then back to O , which will be referred to as $O-S-O$ trip chains. Shopping trips included three subcategories of shopping, namely grocery (82%), clothes (12.7%), and other types of shopping (5.3%), mainly for durables. The vast majority of following trips were trips going home (61.5%), while there was a small percentage of 9.3% of a consecutive shopping trip to a different shopping destination. The alternative modes of transport included car, public transport (PT) – as a combination of bus and rail – and walking.

The first step in the analysis involved the identification of home and work locations per individual, which were not reported initially. The nature of the GPS dataset requires a different way of analysis compared to a traditional dataset, where the destinations are usually defined at the traffic analysis zone (TAZ) level. In the current GPS dataset, the destinations of each trip are represented by a unique pair of latitude/longitude coordinates. Consequently, the identification of unique activity locations included the clustering of all destinations per

individual using Hierarchical Agglomerative Clustering (HAC) with a 200 metres distance threshold. HAC was chosen as it does not require knowledge or a priori assumptions about the number of clusters. The distance threshold was chosen in order to group together in the same cluster points that have a small average straight distance difference among them (100 metres approximately). In total, 6,361 unique clusters were created. Following the clustering analysis, the enumeration of all trip purposes for the tagged trips per cluster was performed. At this point, potential home and work locations were identified as the clusters with the majority of “home” and “work” trips, respectively. In the rare cases where more than one cluster per individual had the same number of home/work trips, home/work locations were assigned to the clusters where the individual spends most of her time during night/early morning (22:00-06:00) and during working hours (09:00-17:00), respectively. The geographical boundary of those clusters was then identified at the Middle Super Output Area (MSOA), Lower Super Output Area (LSOA), and local authority level using the 2011 Census boundaries².

3.3 Definition of general shopping areas

In order to take advantage of the high spatial resolution provided by the GPS data, we decided not to limit our analysis to the usual UK geographical boundaries, such as Middle layer Super Output Areas (MSOA) zones. For that reason, the destination alternatives were defined by clustering the observed elemental shopping destinations. HAC was implemented with a 800 metres distance threshold between the shopping trip destinations. The centroids were defined as the mean of the latitude/longitude coordinates of the points in each cluster and were then used to replace the original destination points of each shopping trip belonging to the cluster. Therefore, the main goal was to choose an appropriate distance threshold that would result in a small average distance difference between the original destination points of a cluster and its centroid. Because of that and after trying different distance thresholds between 500m-1,000m, a 800m distance threshold was selected resulting in small average distance differences of around 4-5 minutes of walking (assuming a 5 km/h average walking speed). A 400m buffer was defined around each cluster centroid, as a final step of creating the aggregate shopping destinations used in the analysis.

In the case of overlapping buffers, especially in Leeds city centre, the polygons within them were assigned to their closest cluster centroid (cf. *Figure 4.6*). This approach was used to ensure that each elemental shopping destination (in the form of polygons/individual stores) would belong to a single aggregate alternative (in the form of the shopping areas defined). This procedure resulted in the creation of 176 general shopping areas around the region of Yorkshire, capturing 76% of the retail polygons, as defined in OpenStreetMaps (OSM), located within the Local Authority of Leeds. It is safe to say that shopping locations exist in other places within the study area, not captured by that process, mainly in areas further away from the city of Leeds. For the purpose of this study, however, it is assumed that those shopping locations have not been considered by the individuals in the sample or that the individuals are not aware of them, hence they have not been included in the subsequent analysis (Thill, 1992).

Shopping clusters were also grouped with regard to their location relative to Leeds city centre. In total, 9 general areas were defined, namely Leeds city centre, North-East-South-West Leeds and North-East-South-West Yorkshire as shown in *Figure 4.7*. The number of trips per mode combination and general area are presented in *Table 4.1*. Most clusters are located around the city of Leeds, while Leeds city centre attracts the vast majority of trips with a preference for more sustainable modes. The remaining areas around Leeds attract a similar number of trips, while from the remaining region of Yorkshire, West Yorkshire, which is the area surrounding the city of Leeds, attracts the highest number of trips. Trips in the rest of the Yorkshire region (North-East-South) are far less frequent, and mostly performed

²Details can be found at <https://census.ukdataservice.ac.uk/use-data/guides/boundary-data.aspx>

3. Data

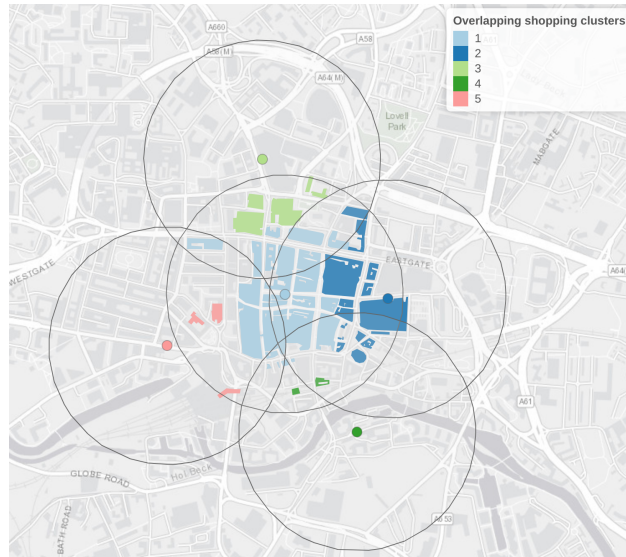


Figure 4.6: Allocation of retail polygons located within overlapping shopping clusters

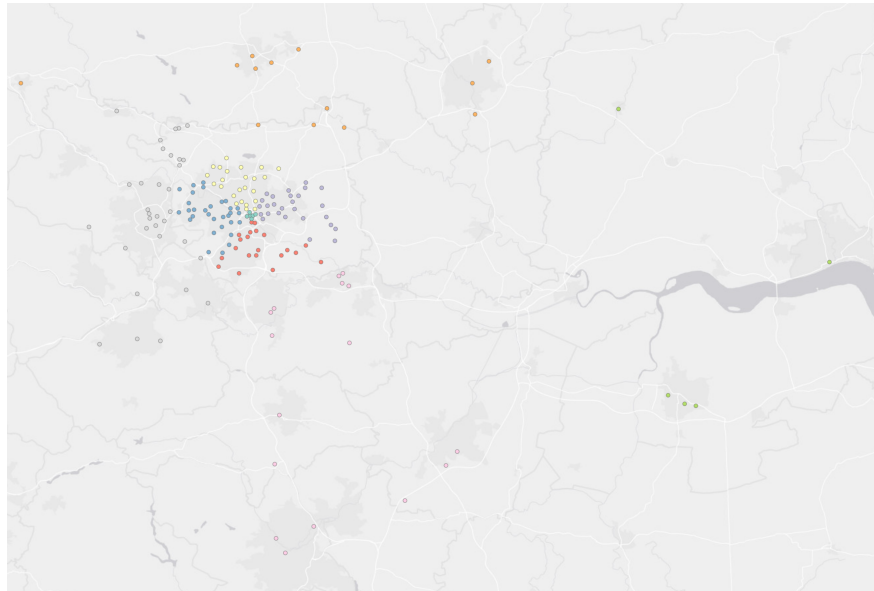


Figure 4.7: General area of shopping destinations in the study area

by car.

3.4 Data enrichment

Additional steps towards data enrichment were necessary to add further information that was important for the specification of a behavioural model. Initially, the dataset contained only the self-reported travel times/distances for the chosen modes, however, the values of the unchosen mode alternatives were also required. For that reason, the Bing maps route API³ was used in order to obtain the travel times and distances for all the modes (car, bus/rail, walking) and for the trips starting from each initial origin to each shopping cluster

³Details can be found here: <https://docs.microsoft.com/en-us/bingmaps/rest-services/routes/>

Table 4.1: Chosen mode and general locations

General location	C-C	C-PT	C-W	PT-C	PT-PT	PT-W	W-C	W-PT	W-W	Total
<i>Leeds city centre</i>	17 (1.1)	–	6 (0.4)	–	28 (1.8)	24 (1.6)	16 (1.0)	59 (3.8)	173 (11.2)	323 (21.0)
<i>Leeds north</i>	120 (7.8)	–	3 (0.3)	–	5 (0.3)	4 (0.3)	7 (0.5)	1 (0.07)	123 (8.0)	264 (17.1)
<i>Leeds east</i>	181 (11.7)	–	12 (0.8)	–	4 (0.3)	3 (0.2)	6 (0.4)	–	20 (1.3)	226 (14.7)
<i>Leeds south</i>	159 (10.3)	–	2 (0.1)	1 (0.07)	4 (0.3)	1 (0.07)	4 (0.3)	1 (0.07)	24 (1.6)	196 (12.7)
<i>Leeds west</i>	197 (12.8)	–	–	–	4 (0.3)	2 (0.1)	5 (0.3)	4 (0.3)	66 (4.3)	278 (18.0)
<i>Yorkshire north</i>	28 (1.8)	–	3 (0.2)	–	1 (0.07)	–	1 (0.07)	1 (0.07)	8 (0.5)	42 (2.7)
<i>Yorkshire east</i>	5 (0.3)	–	–	–	–	–	–	–	–	5 (0.3)
<i>Yorkshire south</i>	27 (1.8)	–	1 (0.07)	–	–	–	4 (0.3)	–	2 (0.1)	34 (2.2)
<i>Yorkshire west</i>	149 (9.7)	1 (0.07)	4 (0.3)	2 (0.1)	–	1 (0.07)	2 (0.1)	–	17 (1.1)	176 (11.4)
Total	880 (57.1)	1 (0.07)	32 (2.1)	3 (0.2)	46 (3.0)	35 (2.3)	45 (2.9)	66 (4.3)	433 (28.1)	1541 (100)

C: Car, PT: Public Transport, W: Walking

and from each shopping cluster to each following destination. For consistency reasons, the travel times/distances of the chosen mode alternatives were recalculated as well, an approach also followed in Calastri et al. (2018). The total number of queries passed to the API was 1,627,296 (1,541 trips \times 176 shopping destinations \times 3 modes \times 2 for the current and the subsequent trip). After that stage, deterministic mode availability was assigned based on logical checks of the results obtained from the API, such as cases of PT trips where the API returned only walking segments, or in specific cases where car was the chosen mode and the participant had to return it back home. For that latter case, special attention was given to the stated size of the party that participated in the trip in order to understand whether the participant of the survey was the actual driver. As such, if the individual was the only person in a car trip, then she was assigned as the car driver and all the remaining modes would become unavailable only in the case where the following trip was to return back home. For other trip purposes for the following trip, it is assumed that the individual is free to consider all the available modes. On the contrary, if there were more than 1 people participating in a car trip, then we could not safely assume that the individual was the driver and all the modes would remain available for the following trip, as well.

Car travel cost was computed using the UK’s official Transport Appraisal Guidance (WEBTag) specifications for fuel and operating costs (Department for Transport, 2014). Parking cost was also calculated for trips with destinations in central areas/high streets across the region of Yorkshire based on information on hourly or fixed parking costs provided by the respective Local Authorities. For PT, an average distance-based fare was used for bus and rail and a total PT cost was calculated per trip based on the distance of the leg performed by bus or rail. A discount was also applied for trips made by season ticket holders.

3.5 Locational variables

Characteristics of the shopping clusters and their respective surrounding areas were also defined. Parking and retail store areas in a buffer zone of 400m around the shopping cluster centroids were calculated using data extracted from OSM. The population of those areas (LSOA level) was extracted from the Office of National Statistics (ONS). Average residential price statistics for the LSOAs in Yorkshire, during the years 2016-2017, were acquired from the ONS, and their average was computed around shopping and home locations. Based on this, a variable was defined to analyse whether the immediate environment around the home location will have an influence on the behaviour of the individual, e.g. whether people living in richer areas are willing to go shopping in poorer areas or vice versa.

Shopping store variability among the elemental shopping destinations within an aggregate destination alternative was captured using Shannon’s entropy (H_d) (Equation 4.11) (Shannon, 1948; Whittaker, 1949), measuring the percentage of the area covered by a specific store type $t \in T$ inside a shopping destination d from a total number of N different store types. Shannon’s entropy has been widely used to quantify land-use variability mostly in studies

related to walkability (Brown et al., 2009; Mavoa et al., 2018) and urban sprawl (Effat and Elshobaki, 2015). In the current study, it is used to examine whether an increased variability in store types adds to the attraction of a shopping destination, since that would enable the completion of more shopping activities within the same trip. All of the aforementioned locational variables were calculated as a weighted average of the respective values of the geographical zones that are overlapped by the 400m buffer zones from each shopping centroid.

$$H_d = -\frac{\sum_{t=1}^T (p_t \ln(p_t))}{\ln N} \quad (4.11)$$

The locations of the most popular retailers per shopping type in the UK market (Rhodes, 2018; Kantar world panel, 2020; Retail Economics, 2020) were also identified across the study area and a binary dummy variable was created for each based on whether they are located within a 400m buffer radius around a shopping centroid.

In order to capture agglomeration effects and the impact of neighbouring shopping destinations on the attraction of a target shopping destination, the same information on the aforementioned locational variables was extracted for additional buffers between 400-1,000m, 1,000-2,000m and 2,000-5,000m from each cluster centroid, similar to the study of Kristoffersson et al. (2018).

3.6 Direction of travel

The effect of the location of the intermediate shopping destination S , in relation to the straight distance between O and D , was also captured by calculating the angles between $OS - OD$ and $SD - OD$. The a priori assumption is that, all else held equal, shopping destinations that require a significant deviation from the straight OD path would be less favoured compared to others. For that purpose, a dummy variable was defined, only for $O-S-D$ trip chains, capturing the impact on utility of a shopping destination located with an angular deviation greater than 90° from either O or D .

4 Results

In this section, we present the results for the destination choice model followed by the mode-destination model, before looking at the calculation of elasticity measures from the model. We contrast the results against those from MNL and NL models.

4.1 Destination model outputs

Five separate models were estimated for destination choice, namely a base MNL, two NL models, a PCL model and finally a CNL model based on the proposed nesting structure. The fit statistics of those specifications as well as the estimated nesting parameters are presented in *Table 4.2*. Detailed estimated parameters for the proposed CNL specification are depicted in *Table 4.3*. The models were estimated using a choice set of 176 destination alternatives. The *NL-dest-1* specification refers to a nesting structure with 9 nests according to the area of the destination, defined as *Leeds city centre*, *north-east-south-west Leeds* and *north-east-south-west Yorkshire* (see *Figure 4.7*). The *NL-dest-2* specification presents a finer segmentation of the destination alternatives into 24 nests according to the administrative area or the city the destinations belong to (*Figure 4.8*). A further segmentation with an even higher resolution, such as based on the MSOA zones, would have resulted in having a nesting structure with many degenerate nests, i.e. nests with just a single alternative, hence it was not attempted. The *CNL-dest* follows the proposed nesting structure with a single generic

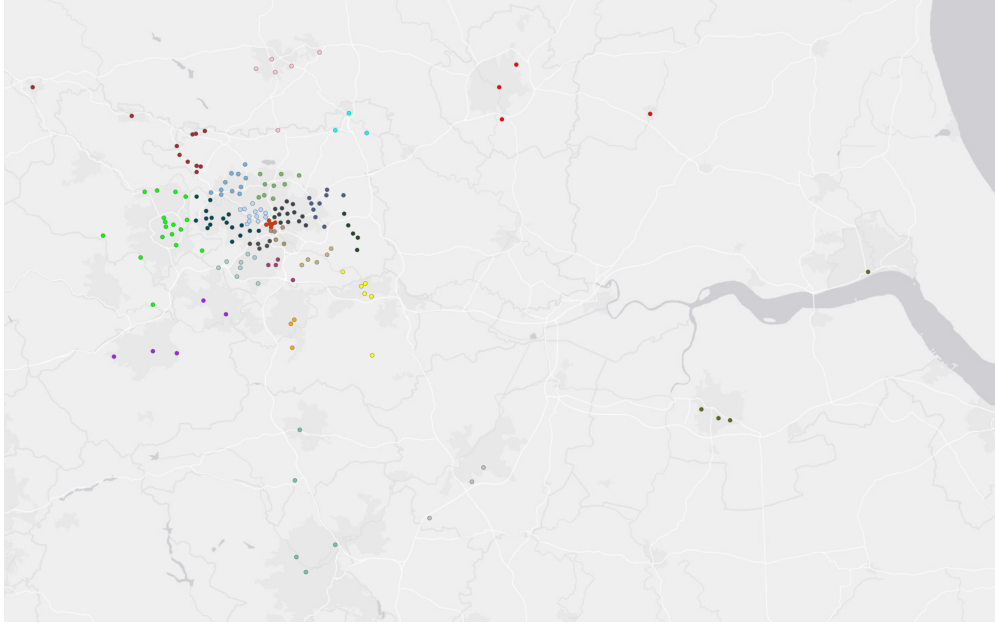


Figure 4.8: Segmentation of destination alternatives based on their administrative area

distance multiplier for the allocation parameters. Finally, a PCL specification having every pair of alternatives in a separate nest was also estimated with a nesting structure of 15,400 nests, in total. Distance based allocation parameters were specified in a similar way to the *CNL-dest*.

The destination choice model presented is conditional on the choice of mode, therefore level-of-service attributes relevant to the chosen mode are used in the utility functions. Socio-demographic variables were included in the model and interacted with the LOS variables as shifts from their base level. Both NL models result in structural parameters (λ) that were outside the theoretically acceptable range (i.e. above 1), meaning that the utilised NL nesting structures were not able to capture any meaningful correlation among the alternatives. Only the first NL model outperforms the MNL model according a likelihood ratio test, but the model is of course itself rejected given the findings for λ . That result provides support to our initial hypothesis that segmenting space into discrete areas/nests, even in more finer segmentations, is not an efficient approach for capturing unobserved correlation among destinations. In contrast, the proposed CNL framework was able to accomplish that with an estimated λ equal to 0.8222 and significantly different than 1.0. The proposed CNL model also provides significant improvements in terms of model fit compared to the MNL model with -5.976 LL units for 2 additional parameters. A PCL specification was also estimated resulting in a worse fit compared to the proposed CNL model (LL=-3,163.735) and with a longer estimation time by a factor of 10. According to the Ben-Akiva & Swait test (Ben-Akiva and Swait, 1986), which is suitable for comparing two non-nested models together, the proposed CNL specification is statistically superior to the PCL model (p-value=0.006). An EC specification could not be estimated due to computational reasons and the large number of alternatives in the choice set.

In general, the estimated parameters were behaviourally reasonable with the expected signs. The ASCs were defined using *destination 1* as the base alternative, which represents the most central shopping mall of Leeds, and constants for the remaining alternatives were specified based on the 9 general areas of the alternatives, as described in Section 3.3. The remaining destinations in the city centre are less likely to be chosen compared to destination 1 (base alternative), while destinations in the remaining study area are even less favourable, especially for modes other than car. All of the specified level-of-service parameters of the

Table 4.2: Fit statistics and nesting parameters of destination choice models

Fit statistics	MNL-dest-base	NL-dest-1	NL-dest-2	PCL-dest	CNL-dest
<i>Log-likelihood (0)</i>			-7,961.332		
<i>Log-likelihood (model)</i>	-3,166.947	-3,163.624	-3,165.307	-3,163.735	-3,160.971
<i>Adjusted ρ^2</i>	0.5972	0.5975	0.5973	0.5973	0.5977
<i>AIC</i>	6,413.89	6,409.25	6,412.61	6411.47	6,405.94
<i>BIC</i>	6,627.5	6,628.2	6,631.56	6635.76	6,630.23
<i>Number of parameters</i>	40	41	41	42	42
<i>Number of individuals</i>			270		
<i>Number of observations</i>			1,541		
Nesting parameters λ		Estimates (Rob. t-ratio w.r.t. 1.0)			
$\lambda_{generic}$	-	1.1267 (1.92)	1.0848 (1.53)	0.4502 (-2.55)	0.8222 (-3.99)

chosen mode were statistically significant validating our approach of explaining destination choice conditional on the choice of mode. The LOS variables of travel time, travel distance and travel cost were specified using a Box-Cox transform as $\frac{x^\lambda - 1}{\lambda}$ in order to capture possible non-linear sensitivities. As a result, statistically significant non-linearities were found for PT time, walking distance and travel cost suggesting that individual sensitivities are decreasing as those variables are increasing. On the other hand, only linear sensitivities were found for car time. Decreasing travel time and walking distance sensitivities were found as the shopping duration increases, while decreasing cost sensitivities were found as personal income increases. Finally, travel time for motorised modes and walking distance sensitivities were slightly higher for the following trip relative to the first shopping trip.

Individuals living in richer areas are less willing to go shopping in poorer areas with very low residential prices with a similar finding also presented in Pellegrini et al. (1997). A Box-Cox transformation was used to capture the preference for parking areas, specifically for trips using car for both legs, uncovering positive but decreasing sensitivities. The presence of major retail attractions per shopping category (clothes, grocery, other) significantly increases the likelihood of visiting the shopping destination for trips of the respective shopping category. The estimated multiplier ϕ of the logarithm of the composite size variable is significantly lower than 1.0 in all of the models presented. According to Kristoffersson et al. (2018), this means that there is significant unobserved correlation among the elemental alternatives within the aggregate shopping destinations used in the choice set. This also gives a behavioural meaning to the clustering approach that was utilised in order to form the aggregate alternatives, described in 3.3. An increased cumulative retail floor area of grocery, clothes and durable stores in a destination acts as a more significant attractor for trips of the respective shopping category than population that was used as the base size variable. Furthermore, an increased store type variability in neighbouring destinations in medium distances (1000-2000 m) will add to the attraction of the shopping destination, when the subsequent trip is also for shopping.

With regard to the direction of travel, shopping destinations located in places where the angular deviation between OS and OD is greater than 90° are less likely to be chosen compared to others, conforming to our initial assumptions. The same dummy variable measuring the impact of an angle above 90° between SD and OD was still negative, but not statistically significant, hence was not included in the specifications reported here. Finally, regarding the estimated distance multipliers, *CNL-dest* results in $\gamma_{dist} = -1.3552$ conforming with our initial assumption of increased correlation among closer destinations, which decreases with distance. The *PCL-dest* specification resulted in an estimated distance multiplier of $\gamma_{dist} = -0.4022$ (rob. t-rat=-4.40) meaning there is a more even allocation to the neighbouring nests.

Table 4.3: Modelling outputs of the proposed CNL destination choice model

Parameter	Estimate (Rob. t-ratio w.r.t. 0)
Locational constants (base: dest 1)	
<i>ASC rest Leeds city centre</i>	-1.1110 (-7.16)
<i>ASC rest Leeds city centre shift for PT-PT</i>	-0.5367 (-1.54)
<i>ASC rest Leeds city centre shift for PT-walking</i>	0.8957 (1.86)
<i>ASC rest Leeds</i>	-0.4782 (-4.32)
<i>ASC rest Leeds shift for PT-PT/ PT-walking/walking-PT</i>	-2.6413 (-7.15)
<i>ASC rest Leeds shift for walking-walking</i>	-1.8334 (-6.15)
<i>ASC rest Yorkshire shift for PT-PT/ PT-walking/walking-walking</i>	-3.8267 (-6.24)
LOS variables	
<i>Travel time for first trip (base)</i>	-0.0924 (-5.24)
<i>Travel time shift for clothes shopping</i>	0.0396 (4.42)
<i>Travel time shift for O-S-O trip chains</i>	0.0201 (2.76)
<i>Travel time shift for HWH tours</i>	-0.0237 (-2.41)
<i>Travel time shift for pm peak/night/weekend evening</i>	-0.0142 (-2.31)
<i>Travel time shift for morning/weekend night</i>	-0.0786 (-3.74)
<i>Travel time shift for grouping size > 1</i>	0.0111 (1.73)
<i>Travel time multiplier for car/PT IVT/ PT first access/PT last egress</i>	1.0000 (-)
<i>Travel time multiplier for following trip</i>	1.2121 (15.88)
<i>Travel time - Shopping duration elasticity</i>	-0.3315 (-8.43)
<i>Box-cox lambda for car travel time</i>	1.1069 (19.91)
<i>Box-cox lambda for PT travel time</i>	0.7696 (10.67)
<i>Travel walking distance for first trip (base)</i>	-1.1904 (-6.73)
<i>Travel walking distance shift for O-S-O trip chains</i>	0.2505 (1.96)
<i>Travel walking distance shift for am peak</i>	-0.7496 (-2.36)
<i>Travel walking distance shift for pm peak/night/ morning/weekend morning/weekend evening</i>	-0.3111 (-2.45)
<i>Travel walking distance multiplier for following trip</i>	1.2467 (11.33)
<i>Box-cox lambda for travel walking distance</i>	0.8246 (12.28)
<i>Travel walking distance - Shopping duration elasticity</i>	-0.2110 (-4.72)
<i>Travel cost</i>	-0.3900 (-3.33)
<i>Box-cox lambda for travel cost</i>	0.6636 (8.32)
<i>Travel cost - Personal income elasticity</i>	-0.5864 (-3.22)
Direction of travel	
<i>Presence of angle > 90° between O-S and O-D</i>	-0.2279 (-2.01)
Locational variables	
<i>Living in rich areas-shopping in poor areas</i>	-0.6316 (-2.61)
<i>Parking areas (400m buffer)</i>	0.1002 (3.96)
<i>Box-cox lambda for parking areas (400m buffer)</i>	0.4547 (6.35)
<i>Major clothes shopping retailers (400m buffer)</i>	1.1264 (5.52)
<i>Major grocery retailers (400m buffer)</i>	0.4506 (5.19)
<i>Major durables retailers (400m buffer)</i>	1.9668 (2.48)
Size variables	
<i>Natural logarithm multiplier ϕ</i>	0.4817 (6.45)
<i>Population (400m buffer) (base)</i>	1.0000 (-)
<i>Retail areas for clothes (400m buffer) (log.)</i>	0.8487 (1.49)
<i>Retail areas for groceries (400m buffer) (log.)</i>	1.5094 (2.80)
<i>Retail areas for durables (400m buffer) (log.)</i>	0.8795 (1.04)
<i>Shopping store variability when following trip purpose is shopping (1000-2000m buffer) (log.)</i>	3.4427 (4.84)
Nesting parameters λ	
<i>$\lambda_{generic}$</i>	0.8222 (-3.99*)
Distance multipliers γ	
<i>γ_{dist}</i>	-1.3552 (-3.90 [†])

4.2 Joint mode and destination model outputs

For the more complex joint mode and destination model, results from the previously described destination model and from simpler mode choice models, conditional on destination, were used as a guideline during the specification search. In that model, the mode and destination choices are assumed to happen at the same time. In total, the choice set of that model includes 1,584 joint destination and mode alternatives (176 destinations \times 3 modes for the shopping trip \times 3 modes for the following trip). A range of different specifications is presented in the following, namely a base MNL model, two NL models utilising an MoD and DoM nesting structure, respectively, a base CNL and finally the proposed CNL specification. In *Table 4.4*, the fit statistics of the different specifications are presented, while in *Table 4.5* the estimated parameters of the proposed CNL model are reported.

For the *NL-joint-MoD* specification, the alternatives were allocated into 9 nests according to the modal combinations of the shopping and the following trip and a generic λ_{mode} was specified assuming the same level of correlation across all nests. Similarly, for the *NL-joint-DoM* specification, 176 nests were specified, one for each shopping destination, with a generic λ_{dest} for each. Regarding the CNL models, the first specification, *CNL-joint-base*, is based on the specification of Ding et al. (2014). Alternatives that use a single mode for both legs are allocated simultaneously into a destination nest and a single mode nest, while alternatives that use different modes across the two legs (e.g. car-walking) fall into a destination nest and two mode nests for different-mode alternatives. We attempted to estimate allocation parameters for this model, but this resulted in numerical issues. An alternative was thus allocated evenly to all the nests it belongs to, meaning a 50-50 split into a destination and a mode nests for single mode alternatives, and an even three-way split into a destination and two mode nests for alternatives using two separate modes.

The second CNL model, *CNL-joint-proposed*, follows the proposed nesting structure with alternatives using the same mode for both legs being allocated to a total of 177 nests (*176 destination nests+1 mode nest*), and alternatives combining different modes being allocated to 178 nests (*176 destination nests+2 mode nests*). In both cases, a generic λ_{dest} is assumed for the destination nests, in addition to three mode-specific λ s for car, PT and walking. For the proposed specification, *CNL-joint-proposed*, the allocation parameters were specified as follows.

- $\alpha_{dest,same\ mode}^{joint}$ was used to scale down the destination α_{sd} of same mode alternatives, as $\alpha_{dest,same\ mode}^{joint}\alpha_{sd}$ (defined in *Equation 4.6*). The allocation parameters of same mode alternatives were computed as $\alpha_{dest,same\ mode}^{joint} = \frac{e^{\alpha_{dest,same\ mode}^{joint*}}}{(e^{\alpha_{dest,same\ mode}^{joint*}})}$ for the destination nest, while for the mode nest the allocation parameter was $1 - \alpha_{dest,same\ mode}^{joint}$.
- $\alpha_{dest,diff.\ mode}^{joint}$ was used to scale down the destination α_{sd} of alternatives with different mode combinations, as $\alpha_{dest,diff.\ mode}^{joint}\alpha_{sd}$ (defined in *Equation 4.6*). The allocation parameters of those alternatives were computed as $\alpha_{dest,diff.\ mode}^{joint} = \frac{e^{\alpha_{dest,diff.\ mode}^{joint*}}}{(e^{\alpha_{dest,diff.\ mode}^{joint*}})}$ for the destination nest, while an equal allocation was assumed for the two mode nests, which was computed as $(1 - \alpha_{dest,diff.\ mode}^{joint})/2$.

*Robust t-ratio w.r.t. 1.0

†The robust standard error was calculated using the delta method (Daly et al., 2012)

The nesting parameters in both of the NL models were not statistically different from 1.0, meaning that those nesting structures were not able to uncover any significant unobserved correlation among the alternatives, in either mode or destination choice dimensions, and those models effectively collapse to the base MNL. The *CNL-joint-base* model presents significant improvements in model fit compared to the *MNL-joint-base*, with 9.75 LL units for 4 additional parameters. It is also able to capture unobserved correlations along the mode dimension for car and PT (although not statistically significant at the 90% confidence level), but not for walking. Using that specification, however, it was not possible to capture any unobserved correlation along the destination dimension, since the estimated λ_{dest} is not statistically different than 1.0. Therefore, using this specification would lead to the conclusion that correlation exists only along the mode dimension for car and PT (again not statistically significant at the 90% confidence level), and not along the destination dimension. That assumption, however, is rejected if we look at the *CNL-joint-proposed* model. That specification resulted in significant model fit improvements over the base MNL model with -25.881 LL units for 9 additional parameters. More importantly, the proposed specification was able to capture significant unobserved correlation along the destination dimension, in addition to car and PT mode dimensions, while again no correlation was captured for walking. Furthermore, the estimated λ_{dest} is smaller than λ_{car} and λ_{PT} , indicating a higher correlation in the destination nests than in car and PT nests.

Table 4.4: Fit statistics and nesting parameters of joint mode and destination choice models

Fit statistics	MNL-joint-base	NL-joint-MoD	NL-joint-DoM	CNL-joint-base	CNL-joint-proposed
<i>Log-likelihood (0)</i>			-11,045.05		
<i>Log-likelihood (model)</i>	-4,093.78	-4,093.339	-4,093.699	-4,084.03	-4,067.899
<i>Adjusted ρ^2</i>	0.6238	0.6238	0.6238	0.6244	0.6254
<i>AIC</i>	8,309.56	8,310.68	8,311.4	8,298.06	8,275.8
<i>BIC</i>	8,635.31	8,641.77	8,642.49	8,645.17	8,649.61
<i>Number of parameters</i>	61	62	62	65	70
<i>Number of individuals</i>			270		
<i>Number of observations</i>			1,541		
Nesting parameters λ		Estimates (Rob. t-ratio w.r.t. 1.0)			
$\lambda_{generic}$	-	0.9491 (-0.86)	1.0267 (0.34)	-	-
λ_{dest}	-	-	-	0.9763 (-0.14)	0.5094 (-6.80)
λ_C	-	-	-	0.8615 (-2.80)	0.7968 (-2.36)
λ_{PT}	-	-	-	0.4846 (-1.60)	0.7708 (1.62)
λ_W	-	-	-	1.2459 (2.89)	1.2474 (2.26)

The ASCs for the joint model were specified in a similar notion as for the destination choice model, but this time the alternative *dest 1/car-car* was used as the base for the remaining 1,583 alternatives, which were grouped according to their general area and their mode combination. The estimated parameters have the expected signs, with mode combinations not including car being more preferred for shopping destinations in the city centre of Leeds, where more sustainable modes are increasingly promoted. The opposite is true, however, for locations in the rest of Leeds, such as suburban stores, and in the rest of the Yorkshire region, where car combinations are more favourable. Nonetheless, destinations in local high streets that are further away from Leeds city centre, are still less likely to be performed by car possibly due to car restriction measures and limited parking availability. Individuals living in households with no car ownership are less likely to use car-car combinations, while shopping trips including more than 1 passenger are more likely to be performed by car, at least for one of the two legs again due to its convenience. Out of all PT-related travel time components, the remaining out-of-vehicle time sensitivity was found to be significantly lower than the base travel time sensitivity (car travel time for first/shopping trips), while the remaining PT travel time components were found to be equal to the base travel time sensitivity, hence their multipliers were fixed to 1.0. Finally, the estimated income elasticity to cost is similar to the empirical evidence suggested by previous studies regarding non-work trips in the UK

(Sanko et al., 2014; Batley et al., 2019). The behavioural interpretation for the remaining level-of-service parameters and for most of the estimated size variables is similar to the destination choice model previously described. This time, however, the cumulative floor area of grocery stores in neighbouring destinations at medium distances (1,000-2,000 m) also adds to the attraction of the shopping destination, when the following trip is again for shopping, albeit at a lower rate than the grocery store area in the immediate neighbourhood of the shopping destination (400m buffer).

In *CNL-joint-proposed*, the distance multipliers were parameterised by mode, which allows for a more detailed analysis of the impact of distance difference among destinations on the allocation of each alternative to the destination nests. In that model, the distance multipliers for a car-car alternative were specified as $\gamma_{dist}^{C-C} = -(\gamma_{dist}^C \times \gamma_{dist}^C) = -e^{2\gamma_{dist}^{C*}}$. In a similar notion, the distance multipliers for a PT-walking alternative were specified as $\gamma_{dist}^{PT-W} = -(\gamma_{dist}^{PT} \times \gamma_{dist}^W) = -[(-e^{\gamma_{dist}^{PT*}}) \times (-e^{\gamma_{dist}^{W*}})]$. It is assumed that combinations such as car-PT and PT-car will have the same γ .

The detailed γ estimates for every mode combination are depicted in *Table 4.6*. Combinations of mechanised modes, i.e. car and PT, lead to lower γ , with the lowest one being for PT-PT trips. That means that individuals travelling by PT for both trip legs will perceive the target destination to be more similar with its neighbouring destinations. On the other hand, mode combinations that include walking on either of the two trip legs have a larger γ with the largest one being for walking-walking trips. That means that individuals walking for both trip legs will perceive their target shopping destinations as a more isolated alternative compared to its neighbouring destinations. In the same Table, the estimated allocation parameters are also presented. According to them, same-mode alternatives will belong with a larger allocation probability to their mode nest, while the opposite is true for different mode alternatives.

Table 4.5: Modelling outputs of the proposed CNL joint mode and destination choice model

Parameter	Estimate (Rob. t-ratio w.r.t. 0)
Households with car ownership (base: car-car/dest 1)	
<i>ASC dest 1 shift Car-PT/Car-Walking</i>	-1.4908 (-2.42)
<i>ASC dest 1 shift PT-PT</i>	0.9859 (2.55)
<i>ASC dest 1 shift Walking-PT</i>	1.8277 (5.85)
<i>ASC dest 1 shift Walking-Walking</i>	2.8060 (8.41)
<i>ASC rest Leeds city centre</i>	-1.6733 (-4.86)
<i>ASC rest Leeds city centre shift for PT-Car/ Walking-Car</i>	0.7783 (1.71)
<i>ASC rest Leeds city centre shift for PT-PT/ PT-Walking</i>	1.4308 (3.00)
<i>ASC rest Leeds city centre shift for Walking-PT</i>	2.2688 (4.67)
<i>ASC rest Leeds city centre shift for Walking-Walking</i>	3.1404 (6.76)
<i>ASC rest Leeds</i>	-0.4705 (-4.01)
<i>ASC rest Leeds shift for Car-PT/Car-Walking</i>	-2.7244 (-8.23)
<i>ASC rest Leeds shift for PT-Car/Walking-Car/ PT-PT/Walking-PT</i>	-1.0093 (-3.50)
<i>ASC rest Leeds shift for PT-Walking</i>	-1.6952 (-3.54)
<i>ASC rest Leeds shift for Walking-Walking</i>	0.4094 (1.32)
<i>ASC rest Yorkshire shift for Car-PT/Car-Walking/ PT-PT/PT-Walking/Walking-PT</i>	-1.8428 (-5.40)
<i>ASC rest Yorkshire shift for PT-Car/Walking-Car</i>	-1.1141 (-2.90)
Shifts for households with no car ownership	
<i>Car-PT/Car-walking/Walking-PT/Walking-Walking</i>	2.1796 (6.83)
<i>PT-PT</i>	3.7996 (8.77)
<i>PT-Walking</i>	2.8590 (5.97)

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Table 4.5 – continued from previous page

Parameter	Estimate (Rob. t-ratio w.r.t. 0)
Shifts for central areas outside Leeds city centre	
<i>PT-Car/Walking-Car</i>	0.9176 (1.72)
<i>Walking-PT/Walking-Walking</i>	2.0684 (4.04)
Shifts for individuals with season ticket ownership	
<i>Walking-Walking</i>	-0.5831 (-1.87)
Shifts for trips with more than 1 passenger	
<i>PT first/shopping trip</i>	-1.3942 (-4.71)
<i>PT following trip</i>	-0.8418 (-2.62)
<i>Walking first/shopping trip</i>	-0.6472 (-3.19)
<i>Walking following trip</i>	-0.4592 (-2.06)
Shifts for students	
<i>Walking-Walking</i>	0.8619 (2.39)
Shifts for married individuals	
<i>Walking-Walking</i>	-0.7207 (-2.76)
Shifts for individuals living in 3-member households	
<i>Walking-Walking</i>	0.7202 (1.97)
LOS variables	
<i>Travel time for first trip (base)</i>	-0.0624 (-4.44)
<i>Travel time shift for clothes shopping</i>	0.0281 (3.54)
<i>Travel time shift for O-S-O trip chains</i>	0.0103 (2.14)
<i>Travel time shift for HWH tours</i>	-0.0321 (-3.70)
<i>Travel time shift for pm peak/night/weekend evening</i>	-0.0076 (-1.70)
<i>Travel time shift for morning/weekend night</i>	-0.0294 (-2.26)
<i>Travel time multiplier for car/PT IVT/ PT first access/PT last egress</i>	1.0000 (-)
<i>Travel time multiplier for remaining PT OVT</i>	0.4655 (2.38)
<i>Travel time multiplier for following trip</i>	1.2522 (14.50)
<i>Travel time - Shopping duration elasticity</i>	-0.3358 (-9.15)
<i>Box-cox lambda for car travel time</i>	1.1047 (20.66)
<i>Box-cox lambda for PT travel time</i>	0.8659 (12.94)
<i>Travel walking distance for first trip (base)</i>	-1.5943 (-11.75)
<i>Travel walking distance shift for O-S-O trip chains</i>	0.1167 (1.09)
<i>Travel walking distance multiplier for following trip</i>	1.3240 (11.89)
<i>Box-cox lambda for travel walking distance</i>	0.8128 (15.23)
<i>Travel walking distance - Shopping duration elasticity</i>	-0.1202 (-3.74)
<i>Travel cost</i>	-0.5138 (-6.95)
<i>Box-cox lambda for travel cost</i>	0.5536 (9.74)
<i>Travel cost - Personal income elasticity</i>	-0.2872 (-2.86)
Direction of travel	
<i>Presence of angle >90° between O-S and O-D</i>	-0.2451 (-2.37)
Locational variables	
<i>Living in rich areas-shopping in poor areas</i>	-0.6460 (-2.76)
<i>Parking areas (400m buffer)</i>	0.0697 (3.40)
<i>Box-cox lambda for parking areas (400m buffer)</i>	0.4576 (5.31)
<i>Major clothes shopping retailers (400m buffer)</i>	1.1858 (6.04)
<i>Major grocery retailers (400m buffer)</i>	0.3661 (3.57)
<i>Major durables retailers (400m buffer)</i>	1.7233 (2.37)
Size variables	
<i>Natural logarithm multiplier ϕ</i>	0.5451 (5.41)
<i>Population (400m buffer) (base)</i>	1.0000 (-)
<i>Retail areas for clothes (400m buffer) (log.)</i>	0.4293 (0.85)
<i>Retail areas for groceries (400m buffer) (log.)</i>	1.1443 (2.35)
<i>Retail areas for durables (400m buffer) (log.)</i>	0.3303 (0.49)
<i>Retail areas for groceries when following trip purpose is shopping (1000-2000m buffer) (log.)</i>	-0.3967 (-0.48)
<i>Shopping store variability when following trip purpose is shopping (1000-2000m buffer) (log.)</i>	2.2730 (1.88)

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4. Results

Table 4.5 – continued from previous page

Parameter	Estimate (Rob. t-ratio w.r.t. 0)
Nesting parameters λ	
λ_{dest}	0.5094 (-6.80*)
λ_C	0.7968 (-2.36*)
λ_{PT}	0.7708 (-1.62*)
λ_W	1.2474 (2.26*)
Distance multipliers γ	
γ_{PT}^C	-1.2279 (-6.48 [†])
γ_{PT}^{dist}	-0.8388 (-4.16 [†])
γ_W^{dist}	-2.3426 (-7.73 [†])
Allocation parameters α	
Dest. allocation for same mode combos $\alpha_{dest,same\ mode}^{joint*}$ (log.)	-0.3765 (-0.50)
Dest. allocation for diff. mode combos $\alpha_{dest,diff.\ mode}^{joint*}$ (log.)	1.7945 (2.85)

Table 4.6: Distance multipliers and allocation probabilities per mode combination

Mode combination	Distance multiplier γ	Allocation to destination nest	Allocation to first mode nest	Allocation to second mode nest
<i>Car-Car</i>	-1.5077	0.4070	0.593	
<i>Car-PT</i>	-1.0299	0.7505	0.1248	0.1248
<i>Car-Walking</i>	-2.8778	0.7505	0.1248	0.1248
<i>PT-Car</i>	-1.0299	0.7505	0.1248	0.1248
<i>PT-PT</i>	-0.7036	0.4070	0.593	
<i>PT-Walking</i>	-1.9658	0.7505	0.1248	0.1248
<i>Walking-Car</i>	-2.8778	0.7505	0.1248	0.1248
<i>Walking-PT</i>	-1.9658	0.7505	0.1248	0.1248
<i>Walking-Walking</i>	-5.4926	0.4070	0.593	

4.3 Demand elasticity analysis

In order to illustrate the importance of accounting for correlation among all destinations in a spatial choice model, either a simple destination or a joint mode and destination choice model, a demand elasticity analysis is performed in both of those cases and presented below.

4.3.1 Destination elasticities

The demand elasticity analysis for the destination choice model has been performed for *MNL-dest-base*, *PCL-dest* and *CNL-dest*. The two NL models, namely *NL-dest-1* and *NL-dest-2* have not been considered, since they collapse to the base MNL. The forecasting scenario involved the increase of car travel cost for destination 47, a suburban shopping centre at the outskirts of Leeds, by 1%. The individual level elasticities and cross-elasticities for a specific participant, who initially chose that shopping destination, are presented in [Table 4.7](#) and are calculated as $\log \frac{demand_{after}}{demand_{base}} / (\log(1.01))$. The cross-elasticities for 3 specific

*Robust t-ratio w.r.t. 1.0

[†]The robust standard error was calculated using the delta method (Daly et al., 2012)

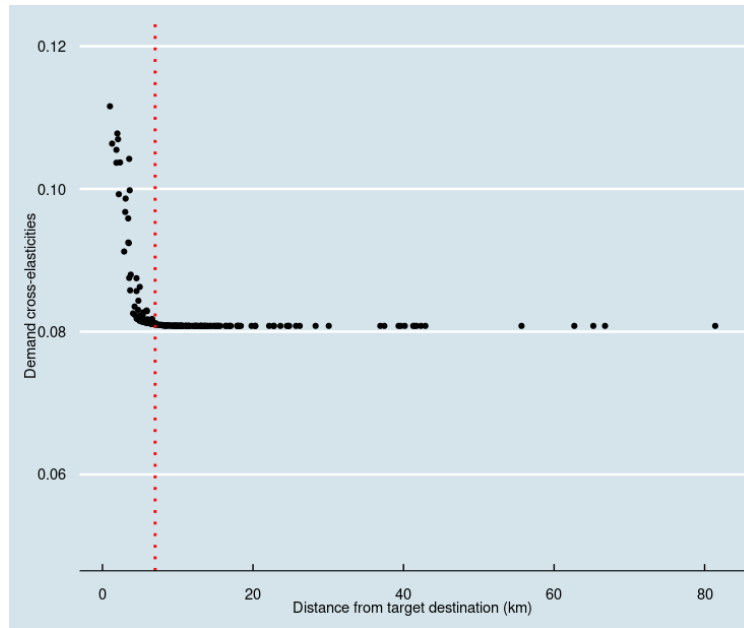


Figure 4.9: Demand cross-elasticities of CNL-dest model for each destination alternative based on their distance from the target alternative for forecasting scenario 1

destinations are examined, where destination 71 is the closest alternative to destination 47 in the choice set at a distance of 0.99km, alternative 34 is located at a distance of 7.88km and finally alternative 131 is located at a distance of 28.31km from the target alternative, destination 47. Looking at the elasticities obtained from *MNL-dest-base*, the impact of the *IIA principle* is clearly visible as it results in a proportionate demand increase across the other three destinations regardless of how far away from the target destination they are located. The *PCL-dest*, also, resulted in an almost proportionate demand increase for the remaining three destinations due to the small estimated distance multiplier. The proposed specification, *CNL-dest*, however, presents more realistic results with the distance between the alternatives now having a more profound impact on the cross-elasticities, as the closer destination, alternative 71, is showing a higher demand increase as a result of the demand decrease of its neighbouring alternative. It is also evident from the same Table that both the *MNL-dest-base* and *PCL-dest* models will significantly underestimate the change in demand of a destination located closer in favour of alternatives that are located at a greater distance. A depiction of the decrease of the estimated cross-elasticities from *CNL-dest* with the increase of distance from the target alternative for the current forecasting scenario is presented in *Figure 4.9*, where there is a steep decline until a distance of about 7km from destination 47, after which they stabilise at around 0.08.

Table 4.7: Individual level demand elasticities for forecasting scenario 1

Model	Destination alternatives			
	Dest 47	Dest 71	Dest 34	Dest 131
<i>Distance (km)</i>	0.00	0.99	7.88	28.31
<i>MNL-dest-base</i>	-0.082	0.084	0.084	0.084
<i>PCL-dest</i>	-0.083	0.079	0.079	0.079
<i>CNL-dest</i>	-0.082	0.112	0.081	0.081

4.3.2 Joint mode and destination elasticities

For the joint mode and destination choice model, a second forecasting example is presented, where car travel cost is increased by one unit for destination 47 again. The demand elasticities and cross-elasticities for the different mode combinations and for different destinations are examined at the individual level –for the same person as before– for *MNL-joint-base*, *CNL-joint-base* and *CNL-joint-proposed* and outlined in *Table 4.8*. Similarly to the elasticity analysis for the destination choice model, the two NL models, namely *NL-joint-Mod* and *NL-joint-DoM*, are not presented, since they both collapse to *MNL-joint-base*. That person chooses car-car initially to travel to destination 47 and to her following activity and PT is not available to her for the first trip. PT is also not available for both trips (shopping/following trips) for destination 71. As in the elasticity analysis for the destination choice model, the impact of the *IIA principle* is clearly evident in the demand elasticities of the *MNL-joint-base* model. The *CNL-joint-base* model results in a higher demand increase for alternative mode combinations in the same destination and those cross-elasticities are stable across the alternatives regardless of their distance from the target destination. Nonetheless, different conclusions can be drawn by examining *CNL-joint-proposed*, where higher cross-elasticities for the same mode combination of car-car for different destinations are estimated. Therefore, *CNL-joint-base* overestimates the shift to alternative mode combinations for the same destination, while *CNL-joint-proposed* suggests that individuals would be more likely to change their destination rather than their mode. This is a key finding, and suggests that not accounting for it could affect policy decisions.

Table 4.8: Individual level demand elasticities for forecasting scenario 2

Destination (density band)	C-C	C-PT	C-W	PT-C	PT-PT	PT-W	W-C	W-PT	W-W
MNL-joint-base model									
47 (second)	-0.122	-0.122	-0.122	–	–	–	0.148	0.148	0.148
71 (second)	0.148	–	0.148	–	–	–	0.148	–	0.148
34 (first)	0.148	0.148	0.148	0.148	0.148	0.148	0.148	0.148	0.148
131 (third)	0.148	0.148	0.148	0.148	0.148	0.148	0.148	0.148	0.148
CNL-joint-base model									
47 (second)	-0.131	-0.148	-0.085	–	–	–	0.165	0.161	0.161
71 (second)	0.168	–	0.159	–	–	–	0.161	–	0.159
34 (first)	0.167	0.163	0.159	0.164	0.160	0.159	0.159	0.159	0.159
131 (third)	0.166	0.162	0.159	0.163	0.160	0.159	0.159	0.159	0.159
CNL-joint-proposed model									
47 (second)	-0.133	-0.174	-0.066	–	–	–	0.175	0.148	0.145
71 (second)	0.199	–	0.145	–	–	–	0.149	–	0.145
34 (first)	0.160	0.158	0.145	0.155	0.146	0.145	0.145	0.145	0.145
131 (third)	0.153	0.153	0.145	0.151	0.146	0.145	0.145	0.145	0.145

C: Car, PT: Public Transport, W: Walking

5 Conclusions

Destination choice is a topic of key interest to the travel behaviour community, and a key issue in this context is how to capture the fact that closer destinations may be better substitutes for each other. The current paper presented a novel correlation structure for a CNL model for destination choice, or for joint mode-destination choices. Distance among alternative destinations was used as a proxy of spatial similarity among alternatives. The proposed

nesting structure, based on Tobler's first law of Geography, was the only specification, out of the MNL, NL and base CNL frameworks examined, that was able to capture significant unobserved correlations among the destination alternatives and provided RUM-consistent λ estimates. The PCL specification was also able to capture spatial correlations among destinations, however the proposed CNL model was able to uncover a much higher impact of distance in addition of being more statistically efficient and resulting in much lower estimation times. Furthermore, the proposed nesting structure can be easily modified to be suitable for the context of a joint mode and destination, where correlation is being captured across all choice dimensions simultaneously.

The results prove that, in general, there is a higher correlation between the error terms of alternatives located closer together than with more distant ones. For the joint mode and destination model, the results showed that mode also has an impact on the allocation parameters. Walking leads to higher allocation parameters for the nest of the target destination, while mechanised modes, i.e. car and PT, result in more balanced allocation parameters between the target and the neighbouring clusters, probably due to the flexibility those modes can provide to the decision-maker compared to walking. The proposed CNL model is also computationally more efficient than its PCL counterpart of Sener et al. (2011) and does not require simulation like the EC model of Weiss and Habib (2017) allowing the analyst to estimate a model using the full choice set.

Other continuous measures can also be used to quantify the spatial similarities among the destinations, such as network travel times among the destinations during different time periods, e.g. am peak, off-peak, pm peak etc. That would allow an additional temporal dimension to be included in the analysis for the purpose of uncovering spatio-temporal similarities among destinations. An interesting finding would be whether the individuals perceive the destinations closer together or further apart based on the time of day due to network traffic in each time period.

Furthermore, the reported specifications in the current study captured similarities among destinations based on their spatial proximity providing an empirical proof of Tobler's first law of Geography. It does not provide an answer, however, as to the most suitable measure of spatial similarity, which could be a function of both spatial proximity, but also of demographic characteristics (social distance), network topology etc. Machine Learning algorithms can help in this regard to identify more complex spatio-temporal similarities among destinations. Similarities could also differ based on the context of the choice problem itself with different attributes influencing perceived similarity in a shopping location than in a residential location choice model.

In addition to the insights of individual behaviour, the present study offers a specification that can be used to enhance current national travel demand models (Department for Transport, 2020). Furthermore, agent-based models or individual components of land use-transport interaction models could be enhanced with such a specification to better capture the effect of spatial similarity in the decision-making process that would most likely lead to different distribution of activities through space and hence to different dynamic interactions among agents or between land use developments and the transport system.

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Chapter 5

Augmenting Choice Models with Machine Learning techniques to capture the heterogeneity in Travel Behaviour

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Abstract

In the era of big data, machine learning (ML) has emerged as a strong competitor to econometric modelling. In particular, machine learning models offer flexible classification methods that are well-suited to capture the heterogeneity among the decision makers and improve model fit. A key limitation of the purely data driven models, however, is the difficulty in the calculation of welfare measures, such as value of travel time estimates (VTT) that feed into the cost-benefit analyses. This motivates the current study which focuses on combining ML-based segmentation approaches with DCM to get the best of both - a ML-based component to capture the heterogeneity among the travellers and a utility based choice component that is suitable for quantifying VTT estimates. In the proposed hybrid framework, the travellers are probabilistically allocated into clusters based on their degree of similarity from each cluster and cluster-specific random-utility-based mode choice models are estimated simultaneously. The proposed hybrid framework is tested on two different datasets and in a range of different behavioural contexts related to mode and destination choice behaviour. The performance of the proposed hybrid model (H-LCCM) is compared with that of the traditional latent class choice models (LCCM), where both the class membership and mode choice components are based on utility-based frameworks. Results indicate that H-LCCM outperforms the LCCM in most of the contexts examined, and are particularly suited for contexts with a large number of observations (which is the case for big data sources). The proposed framework is practically applicable for policy making as it allows calculation of VTT estimates, therefore not sacrificing the microeconomic interpretability of the traditional choice models. The results are thus promising, especially in the current era of big data and are expected to contribute to the emerging literature looking at cross-synergies between traditional econometric approaches and new data-driven methods.

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1 Introduction

During the last decade, the abundance of passively generated location data has provided interesting insights into human mobility behaviour. For instance, GPS traces, mobile phone call detail records, public transport smart card data, etc. not only provide location data at a high temporal and spatial resolution, but also have repeated observations of the same individual. The panel nature of the data provides rich insights about the similarity/dissimilarity of the travellers, which can be used to better capture the heterogeneity in their travel decisions.

Deriving 'value' out of these new forms of data, however, typically requires significant pre-processing and the use of methods from different fields of research (e.g. Computer Science) (Antoniou et al., 2019). In addition to that, the massive size of the data has started to highlight the limitations of well-established tools and methods for their analysis and the scope for improvements (Milne and Watling, 2019). That led to an increase in the popularity of Machine Learning (ML) techniques due to their efficiency in capturing patterns in the data, which could prove to be useful in capturing the heterogeneity among the behaviour of different decision-makers.

Originating from the field of Computer Science, ML algorithms are generally characterised as non-parametric methods (with some exceptions) aiming to minimise the errors between actual and predicted outcomes without relying on any behavioural assumptions about the underlying model. ML encompasses a large array of algorithms, which can be broadly categorised into supervised and unsupervised learning. A wide range of studies has implemented clustering algorithms (unsupervised learning) to analyse individual behaviour and uncover mobility patterns (see Anda et al. (2017) for details). Though such studies provide good insights about the state of the network, they have limited applications in the context of predictions and/or valuation (e.g. calculation of value of time estimates to feed into the cost-benefit analyses).

The literature of travel demand modelling has arguably shown a larger interest in the use of supervised ML algorithms, such as Artificial Neural Networks and Random Forests, and on their comparison with traditional econometric Discrete Choice Modelling (DCM) frameworks, such as Multinomial logit (MNL) and Nested Logit models, usually in the context of mode choice (Hensher and Ton, 2000; Xie et al., 2003; Cantarella and de Luca, 2005; Zhang and Xie, 2008; Sekhar et al., 2016; Hagenauer and Helbich, 2017). Their findings at large suggest that ML algorithms have the potential to be used as an alternative method for behavioural modelling due to their superior predictive performance, although Hensher and Ton (2000) also highlight the limitations associated with the lack of interpretable results compared to a DCM framework.

The majority of studies from that initial stream of literature is subject to three key limitations. Firstly, they relied on "traditional" samples with regard to their data collection methods (e.g. single RP choice scenarios, short trip diaries, etc.) and it is worth investigating the performance of similar approaches with passively collected larger samples (more participants and/or longer panels). Secondly, these studies did not compare the model performances with more advanced discrete choice models that account for heterogeneity among groups of decision makers. Thirdly, those earlier studies focused on comparing the goodness of fit and/or prediction capabilities of ML and DCM as opposed to a more in-depth effort of formulating models that combine the best of both worlds – the computational advantages on ML that can more efficiently distinguish the signal among the noise and the behavioural interpretation of DCM that can produce outputs suitable for valuation and cost-benefit analysis. Wang et al. (2021) aimed to generalise the empirical results of the studies so far by comparing a vast range of ML algorithms and choice models and on a range of different datasets concluding that it would be advantageous to use ML algorithms for predicting travel behaviour, while also highlighted the need for DCM to improve their computational efficiency to be more suitable for estimating models on large datasets. These initial studies, have also motivated researchers to investigate methodologies to combine the ML and DCM paradigms. DCM,

with their grounding on strong theoretical underpinnings of human behaviour (McFadden, 1973; McFadden, 1978; Ben-Akiva and Lerman, 1985; McFadden, 2000; Train, 2009) are suitable for policy making, while also providing clear interpretations on the impact of the utilised independent variables and their statistical significance. Hence, cross-fertilisation of ML approaches with DCM is very appealing for policy analyses to get the best out of both worlds. Prominent examples of combining DCM and ML are presented in the studies of Sifringer et al. (2020) and Wang, Mo and Zhao (2021) in both of which Deep Learning architectures have been integrated with DCM specifications in the context of mode choice, risk and time preference.

In a similar notion, there have been attempts to harness the power of unsupervised learning for uncovering latent segments of the population to aid the estimation of advanced choice models, namely Latent Class Choice Models (LCCM) (Kamakura and Russell, 1989). In a recent series of studies, Sfeir et al. (2021) and Sfeir et al. (2022) provided significant research advancements towards that direction by integrating probabilistic ML algorithms, namely gaussian mixture models and gaussian processes respectively, into a Latent Class Choice Model (LCCM) framework effectively replacing the random utility-based class allocation component with ML algorithms. In both cases, their proposed specifications were tested on models of mode choice behaviour using traditional Revealed (RP) and Stated Preference (SP) datasets. Overall, the non-parametric gaussian processes outperformed the gaussian mixture variants of LCCM and the traditional LCCM in terms of model fit and estimation stability, while also resulting in estimates with behaviourally consistent signs. Nonetheless, the models in those studies were estimated only on traditional RP and SP data and it is not clear if that ML-DCM integration can provide additional benefits when used for modelling travel behaviour in the context of passively generated big data sources where the increased number of observations per traveller could offer a more detailed depiction of the underlying heterogeneity.

The current research aims to contribute to that stream of literature by proposing a novel approach of integrating a clustering algorithm, namely K-means clustering, in the context of an LCCM. The main goal of the study is to illustrate that an integration of a clustering algorithm can provide model fit improvements to a LCCM specification estimated on large data sets, contrary to a traditional econometric framework. Several studies have used clustering techniques for market/sample segmentation (Salomon and Ben-Akiva, 1983; Lanzendorf, 2002; Krizek and Waddell, 2003) reporting that different lifestyle clusters (empirically identified) could have different choice elasticities. Nonetheless, the clustering algorithms in those studies were used to deterministically allocate individuals into clusters, while the clustering process was independent from the choice behaviour itself. The novelty in the framework proposed in the current paper is to illustrate how a deterministic clustering algorithm can be transformed effectively into a probabilistic one enabling a simultaneous estimation of parameters of class membership and choice components. Therefore, the aim of the current study is to combine a clustering ML algorithm and a DCM specification (MNL model at the lower level) in a combined LCCM framework, while still being able to produce outputs that can be used for valuation.

The proposed methodology is tested empirically on 2 RP datasets, a GPS diary and a traditional household survey, and on 3 different choice contexts providing a range of different sample sizes and data complexity. The results indicate that the proposed approach could prove to be advantageous in datasets with larger sample sizes, either in terms of observations or in terms of the number of individuals. The three case studies utilised for the empirical application of the proposed approach are the following:

1. a mode choice model estimated using a GPS trip diary
2. a shopping destination choice model estimated using a GPS trip diary
3. a mode choice model estimated using a traditional trip diary

The remainder of this paper is structured as follows. In Sections 2 and 3, the methodological framework and the different datasets used for the study’s practical applications are described, respectively. Section 4 focuses on the results and the comparison among the different approaches. The main conclusions and a potential direction for future research are summarized in the final section.

2 Methodology

2.1 Latent Class Choice Model

DCM and the MNL model specifically has been the main behavioural framework for analysing individual preferences since the seminal study of McFadden (1973). According to that framework, an individual n facing a specific choice task t will choose the alternative i that provides the largest utility U_{int} among a choice set of J alternatives. The utility U_{int} is a latent construct consisting of two parts, a deterministic utility V_{int} and a disturbance term ϵ_{int} . The deterministic part of the utility is a function of individual- and alternative-specific attributes x_{int} and parameters β to be estimated, as shown in Equation 5.1. Different distributional assumptions about the disturbance term will lead to different specifications, with independent and identically distributed (iid) extreme value error terms leading to an MNL model. The probability of choosing alternative i can be calculated using Equation 5.2.

$$U_{int} = V_{int} + \epsilon_{int} = f(\beta, x_{int}) + \epsilon_{int} \quad (5.1)$$

$$P_{int}(\beta) = \frac{e^{V_{int}}}{\sum_{j=1}^J e^{V_{jnt}}} \quad (5.2)$$

Heterogeneity in an MNL model can be captured by specifying interactions between socio-demographics characteristics and level-of-service variables/alternative specific constants. Those interactions are usually specified as shifts of taste parameters from their base level. Despite those interactions, however, a significant portion of unobserved heterogeneity is likely to remain uncaptured with an MNL model. LCCMs together with mixed logit models (McFadden and Train, 2000) have been established as important behavioural modelling specifications capable of uncovering unobserved individual choice heterogeneity. The former achieves that by probabilistically segmenting the sample into a finite number of latent classes based on the individuals’ socio-demographic characteristics and their observed choice behaviour. It uses two model components that are jointly estimated, a class allocation model at the upper level and a choice model at the lower model. Mixed logit models, on the other hand, require the specification of continuous distributions over the individual taste parameters, thus resulting in non-closed form solutions that usually require the use of simulated estimation procedures (Train, 2009). Besides its closed form solution, the LCCM provides the additional benefit of a more straightforward interpretation of the context of each estimated class, since they are directly linked with socio-demographic characteristics for each class (given that covariates are included in the class allocation component) that could be important from a policy perspective.

In a LCCM, it is assumed that the sample can be segmented into a finite number of S heterogeneous classes. The class allocation component of the LCCM, commonly specified as an MNL model, is responsible for probabilistically allocating individuals into the latent classes. Socio-demographic characteristics x_n are included in the class allocation model as covariates, while additional parameters γ_s are estimated per class together with $S - 1$ constants, δ_s . The probability π_s of an individual belonging into class s is thus calculated as per Equation 5.3,

2. Methodology

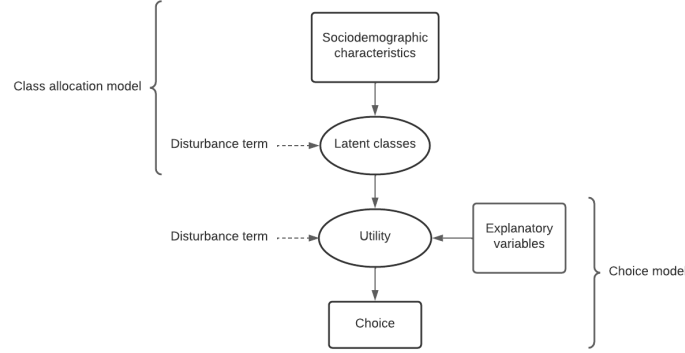


Figure 5.1: Schematic diagram of the LCCM framework and its constituent components

with $0 < \pi_s < 1$ and $\sum_{s=1}^S \pi_s = 1$ for each individual n . Homogeneity of preferences is usually assumed to hold within each class, although there is also the possibility to capture additional within-class heterogeneity by specifying continuous distributions over covariates (Hess, 2014).

$$\pi_s = \frac{e^{\delta_s + \gamma_s x_n}}{\sum_{r=1}^S e^{\delta_r + \gamma_r x_n}} \quad (5.3)$$

A choice model at the lower level is being estimated conditional on the class, as depicted in *Figure 5.1*. The choice probabilities for the class-specific model are calculated from *Equation 5.4*. Finally, the unconditional likelihood of observing a sequence of choices for individual n is calculated as *Equation 5.5* in which class probabilities are used to weight the respective class-specific conditional probabilities for each alternative j . The coefficients of both levels are jointly determined by maximising the logarithm of the likelihood function.

$$P_{sint} = \frac{e^{V_{sint}}}{\sum_{j=1}^J e^{V_{sjnt}}} \quad (5.4)$$

$$L_n(\beta, \pi) = \sum_{s=1}^S \pi_s \prod_{t=1}^T P_{sint} \quad (5.5)$$

2.2 Clustering - Latent Class Choice Model

Focusing now on our proposed modelling framework, the main idea is to incorporate a clustering algorithm into an LCCM modelling framework to take the role of the class allocation model. In the current study, we use the K-means clustering algorithm to take that role, mainly for its simplicity, but the same principles can be applied to more advanced algorithms, as well. The K-means clustering algorithm (Lloyd, 1982) allocates individuals deterministically into a finite K number of clusters based on specific D socio-demographic characteristics, which are found after a specification search similarly to the covariates in a class allocation model. The clustering process itself is an iterative algorithm that tries to minimise a measure of distance among the data points (i.e. individuals) and their respective allocated cluster centroid (within cluster sum of square distance), while at the same time maximise their distance to the centroids of the remaining cluster centroids (between cluster

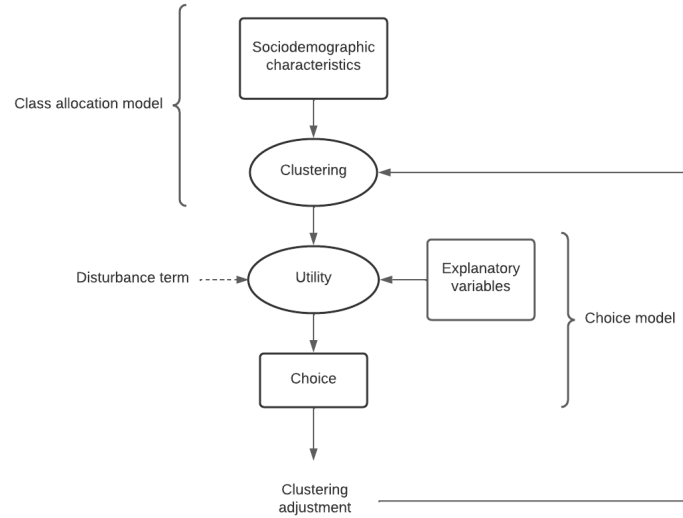


Figure 5.2: Schematic diagram of the H-LCCM framework and its constituent components

sum of square distance) (Ripley, 2009). Different measures of distance can be used for that purpose, such as the euclidean or the manhattan distance (Bishop, 2006; Singh et al., 2013; Bora and Gupta, 2014), with the former being implemented in the current paper *Equation 5.6*. In order to avoid the calculated distance measure being influenced by the scale discrepancies among the different variables used for clustering, it is important to scale the variables prior of the initialisation of the clustering algorithm, either by normalising or by standardising the variables, with the latter approach being utilised here.

$$d_{nk} = \sqrt{\sum_{d=1}^D (X_{nd}^* - X_{kd}^*)^2} \quad (5.6)$$

The proposed hybrid methodological framework, *H-LCCM*, developed for this study involves the implementation of a probabilistic transformation of the traditional deterministic K-means clustering algorithm for its efficient integration into an LCCM specification. The probabilistic K-means algorithm is designed to handle the identification of latent segments of travellers based on specific socio-demographic characteristics, while it gets adjusted with information provided by the choice model with a feedback loop as depicted in *Figure 5.2*.

The class allocation model in a traditional LCCM framework is used to probabilistically allocate individuals into latent classes based on their sociodemographics and their observed behaviour with regard to a specific choice situation. The two important things to note here is first that each individual is allocated with a non-zero probability to every class and second that the class allocation model is getting feedback from the choice model at the lower level. In order to mimic that specification with a K-means algorithm, the first step is to transform it from a deterministic algorithm into a probabilistic one. That is achieved by taking advantage of the fact that each data point n is allocated to its closest centroid k , but there still is a non-zero distance $d_{nk} > 0$ with $d_{nk} < d_{nl}$ and $k, l \in K$. Therefore, instead of assuming that an individual n would be allocated entirely into the closest centroid, we re-define her allocation by taking into account her distance from all centroids. In our framework the class allocation probability is defined as:

$$\pi_{nk} = \frac{e^{\gamma_{dist}^k d_{nk}}}{\sum_{l=1}^K e^{\gamma_{dist}^k d_{nl}}} \quad (5.7)$$

where π_{nk} is the allocation probability of individual n to her closest centroid k , d_{nl} is the distance of individual n from centroid l and finally γ_{dist}^k is a parameter to be estimated controlling the allocation to the closest centroid k relative to the remaining ones. If $\gamma_{dist}^k > 0$ it means that the individual is allocated with a higher probability to the closest centroid k relative to the rest, while the opposite would be true in the case of $\gamma_{dist}^k < 0$ signifying the need for readjusting the allocation of individuals into the clusters. Finally, the use of $\gamma_{dist}^k = 0$ would result into an equal allocation to every cluster.

Regarding cluster initialisation, the K-means++ algorithm (Arthur and Vassilvitskii, 2007) was implemented. According to that, a data point, i.e. an individual, is randomly selected and assigned as the centroid of the first cluster k_1 . The distance d_{nk_1} of all data points n from that initial centroid k_1 are calculated and the second centroid is sampled with a probability equal to $\frac{d_{nk_1}^2}{\sum d_{mk_1}^2}$. That means that data points further away from the initial centroid will have a higher probability of being selected as the second centroid from that process. For the third centroid, the distances of all data points from the two selected centroids are calculated and the next centroid is sampled with a probability based on the square of the minimum distance from the other two centroids. In a similar way, the remaining centroids are sampled until the predetermined number of centroids is reached. Following that, the K-means algorithm can initialise using the previously sampled centroids during the first iteration. Alternatively, the analyst can define specific centroids manually by trying different sign combinations for the clustering covariates (i.e. same or different sign per cluster etc.). Both of the aforementioned initialisation approaches were implemented in the current study.

The developed algorithm behind H-LCCM is presented in the flow chart of *Figure 5.3*, which consists of the following steps:

1. Scaling of variables used as covariates in the clustering process. Define minimum difference threshold for reaching convergence.
2. Define starting values for parameters.²
3. Initialisation of centroids using the K-means++ algorithm.
4. Distance calculation of data points (individuals) from the initial centroids to define initial cluster allocation.
5. Estimation of choice model for the first iteration using Maximum Likelihood.
6. Update of cluster allocation based on new estimated γ_{dist}^k and the previously defined centroids.
7. Definition of new centroids for following iteration as the mean of the covariates of the individuals that are being attracted with a higher probability to the same cluster.
8. Compute distance between previous and new centroids and compare that with the threshold defined in step 1.
9. If the difference is larger than the threshold, then estimate a new choice model for next iteration and repeat steps 6-8. If the difference is smaller than the threshold, then convergence is reached.

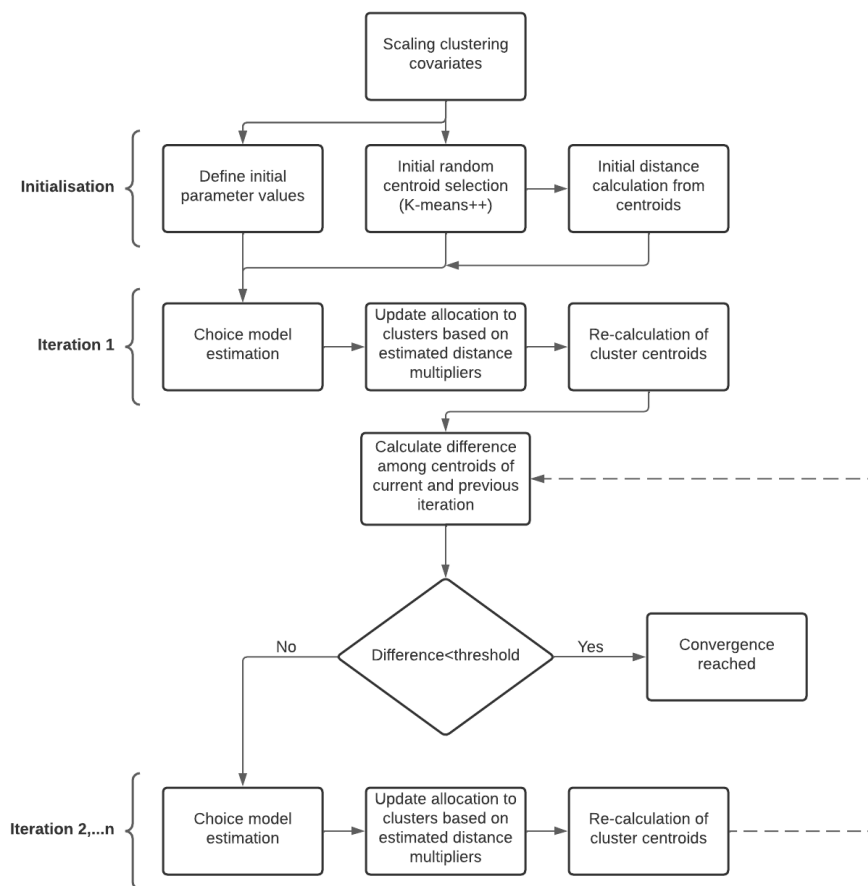


Figure 5.3: Flow chart of the H-LCCM algorithm

After reaching a stable point and terminating the iterative estimation process, additional linear regressions can be specified in order to capture the impact and the statistical significance of the covariates used for clustering by using the logarithm of the estimated shares, $\log \pi_{nk}$, as the dependent variable. Specifically, $K - 1$ linear regression models are estimated, where K is the total number of cluster centroids specified. One centroid is kept fixed by subtracting its logarithm of shares, $\log \pi_{n0}$, from the remaining ones, while the covariates used for the clustering, X_{nd} , take the role of the independent variables with parameters ξ_d capturing their impact (*Equation 5.8*).

$$\log \pi_{nk} - \log \pi_{n0} = \xi_{nk0} + \sum_{d=1}^D \xi_d X_{nd} \quad (5.8)$$

3 Data

The empirical application of the proposed methodology was performed using two datasets, which are described in the following, together with a brief description of the choice context of each of the three case studies. Case studies 1 and 2 utilised a GPS trip diary ("DECISIONS"), while Case study 3 utilised a traditional pen and paper trip diary for London.

3.1 DECISIONS dataset

The first dataset used was collected as part of the research project "DECISIONS" conducted at the University of Leeds between October 2016-March 2017. The dataset includes several submodules aiming to capture different aspects of everyday individual behaviour, such as indoor/outdoor activity behaviour, energy consumption, social networks etc. More information on the range of the different submodules of the dataset can be found in Calastri et al. (2020). In the current study, two specific submodules are being utilised, namely a 2-week GPS-based trip diary captured through a smart-phone application and a household survey capturing important sociodemographic information of the participants. The survey captured trips across all of the UK, but with the vast majority of those being around the region of Yorkshire and more specifically the city of Leeds, which most of the participants were residents of.

Two different subsets of the DECISIONS dataset were used, namely one for the mode choice (*Case study 1*) and one for the shopping destination choice model (*Case study 2*). For both of them, only the trips within the region of Yorkshire were selected. Data enriching steps followed the initial data cleaning stages, during which the dataset was augmented with travel time and travel cost information for all the alternatives. More specifically, travel times and distances were estimated for both chosen and unchosen alternatives (for consistency reasons) using a combination of the "Directions" Google API and Bing maps API. Both APIs allow for a detailed routing plan between an Origin and a Destination for different transport modes and times of day, while also accounting for traffic for car trips and for service timetable for public transport (PT) trips. Travel costs for car trips were calculated using WEBTag's official specifications for fuel and operating costs, while bus and rail travel costs were calculated based on average distance-based costs of PT services operating in the region. A discount was applied for season ticket holders. The final mode choice dataset utilised for model estimation included 12,524 performed by 540 individuals and a choice set of six alternative modes of transport, namely car, bus, rail, taxi, cycling and walking. Out of those trips, 47.6% were performed by car, 14.6% by bus, 5.2% by rail, 3.2% by taxi, 3.3% by cycling and finally 26.1% by walking.

²For the initialisation of γ_{dist}^k , an initial value of 1.0 is assigned in the current study assuming a higher allocation probability of each individual to their initially defined closest centroid, but any value would work since the initial centroids are randomly assigned without having any behaviourally connection with the decision making process under examination.

A further subset of the mode choice dataset was selected for the shopping destination choice model, which included only shopping trips (for groceries, clothes and durables) from an initial origin O to a shopping location j and the trips to the following destination D . In total, 1541 trip pairs were included in the dataset performed by 270 individuals with 82% of them being for groceries, 12.7% for clothing and 5.3% for durables. The purpose of including the subsequent trip, as well, was to study the impact of the following destination D (considered fixed in that study) on the choice of the intermediate shopping location. The choice set in the destination model was defined by clustering the observed elemental locations utilising the Hierarchical Agglomerative Clustering (HAC) algorithm with a 800m distance threshold. HAC was chosen since it does not require the analyst to make a priori assumptions regarding the number of clusters. The aforementioned procedure resulted in the creation of a choice set of 176 shopping destinations, most of them within the administrative boundaries of the local authority of Leeds. The main shopping mall of Leeds city centre attracted the majority of shopping trips, namely 11.3%. The remaining 5 shopping locations in the city centre attracted 9.7% of trips followed by the 103 locations in remaining city of Leeds (62.6%) and finally the 67 locations in the remaining region of Yorkshire (16.7%). More details regarding the data cleaning/enriching steps and the approach followed to define the availability of mode and destination alternatives in both subsets can be found in *Chapters 2-4*.

3.2 London travel demand survey

The second dataset utilised for *Case study 4* in the empirical application is the openly available London Passenger Mode Choice (LPMC), collected as part of the London travel demand survey, in which the individuals had to choose a mode of transport among a choice set of four alternatives, namely walking, cycling, transit and car. The dataset was augmented at a later stage by Hillel et al. (2018) with travel cost and travel time information for chosen and unchosen alternatives using the “Directions” Google API, in a similar way as in the DECISIONS dataset. An additional interesting variable was defined during that data enriching stage measuring the traffic variability for car trips as captured by the different routing procedures of the Google API. More details about the specific dataset can be found in Hillel et al. (2018). For the current application, a subset of only home-based trips performed by individuals of at least 12 years of age was selected, similarly to the study of Krueger et al. (2020) and Hancock et al. (2021). The resulting dataset contains a total of 58,584 trip observations performed by 26,904 individuals.

In terms of the observed mode choices, 42.8% of trips were performed by car, followed by 37.6% of PT trips, 16.6% walking and finally 3.2% cycling trips. With regard to socio-demographic, 53.5% are females, the mean age is 42 years old and 69.8% of participants have at least one car in their household. Besides the richness of individual mobility information, an important limitation of the London dataset is the absence of any income information, personal or household.

4 Results

The proposed hybrid specification, *H-LCCM*, is compared against a base MNL model, *MNL-base*, a traditional *LCCM* model and a two-stage clustering choice model, *C-MNL*, where K-means is used at the first stage to allocate individuals into latent clusters based solely on sociodemographic characteristics, and then a choice model is estimated per cluster at the second stage. The final log-likelihood of that model is calculated by adding the log-likelihoods of the K cluster-specific models and the remaining fit statistics are computed relative to that. In all cases, the same specification was used in terms of covariates in the clustering/class allocation model and explanatory variables in the utility functions to ensure consistency in our evaluation comparison. The number of classes and the specified covariates in the final

specification reported in the following for each case refer to the one which resulted in the best model fit for the traditional *LCCM* model.

4.1 Case study 1: Yorkshire mode choice

4.1.1 Model specification

The specification of the Yorkshire mode choice model presented in the following contains 5 alternative specific constants (ASCs) with the ASC for car being kept fixed as the base. Mode-specific linear travel time sensitivities were specified in addition to a logarithmic generic specification for travel cost for the purpose of capturing cost damping effects (Daly, 2010).

4.1.2 Model outputs

The fit statistics of the specifications for *Case study 1* are presented in *Table 5.1*. All models that are capturing individual unobserved heterogeneity are able to outperform the *MNL-base* model, even the *C-MNL*, in which the sample is segmented into clusters solely based on socio-demographic characteristics. As expected, however, more significant heterogeneity can be captured by including the choice behaviour in that process as illustrated by the remaining two models, namely *LCCM* and *H-LCCM*. Out of those two specifications, the proposed *H-LCCM* is able to outperform in terms of model fit the traditional *LCCM* by 5.38 LL units with 19 parameters less. Those improvements in model fit are more evident by looking at the adjusted ρ^2 , the AIC and BIC statistics.

A closer comparison between the estimated parameters of *LCCM* and *H-LCCM* is depicted in *Table 5.2*. The specification search resulted in a model with 5 classes and with gender, age, number of cars, season ticket ownership and household income in the class allocation. An equivalent specification was estimated for *H-LCCM*. An increase to 6 classes resulted in numerical issues in the covariance matrix, hence no attempt was made to estimate a model with 6 clusters for *H-LCCM*. Furthermore, only a generic ASC for cycling was used across classes, since a class-specific parameter led to numerical issues even in the case of two classes, possibly due to the low number of cycling trips (3.3%). Having said that, however, it should also be noted that the equally low number of taxi trips (3.2%) did not pose a problem for specifying class-specific ASCs.

Overall, the *H-LCCM* results in more balanced cluster membership probabilities compared to *LCCM*, with cluster 5 representing the largest segment of the sample (23.0%) followed by cluster 2 (21.0%). Furthermore, by examining the estimated distance multipliers γ of *H-LCCM*, it is evident that individuals of cluster 5 are allocated to their class with a higher probability relative to others (48.2% to cluster 5 on average), while there is a higher degree of uncertainty in the allocation of individuals of cluster 4 (26.0% to cluster 4 on average). On the other hand, *LCCM* leads to more imbalanced class allocation with the majority of the sample (43%) being allocated to class 1. All level-of-service parameters have the expected negative sign in both models. A non cost sensitive class is identified in *LCCM*, class 5, representing the smallest segment of the sample (9%). Contrary to that, all clusters of *H-LCCM* show significant cost sensitivities, which illustrates the discrepancies of the two approaches in the heterogeneity they are able to capture. The estimated parameters of the covariates used in the class allocation of *LCCM* are presented in the same *Table 5.2*. The respective parameters for *H-LCCM* are obtained from four linear regression models on the log of shares and are reported in *Table 5.3*. In both cases, class/cluster 5 was used as the base and the remaining parameters were estimated relative to that.

A closer look at the average probabilities per sociodemographic group and their respective average values allows us to get a better understanding of the profile of each class/cluster (*Figure 5.4*). Regarding the classes resulting from the *LCCM*, class 1 is more likely to contain car dependent (average number of cars=1.1/average season ticket ownership=0.16), middle-aged

individuals (average age=42.8) of higher household income (average income=£55,731). Class 2 is more likely to contain individuals who are frequent public transport users (average season ticket ownership=0.6) have a lower than average number of cars in their household (average number of cars=0.76) and a lower household income (average income=£40,760). Class 3 is more likely to have younger (average age=29.2) female (average value for female=0.63) individuals with both a low number of season ticket ownership (average season ticket ownership=0.12) and number of cars (average number of cars=0.66). Class 4 has a higher share of younger (average age=34.5) male (average value for female=0.5) individuals, and finally class 5 has the highest share of female individuals (average value for female=0.72) with the lowest number of cars (average number of cars=0.4) and a high season ticket ownership (average season ticket ownership=0.46).

Moving on to the behavioural profiling of the clusters estimated from *H-LCCM*, cluster 1 can be characterised by mostly higher income individuals (average income=£59,650) with a high number of cars in their household (average number of cars=1.15). Cluster 2 contains a high share of female individuals (average value for female=0.60) together with the highest share of season ticket holders (average season ticket ownership=0.56), a low number of cars (average number of cars=0.64) and low household income (average income=£43,970). Cluster 3 has a high share of younger individuals (average age=32.1) with a low number of cars (average number of cars=0.64) and of low income (average income=£44,140). They are also the most cost sensitive according to their estimated travel cost parameter. Cluster 4 can be characterised by younger (average age=36.86) female (average value for female=0.60) with the lowest share of season ticket ownership (average season ticket ownership=0.11). Finally, cluster 5 contains the highest share of older (average age=44.91) male (average value for female=0.53) individuals with a higher than average number of cars (average number of cars=0.97) and with a quite low season ticket ownership (average season ticket ownership=0.18).

Table 5.1: Fit statistics of the Yorkshire mode choice models

Fit statistics	MNL-base	C-MNL	LCCM	H-LCCM
<i>Log-likelihood (0)</i>			-14,974.45	
<i>Log-likelihood (model)</i>	-5,275.415	-4,928.319	-3,956.388	-3,951.008
<i>Adjusted ρ^2</i>	0.6469	0.6669	0.7304	0.7321
<i>AIC</i>	10,574.83	9,976.638	8,072.78	8,024.02
<i>BIC</i>	10,664.05	10,422.76	8,667.61	8,477.58
<i>Number of parameters</i>	12	60	80	61
<i>Number of individuals</i>			540	
<i>Number of observations</i>			12,524	

Table 5.2: Modelling estimates of LCCM and H-LCCM models for the Yorkshire mode choice context

Parameter	LCCM	H-LCCM
Alternative-specific constants		
<i>Constant Car (base)</i>	-	-
<i>Constant Bus - class 1</i>	-5.2404 (-12.17)	-2.8387 (-4.25)
<i>Constant Bus - class 2</i>	-1.3781 (-3.79)	-1.3895 (-3.00)
<i>Constant Bus - class 3</i>	-0.3819 (-0.32)	1.1986 (1.28)
<i>Constant Bus - class 4</i>	-3.4909 (-5.23)	-5.9098 (-10.92)
<i>Constant Bus - class 5</i>	-2.7507 (-4.49)	-3.7478 (-5.21)
<i>Constant Rail - class 1</i>	-2.8864 (-3.31)	0.2058 (0.27)
<i>Constant Rail - class 2</i>	-0.5536 (-0.57)	-0.7345 (-0.93)
<i>Constant Rail - class 3</i>	-4.2090 (-1.65)	-3.4585 (-2.62)

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4. Results

Table 5.2 – continued from previous page

Parameter	LCCM	H-LCCM
<i>Constant Rail - class 4</i>	-1.3919 (-1.11)	-4.3949 (-7.00)
<i>Constant Rail - class 5</i>	-8.8327 (-5.18)	-3.7627 (-2.61)
<i>Constant Taxi - class 1</i>	-4.6140 (-6.95)	-3.4106 (-6.02)
<i>Constant Taxi - class 2</i>	-7.1176 (-1.71)	-1.9408 (-3.39)
<i>Constant Taxi - class 3</i>	1.2652 (0.52)	4.8698 (4.48)
<i>Constant Taxi - class 4</i>	-0.4390 (-0.67)	-3.5561 (-5.61)
<i>Constant Taxi - class 5</i>	-4.3879 (-5.22)	-4.7877 (-6.78)
<i>Constant Cycling</i>	-2.2052 (-4.59)	-2.9060 (-5.12)
<i>Constant Walking - class 1</i>	0.2032 (0.35)	3.2223 (3.74)
<i>Constant Walking - class 2</i>	1.4334 (2.43)	0.9795 (1.56)
<i>Constant Walking - class 3</i>	3.4196 (2.49)	4.9729 (5.92)
<i>Constant Walking - class 4</i>	2.4570 (3.43)	0.1633 (0.31)
<i>Constant Walking - class 5</i>	-0.7686 (-1.15)	0.1578 (0.26)
LOS parameters		
<i>Car travel time (mins) - class 1</i>	-0.1712 (-10.35)	-0.0711 (-2.87)
<i>Car travel time (mins) - class 2</i>	-0.0864 (-1.17)	-0.2551 (-6.96)
<i>Car travel time (mins) - class 3</i>	-0.1707 (-4.68)	-0.1617 (-2.36)
<i>Car travel time (mins) - class 4</i>	-0.0930 (-3.48)	-0.1676 (-5.25)
<i>Car travel time (mins) - class 5</i>	-0.2880 (-6.46)	-0.0293 (-0.75)
<i>Bus travel time (mins) - class 1</i>	-0.0791 (-9.04)	-0.0677 (-5.87)
<i>Bus travel time (mins) - class 2</i>	-0.0325 (-1.06)	-0.1045 (-8.11)
<i>Bus travel time (mins) - class 3</i>	-0.1112 (-3.49)	-0.1561 (-6.04)
<i>Bus travel time (mins) - class 4</i>	-0.0645 (-4.35)	-0.0572 (-3.60)
<i>Bus travel time (mins) - class 5</i>	-0.0956 (-4.94)	-0.0088 (-2.81)
<i>Rail travel time (mins) - class 1</i>	-0.0988 (-9.13)	-0.0576 (-4.53)
<i>Rail travel time (mins) - class 2</i>	-0.0729 (-2.49)	-0.1578 (-9.21)
<i>Rail travel time (mins) - class 3</i>	-0.0791 (-1.71)	-0.0245 (-1.35)
<i>Rail travel time (mins) - class 4</i>	-0.0367 (-2.07)	-0.0812 (-2.40)
<i>Rail travel time (mins) - class 5</i>	-0.0604 (-2.08)	-0.1515 (-4.50)
<i>Taxi travel time (mins) - class 1</i>	-0.2411 (-5.72)	-0.0749 (-1.53)
<i>Taxi travel time (mins) - class 2</i>	-0.0201 (-0.11)	-0.2870 (-6.20)
<i>Taxi travel time (mins) - class 3</i>	-0.2804 (-2.14)	-0.4870 (-6.74)
<i>Taxi travel time (mins) - class 4</i>	-0.1247 (-2.28)	-0.1380 (-3.56)
<i>Taxi travel time (mins) - class 5</i>	-0.1977 (-3.32)	-0.1007 (-1.77)
<i>Cycling travel time (mins) - class 1</i>	-1.0019 (-6.60)	-0.1832 (-2.90)
<i>Cycling travel time (mins) - class 2</i>	-0.3389 (-3.23)	-0.2839 (-3.19)
<i>Cycling travel time (mins) - class 3</i>	-0.1757 (-3.42)	-0.0939 (-2.58)
<i>Cycling travel time (mins) - class 4</i>	-0.0644 (-4.87)	-0.0701 (-5.03)
<i>Cycling travel time (mins) - class 5</i>	-0.1132 (-3.92)	-1.9796 (-12.57)
<i>Walking travel time (mins) - class 1</i>	-0.1980 (-10.76)	-0.2324 (-10.09)
<i>Walking travel time (mins) - class 2</i>	-0.1572 (-5.13)	-0.2091 (-9.03)
<i>Walking travel time (mins) - class 3</i>	-0.1065 (-2.89)	-0.1398 (-5.73)
<i>Walking travel time (mins) - class 4</i>	-0.2249 (-8.86)	-0.1935 (-8.28)
<i>Walking travel time (mins) - class 5</i>	-0.1781 (-5.40)	-0.1397 (-6.80)
<i>Natural logarithm of travel cost (£) - class 1</i>	-0.3764 (-1.94)	-1.0772 (-4.34)
<i>Natural logarithm of travel cost (£) - class 2</i>	-0.4822 (-2.51)	-0.4916 (-2.79)
<i>Natural logarithm of travel cost (£) - class 3</i>	-0.9810 (-2.21)	-1.7831 (-6.39)
<i>Natural logarithm of travel cost (£) - class 4</i>	-1.7228 (-11.10)	-0.6018 (-2.55)
<i>Natural logarithm of travel cost (£) - class 5</i>	-0.1566 (-0.70)	-0.9708 (-4.40)
Class allocation parameters		
<i>Constant - class 1</i>	1.6204 (1.59)	–
<i>Season ticket ownership - class 1</i>	-1.2191 (-2.48)	–
<i>Number of cars in household - class 1</i>	2.1653 (4.14)	–
<i>Age - class 1</i>	-0.0097 (-0.53)	–
<i>Female - class 1</i>	-0.7614 (-1.37)	–
<i>Annual household income (£1,000) - class 1</i>	-0.0072 (-0.73)	–
<i>Constant - class 2</i>	1.2963 (1.22)	–
<i>Season ticket ownership - class 2</i>	0.7863 (1.36)	–

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Table 5.2 – continued from previous page

Parameter	LCCM	H-LCCM
<i>Number of cars in household - class 2</i>	1.8449 (3.19)	–
<i>Age - class 2</i>	-0.0053 (-0.26)	–
<i>Female - class 2</i>	-0.9181 (-1.55)	–
<i>Annual household income (£1,000) - class 2</i>	-0.0303 (-2.57)	–
<i>Constant - class 3</i>	4.2543 (3.92)	–
<i>Season ticket ownership - class 3</i>	-1.7149 (-2.22)	–
<i>Number of cars in household - class 3</i>	1.8877 (3.01)	–
<i>Age - class 3</i>	-0.1059 (-3.83)	–
<i>Female - class 3</i>	-0.8211 (-1.16)	–
<i>Annual household income (£1,000) - class 3</i>	-0.0147 (-1.27)	–
<i>Constant - class 4</i>	3.7937 (3.59)	–
<i>Season ticket ownership - class 4</i>	-0.9634 (-1.49)	–
<i>Number of cars in household - class 4</i>	2.2705 (4.23)	–
<i>Age - class 4</i>	-0.0667 (-3.10)	–
<i>Female - class 4</i>	-1.3330 (-2.19)	–
<i>Annual household income (£1,000) - class 4</i>	-0.0180 (-1.69)	–
Clustering distance parameters		
<i>Distance multiplier γ - cluster 1</i>	–	0.7310 (3.23)
<i>Distance multiplier γ - cluster 2</i>	–	0.7254 (3.73)
<i>Distance multiplier γ - cluster 3</i>	–	0.3633 (1.69)
<i>Distance multiplier γ - cluster 4</i>	–	0.2274 (1.56)
<i>Distance multiplier γ - cluster 5</i>	–	1.0895 (5.09)
Class/cluster membership probabilities		
<i>Class/cluster 1</i>	0.43	0.19
<i>Class/cluster 2</i>	0.17	0.21
<i>Class/cluster 3</i>	0.10	0.18
<i>Class/cluster 4</i>	0.21	0.19
<i>Class/cluster 5</i>	0.09	0.23

Table 5.3: Estimated parameters of clustering covariates for the Yorkshire mode choice model

Parameters	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5
<i>Constant</i>	-0.0734 (-1.40)	0.9180 (17.04)	1.8914 (39.02)	0.9561 (22.49)	–
<i>Season ticket ownership</i>	0.0898 (2.89)	1.5482 (48.67)	0.1960 (6.85)	0.2493 (9.93)	–
<i>Number of cars</i>	0.3314 (14.27)	-0.1527 (-6.41)	-0.2246 (-10.48)	-0.0858 (-4.57)	–
<i>Age</i>	-0.0322 (-29.66)	-0.0409 (-36.76)	-0.0481 (-48.12)	-0.0391 (-44.63)	–
<i>Female</i>	0.1831 (6.67)	0.1927 (6.85)	-0.3479 (-13.75)	0.6190 (27.90)	–
<i>Annual household income</i>	0.0143 (28.24)	0.0030 (5.70)	0.0029 (4.24)	0.0023 (5.62)	–

As a further measure of validation, the estimated Values of Travel Time (VTT) are presented in *Table 5.4*. The VTT estimates from all models are close to the latest official values suggested by the Department for Transport (no official VTT estimates for taxi) (Batley et al., 2019) with the exception of *LCCM* resulting in significantly higher VTTs. The reason for the higher VTTs of *LCCM* is the low and non-statistically significant travel cost parameter for class 5, which increases the weighted average across all classes. That finding can act as a further supporting argument for considering the *H-LCCM* framework for real-world policy making, since it has the ability to lead to more behaviourally accurate valuation measures, at least in the current study.

Table 5.4: Values of Travel Time estimates (£/hr)

VTT estimate	MNL-base	C-MNL	LCCM	H-LCCM
<i>Car</i>	12.01	15.87	34.80	14.98
<i>Bus</i>	6.14	7.52	16.93	8.27
<i>Rail</i>	32.09	35.84	68.74	52.8
<i>Taxi</i>	82.11	122.81	198.33	120.54

4.2 Case study 2: Yorkshire shopping destination choice

4.2.1 Model specification

The specification of the models presented in the following is based on the size variable specification of Daly (1982) and more specifically of Kristoffersson et al. (2018). According to that, the attraction of a destination j is captured with the addition in the utility function of a composite term A_j inside a logarithmic function, i.e. $\log(A_j)$. The composite term A_j includes various variables aiming at capturing the attraction of the target destination j and their respective parameters, as $A_j = a_{1j} + \sum_{r>1} \exp(\gamma_r) a_{rj}$, where one attraction variable, a_{1j} , is defined as the base and its parameter is kept fixed to 1.0. The remaining attraction/size variables a_{rj} are estimated relative to the base one with parameters γ_r , which are usually specified as exponentials to guarantee their positive sign.

The final specification was able to uncover 2 latent classes/clusters of heterogeneous decision-makers using annual personal income and the areal measure of Index of Multiple Deprivation (IMD) calculated for a 400m buffer around home locations. The IMD is a composite measure developed by the Office for National Statistics (ONS) aimed to capture deprivation among a range of different domains, such as crime, environment and housing among others and at a high spatial resolution (Lower Super Output Areas). The IMD is calculated as a weighted measurement of the constituent deprivation domains with a higher number signifying a more deprived area. More details can be found at the IMD technical report in Smith et al. (2015). The IMD indices for the year 2015 were used in the current study.

4.2.2 Model outputs

The fit statistics for *Case study 2* are presented in Table 5.5. Capturing latent heterogeneity resulted again in model fit improvements compared to the *MNL-base*, even with the simpler *C-MNL* specification. A slightly better LL is achieved for *LCCM* compared to *H-LCCM* by only 0.742 LL units, but with one additional parameter. Therefore, *H-LCCM* presents a more efficient approach for capturing heterogeneity in that choice context, as shown by the fit statistics of adjusted ρ^2 , AIC and BIC.

The estimated parameters of *LCCM* and *H-LCCM* are detailed in Table 5.6. In that case, the estimates of the two specifications are almost identical with only negligible discrepancies. LOS variables were allowed to vary across classes capturing significant taste differences. Most of the remaining parameters, however, such as the size variables, the locational variables, the direction of travel etc. remained the same across classes either because they did not show any significant differences or because they led to numerical issues during estimation. The central shopping mall of Leeds, destination 1, was selected as the base alternative. The specified ASCs were grouped separately for the remaining destinations of the city centre, the remaining destinations of Leeds outside of the city centre and the destinations located in the remaining region of Yorkshire. Additional interactions were also specified for season ticket holders and individuals with no car in their household for the destinations outside the city centre and outside Leeds. The purpose of those interactions was to capture the additional

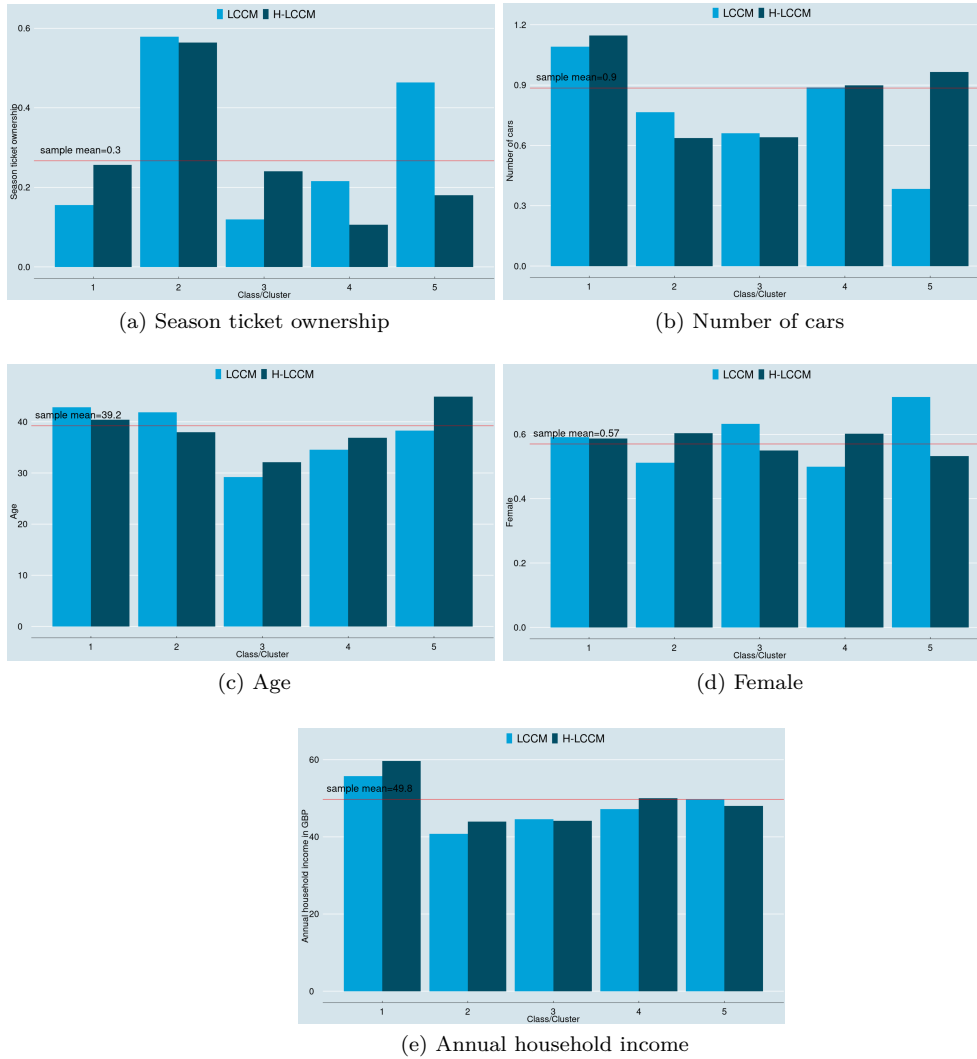


Figure 5.4: Class-specific average values of covariates across LCCM and H-LCCM for Yorkshire mode choice model

disutility of travelling to those places, which are located further away from the city centre with worse provision of PT infrastructure and without the convenience of a private vehicle. Significant non-linearities were captured for PT travel time, walking distance and travel cost sensitivities using a Box-Cox transformation, while only linear sensitivities were uncovered for car travel time. A similar Box-Cox transformation was also used for parking areas for car trips capturing significant non-linear sensitivities, as well.

The class allocation of *LCCM* resulted in a sample segmentation with 56% of the sample allocated in class 1 and 44% in class 2. Similarly, the clustering procedure of *H-LCCM* allocated individuals by 59% to class 1 and 41% to class 2. According to the estimated distance multipliers γ of *H-LCCM*, the individuals of cluster 1 are allocated with a higher probability to their class (66.6% to class 1 on average) compared to individuals of class 2 (58.0% to class 2 on average).

The small number of identified classes allows us to perform an easier behavioural profiling compared to the five classes of *Case study 1*. Overall, the insights derived from the covariates of the class allocation, presented in *Table 5.6*, and the linear regression on the log of shares

from clustering, depicted in *Table 5.7*, are in agreement with the sensitivities between the two classes/clusters. Individuals allocated into class/cluster 1 have a higher personal income (average personal income=£28,716 from *LCCM* and £27,836 from *H-LCCM*) and are living in less deprived areas (average home IMD=20.0 from *LCCM* and 20.2 from *H-LCCM*), while also showing higher time and distance and lower cost sensitivities. Furthermore, they show significant cost damping effects compared to class 2 and their cost sensitivity decreases as their personal income increases, although the latter was not statistically significant. Finally, those living in richer areas with higher house prices (4th quartile) are less willing to go shopping in poorer areas (1st quartile). On the contrary, individuals in class/cluster 2 are more likely to have a lower personal income (average personal income=£21,941 from *LCCM* and £22,778 from *H-LCCM*) and reside in more deprived areas (average home IMD=26.7 from *LCCM* and 26.8 from *H-LCCM*). They are characterised by higher cost and lower time and distance sensitivities, i.e. they are willing to travel further with cheaper modes probably to reach stores offering cheaper/more affordable products. Their sensitivities for travel time with PT further decreases as travel time increases as captured by the Box-Cox λ . In addition, individuals of class 2 living in areas of higher house prices show no significant taste variation for shopping in equally rich or poorer areas. The aforementioned comparison of the behavioural profiling of the estimated classes/clusters is also depicted in *Figure 5.5*.

Regarding the remaining generic parameters, the presence of major clothing, grocery and durable retailers -captured as elemental stores from OpenStreetMaps- increases the utility of the aggregate destination alternative for the respective shopping type trip (i.e. clothes, grocery, durables shopping). As expected, the presence of parking areas is a significant factor for car trips, but that utility is decreasing with the increase of parking spaces, as captured by the estimated λ parameter of the Box-Cox transformation. The directionality of travel is also an important factor with intermediate shopping destinations that require a significant deviation (above 90°) from the straight path between the previous origin and the following destination are less likely to be chosen compared to others.

An interesting finding is that individuals living in areas with a higher percentage of white residents (4th quartile) are less willing to go shopping at more racially diverse locations (1st quartile) relative to less diverse locations. On the contrary, individuals from more diverse locations show no significant taste variation for shopping at predominantly “white” locations, while they are more willing to go shopping in locations in the 2nd and 3rd quartile of white residents percentage. That finding together with the dispreference of individuals from richer neighbourhoods to shop in poorer areas hints to instances of economic and racial inequality in the region of Yorkshire, where wealth is not distributed equally across space and in fact it is distributed disproportionately in favour of the already affluent areas.

The multiplier of the composite log term for the size variables is significantly less than 1.0. According to Kristoffersson et al. (2018) that implies the existence of correlation among the elemental alternatives inside the aggregated destination alternatives, thus providing a behavioural meaning behind the alternative aggregation, in that case the implementation of HAC. The population in a 400m buffer around the shopping destinations was used as the base size variable. The remaining size variables, namely retail, grocery and durable shopping areas attract significantly more trips relative to the base size variable. Specifically, for the case of a consecutive shopping trip, the shopping variability of neighbouring locations at a distance of 1,000-2,000m (captured using Shannon’s entropy (Shannon, 1948)) also adds to the attraction of the target destination. This means that destinations closer to others with a variety of shopping stores are more likely to be chosen relative to more isolated ones, which also signifies that individuals are likely to have a pre-planned daily activity schedule.

Table 5.5: Fit statistics of the Yorkshire shopping destination choice models

Fit statistics	MNL-base	C-MNL	LCCM	H-LCCM
<i>Log-likelihood (0)</i>		-7,961.332		
<i>Log-likelihood (model)</i>	-3,369.363	-3,341.002	-3,310.953	-3,311.695
<i>Adjusted ρ^2</i>	0.5734	0.5736	0.5792	0.5793
<i>AIC</i>	6,792.73	6,790.004	6,699.91	6,699.39
<i>BIC</i>	6,936.91	7,078.374	6,908.17	6,902.32
<i>Number of parameters</i>	27	54	39	38
<i>Number of individuals</i>			270	
<i>Number of observations</i>			1,541	

Table 5.6: Modelling estimates of LCCM and H-LCCM models for the Yorkshire shopping destination choice context

Parameter	LCCM	H-LCCM
Alternative-specific constants		
<i>Constant Leeds city centre/destination 1 (base)</i>	-	-
<i>Constant Leeds city centre/remaining destinations - class 1</i>	-1.8618 (-7.66)	-1.8077 (-7.11)
<i>Constant Leeds city centre/remaining destinations - class 2</i>	-0.5778 (-2.12)	-0.5634 (-1.87)
<i>Constant Remaining Leeds</i>	-1.3988 (-6.65)	-1.4033 (-6.64)
<i>Constant Remaining Leeds shift for season ticket owners/no car ownership</i>	-0.8056 (-3.29)	-0.7994 (-3.27)
<i>Constant Remaining Yorkshire</i>	-0.7394 (-2.73)	-0.7467 (-2.76)
<i>Constant Remaining Yorkshire shift for season ticket owners/no car ownership</i>	-0.9537 (-2.25)	-0.9337 (-2.20)
LOS parameters		
<i>Travel time car,PT (mins) - class 1</i>	-0.1242 (-9.08)	-0.1227 (-8.87)
<i>Travel time car,PT (mins) - class 2</i>	-0.0922 (-2.40)	-0.0942 (-2.03)
<i>Box-Cox λ car</i>	1.0000 (-)	1.0000 (-)
<i>Box-Cox λ PT time - class 1</i>	0.8098 (11.63)	0.8095 (11.37)
<i>Box-Cox λ PT time - class 2</i>	0.0462 (1.23)	0.0483 (1.06)
<i>Walking distance (km) - class 1</i>	-2.2367 (-9.42)	-2.1877 (-8.20)
<i>Walking distance (km) - class 2</i>	-1.4802 (-10.37)	-1.4685 (-9.26)
<i>Box-Cox λ walking distance - class 1</i>	0.5958 (3.32)	0.6042 (3.60)
<i>Box-Cox λ walking distance - class 2</i>	0.8302 (6.34)	0.8382 (5.96)
<i>Travel cost (£) - class 1</i>	-0.2354 (-1.91)	-0.2607 (-2.05)
<i>Travel cost (£) - class 2</i>	-2.4754 (-4.72)	-2.5341 (-3.94)
<i>Box-Cox λ travel cost - class 1</i>	0.3811 (3.33)	0.4170 (4.15)
<i>Box-Cox λ travel cost - class 2</i>	0.8345 (9.73)	0.8330 (9.20)
<i>Personal income-cost elasticity - class 1</i>	-0.1861 (-0.48)	-0.3362 (-1.02)
<i>Personal income-cost elasticity - class 2</i>	0.1052 (1.34)	0.1162 (1.39)
Direction of travel		
<i>Presence of angle > 90° between O-S and O-D</i>	-0.4748 (-4.41)	-0.4743 (-4.40)
Locational variables		
<i>Living in areas with high house prices (quart.4)- shopping in areas with low house prices (quart.1) - class 1</i>	-1.2184 (-2.85)	-1.2538 (-2.86)
<i>Living in areas with high house prices (quart.4)- shopping in areas with low house prices (quart.1) - class 2</i>	0.3311 (0.84)	0.4017 (1.02)
<i>Living in areas with high % of whites (quart.4)- shopping in low % whites (quart.1)</i>	-0.5956 (-2.31)	-0.6012 (-2.33)
<i>Living in areas with low % of whites (quart.1)- shopping in medium % whites (quart.2-3)</i>	0.5762 (2.62)	0.5758 (2.63)
<i>Living in areas with low % of whites (quart.1) shopping in high % whites (quart.4)</i>	0.2761 (0.90)	0.2783 (0.91)
<i>Parking areas (400m buffer)</i>	0.1184 (4.29)	0.1177 (4.28)
<i>Box-Cox λ for parking areas (400m buffer)</i>	0.4350 (6.56)	0.4366 (6.58)

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4. Results

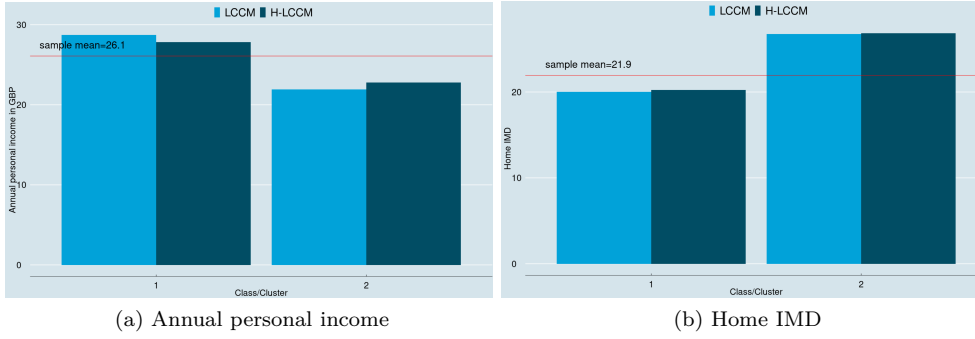


Figure 5.5: Class-specific average values of covariates across LCCM and H-LCCM for Yorkshire shopping destination choice model

Table 5.6 – continued from previous page

Parameter	LCCM	H-LCCM
<i>Major clothes shopping retailers (400m buffer)</i>	1.6041 (6.60)	1.5978 (6.59)
<i>Major grocery retailers (400m buffer)</i>	0.4516 (4.52)	0.4541 (4.54)
<i>Major durables retailers (400m buffer)</i>	2.1775 (2.96)	2.1696 (2.91)
Size variables		
<i>Natural logarithm multiplier ϕ</i>	0.5526 (7.04)	0.5545 (7.05)
<i>Population (400m buffer) (base)</i>	1.0000 (–)	1.0000 (–)
<i>Retail areas for clothes (400m buffer) (exp.)</i>	0.8992 (1.47)	0.8863 (1.46)
<i>Retail areas for groceries (400m buffer) (exp.)</i>	1.2434 (2.75)	1.2352 (2.73)
<i>Retail areas for durables (400m buffer) (exp.)</i>	0.8663 (1.08)	0.8605 (1.07)
<i>Shopping store variability when following trip purpose is shopping (1000-2000m buffer) (exp.)</i>	3.3918 (4.56)	3.3657 (4.53)
Class allocation parameters		
<i>Constant - class 1</i>	0.3114 (0.47)	–
<i>Annual personal income (£1,000) - class 1</i>	0.0285 (1.75)	–
<i>Home IMD - class 1</i>	-0.0332 (-1.99)	–
Clustering distance parameters		
<i>Distance multiplier γ - cluster 1</i>	–	0.6113 (3.27)
<i>Distance multiplier γ - cluster 2</i>	–	0.3013 (0.88)
Class/cluster membership probabilities		
<i>Class/cluster 1</i>	0.56	0.59
<i>Class/cluster 2</i>	0.44	0.41

Table 5.7: Estimated parameters of clustering covariates for the Yorkshire shopping destination choice model

Parameters	Cluster 1	Cluster 2
<i>Constant</i>	0.9779 (24.57)	–
<i>Annual personal income (£1,000)</i>	0.0068 (9.46)	–
<i>Home IMD</i>	-0.0350 (-33.74)	–

4.3 Case study 3: London mode choice

4.3.1 Model specification

Regarding the mode choice model for the London dataset, the *MNL-base* model follows the specification presented in Krueger et al. (2020) and Hancock et al. (2021). In addition to ASCs and interactions with socio-demographic (e.g. gender, number of cars, age etc.) and trip characteristics (e.g. month of the year), the utility function also includes generic in-vehicle travel time parameters for motorised modes (car, transit) and out-of-vehicle time for the access-egress segments of transit, cycling and walking. Moreover, there are parameters capturing the impact of traffic variability for car trips and the number of necessary transfers for transit trips. The specification of *LCCM* was able to identify two latent classes of individuals, while failing to identify a third class. The number of cars owned per household and the age of the individuals were used as covariates in the class allocation model in the absence of any measure of personal or household income. The same socio-demographics were also included in the class-specific mode choice models at the lower level with different parameters specified for each case, similar to the study of Calastri et al. (2018). The estimated parameters of each component will inform the analyst whether a specific socio-demographic attribute might be better at explaining the allocation of the individuals into the classes/clusters or their observed choices. An equivalent specification was also used for *C-MNL* and *H-LCCM* for evaluation purposes, similar to the previous case studies already discussed.

4.3.2 Model outputs

The fit statistics of the four specifications are depicted in *Table 5.8*, while the detailed estimated parameters of *LCCM* and *H-LCCM*, along with their robust t-ratios, are reported in *Table 5.9*. Overall the proposed specification is able to provide significant model fit improvements compared to *LCCM* with 460.15 LL units of improvement, while also having 1 parameter less. The remaining fit statistics of *H-LCCM* are also improved compared to *LCCM*. Besides the improvements in model fit, however, the advantages of our proposed methodology are more evident in the behavioural interpretation of the estimated classes/clusters (*Figure 5.6*). According to *LCCM*, class 1 is characterised by mostly older individuals (average age=44.6) with a lower than average number of cars in their households (average number of cars=0.89), while the opposite is true for class 2 including younger individuals (average age=39.1) with a higher than average number of cars in their possession (average number of cars=0.98). It is fair to say that the behavioural interpretation of the covariates of *LCCM* is not intuitive enough, since age and the number of cars were used as proxy measures of income. As such, our prior assumption was that older individuals would likely also be in the possession of more cars, relative to younger individuals, acting as a manifestation of an increased income accumulation over their lifetime.

Contrary to this, the clusters of *H-LCCM* represent a more intuitive behavioural profiling. First of all, based on the estimated distance multipliers γ , there is high certainty for allocating individuals into cluster 1 with a probability of 81.5% on average to belong to that cluster, while individuals of cluster 2 have an average probability of 61.4% to be allocated into cluster 2. Cluster 1 is more likely to include younger individuals (average age=38.9) with a lower than average number of cars (average number of cars=0.88), while older individuals (average age=44.7) with a higher than average number of cars (average number of cars=0.99) are more likely to be allocated into cluster 2. Individuals in cluster 1 are also more cost sensitive and less sensitive for in-vehicle car and transit time compared to individuals in cluster 2.

A range of willingness-to-pay (WTP) estimates, derived from the four specifications, are also presented in *Table 5.11*, specifically for in-vehicle travel times for car and transit, for out-of-vehicle times for transit, for traffic variability for car and for transit transfers. The values are similar across all models, but an interesting thing to note here is that *H-LCCM* results in higher WTP for IVTT relative to the rest and specifically compared to *LCCM*

4. Results

by around 5£/hr. Taking into account the VTTs for the Yorkshire mode choice model (see Table 5.4) and the inherently increased average income of London residents, which is subset by the increased cost of living, the higher VTT for IVTT of *H-LCCM* presented in Table 5.11 could be considered as a more accurate behavioural representation of the trade-offs that individuals in London are willing to make. From that Table, the ratio among OVT/IVT can also be calculated across the four specifications, which results in 2.09, 2.03, 2.32 and 1.40, respectively, indicating a lower estimated importance of OVT relative to IVT from the proposed H-LCCM model compared to the rest.

Table 5.8: Fit statistics of the London mode choice models

Fit statistics	MNL-base	C-MNL	LCCM	H-LCCM
<i>Log-likelihood (0)</i>		-81,214.67		
<i>Log-likelihood (model)</i>	-44,309.01	-43,854.73	-37,597.26	-37,137.11
<i>Adjusted ρ^2</i>	0.4542	0.4596	0.5366	0.5423
<i>AIC</i>	88,654.03	87,773.46	75,272.52	74,350.23
<i>BIC</i>	88,815.63	88,060.76	75,622.67	74,691.4
<i>Number of parameters</i>	18	32	39	38
<i>Number of individuals</i>			26,904	
<i>Number of observations</i>			58,584	

Table 5.9: Modelling estimates of LCCM and H-LCCM for the London mode choice context

Parameter	LCCM	H-LCCM
Alternative-specific constants		
<i>Constant Walking (base)</i>	-	-
<i>Constant Cycling - class 1</i>	-7.6354 (-7.05)	-7.7086 (-9.42)
<i>Shift Cycling for females - class 1</i>	-0.8494 (-0.75)	-7.1144 (-11.08)
<i>Shift Cycling for winter (November-March) - class 1</i>	1.1809 (0.91)	-1.5958 (-1.06)
<i>Shift Cycling for age below 18 or above 64 - class 1</i>	-9.5609 (-12.94)	-0.1846 (-0.14)
<i>Constant Cycling - class 2</i>	-3.2261 (-32.62)	-1.6507 (-11.51)
<i>Shift Cycling for females - class 2</i>	-1.1075 (-11.09)	-1.0203 (-6.50)
<i>Shift Cycling for winter (November-March) - class 2</i>	-0.3090 (-3.47)	-0.3227 (-3.80)
<i>Shift Cycling for age below 18 or above 64 - class 2</i>	-0.6358 (-4.16)	-1.3231 (-5.18)
<i>Constant Transit - class 1</i>	-1.7203 (-13.24)	-2.0758 (-11.47)
<i>Shift Transit for females - class 1</i>	0.3339 (2.50)	0.3186 (4.58)
<i>Shift Transit for age below 18 - class 1</i>	-0.7387 (-0.81)	0.2925 (1.56)
<i>Shift Transit for age above 64 - class 1</i>	0.9919 (5.27)	0.6414 (5.96)
<i>Constant Transit - class 2</i>	-2.2070 (-26.06)	-1.9745 (-11.05)
<i>Shift Transit for females - class 2</i>	0.2583 (3.68)	0.3881 (2.35)
<i>Shift Transit for age below 18 - class 2</i>	0.7975 (3.13)	0.1651 (0.49)
<i>Shift Transit for age above 64 - class 2</i>	0.4306 (4.18)	-0.0379 (-0.15)
<i>Constant Car - class 1</i>	-4.7424 (-18.60)	-6.3640 (-9.91)
<i>Shift Car for females - class 1</i>	0.4735 (3.19)	0.4468 (2.58)
<i>Shift Car for age below 18 - class 1</i>	-1.5875 (-2.57)	-1.7334 (-4.46)
<i>Shift Car for age above 64 - class 1</i>	1.5389 (6.49)	0.6141 (2.29)
<i>Shift Car for car ownership - class 1</i>	4.3621 (29.95)	1.6926 (13.46)
<i>Constant Car - class 2</i>	-5.8963 (-27.31)	-0.6286 (-2.28)
<i>Shift Car for females - class 2</i>	0.3270 (3.42)	0.0701 (0.51)
<i>Shift Car for age below 18 - class 2</i>	-0.7333 (-3.10)	-1.6307 (-6.19)
<i>Shift Car for age above 64 - class 2</i>	-0.1673 (-1.18)	0.1112 (0.58)
<i>Shift Car for car ownership - class 2</i>	2.1917 (23.02)	1.2616 (16.38)
LOS parameters		
<i>Travel cost (£) - class 1</i>	-0.2757 (-13.36)	-0.5484 (-7.07)
<i>Travel cost (£) - class 2</i>	-0.3607 (-11.30)	-0.1891 (-16.67)

Continued on next page

Table 5.9 – continued from previous page

Parameter	LCCM	H-LCCM
<i>Out-of-vehicle travel time for walking, cycling and transit (hrs) - class 1</i>	-13.3327 (-30.10)	-10.1507 (-7.57)
<i>Out-of-vehicle travel time for walking, cycling and transit (hrs) - class 2</i>	-7.1890 (-37.46)	-7.5145 (-5.02)
<i>In-vehicle travel time for transit and car (hrs) - class 1</i>	-6.0404 (-15.92)	-3.6914 (-5.90)
<i>In-vehicle travel time for transit and car (hrs) - class 2</i>	-2.6818 (-13.46)	-6.6554 (-4.90)
<i>Traffic variability for car - class 1</i>	-3.3284 (-13.21)	-7.5255 (-11.31)
<i>Traffic variability for car - class 2</i>	-5.5894 (-20.00)	-2.8760 (-13.69)
<i>Number of transfers for transit - class 1</i>	-0.4640 (-5.79)	-0.3665 (-2.97)
<i>Number of transfers for transit - class 2</i>	-0.0620 (-1.02)	-0.0267 (-0.24)
Class allocation parameters		
<i>Constant - class 1</i>	-0.4306 (-4.53)	–
<i>Number of cars - class 1</i>	-0.1861 (-3.36)	–
<i>Age - class 1</i>	0.0173 (14.71)	–
Clustering distance parameters		
<i>Distance multiplier γ - class 1</i>	–	1.2584 (21.65)
<i>Distance multiplier γ - class 2</i>	–	0.4785 (9.80)
Class/cluster membership probabilities		
<i>Class/cluster 1</i>	0.53	0.52
<i>Class/cluster 2</i>	0.47	0.48

Table 5.10: Estimated parameters of clustering covariates for the London mode choice model

Parameters	Cluster 1	Cluster 2
<i>Constant</i>	1.4311 (208.5)	–
<i>Number of cars</i>	-1.1826 (-347.7)	–
<i>Age</i>	-0.0039 (-28.0)	–

Table 5.11: Willingness-to-pay estimates (£/hr) for the London dataset

WTP estimate	MNL-base	C-MNL	LCCM	H-LCCM
<i>IVTT for Car, Transit</i>	17.28	16.93	15.10	20.54
<i>OVTT Transit</i>	36.08	34.38	34.98	28.80
<i>Car traffic variability</i>	19.00	17.54	13.68	14.44
<i>Transit transfers</i>	0.28	0.31	0.97	0.41

5 Conclusions

The current study showcased the integration of a ML clustering algorithm into a state-of-the-art econometric framework for the purpose of capturing individual heterogeneity in the sample. The novelty of our approach compared to existing studies in the literature is the transformation of a deterministic clustering algorithm into a probabilistic one in order to effectively take the role of a class allocation model. The same methodology developed can also be applied to different and more advanced deterministic clustering approaches and using different distance measures, as well. Furthermore, the same framework and its fundamental principles can be used to accommodate unconventional data, such as text, in the

5. Conclusions

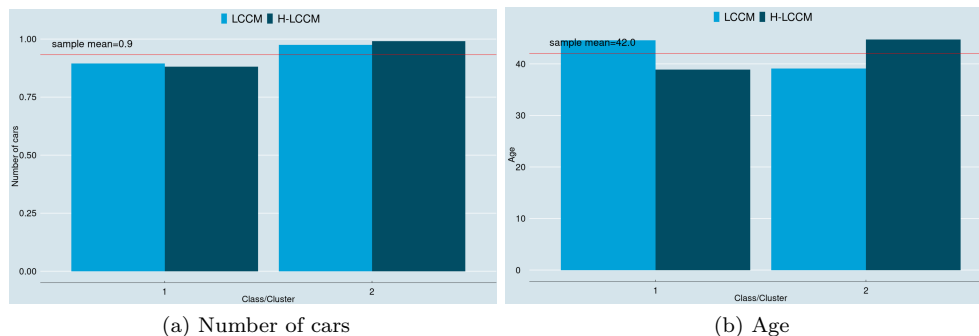


Figure 5.6: Class-specific average values of covariates across LCCM and H-LCCM for the London mode choice model

clustering/class allocation part of the model, as long as those types of data can be decoded in a lower dimensionality representation as numeric vectors.

From all case studies analysed, the proposed methodology is able to achieve at worst comparable results with the traditional econometric specification in terms of model fit. More benefits were achieved with larger samples including more individuals and trips (*Case studies 1, 3*) indicating that an ML algorithm might excel at identifying more complex patterns with more data. In terms of behavioural interpretation, however, it was possible to achieve more intuitive clustering profilings and WTP estimates compared to the traditional econometric model in all of the case studies.

The proposed methodology is subject of course to certain limitations, the most important of which being the centroid initialisation process. The estimation is highly dependent on the initial centroid that is randomly selected, and under the K-means++ initialisation process, that initial centroid forms the basis for the selection of the remaining centroids, as well. Prior assumptions regarding the signs of the scaled clustering variables can help to reach a better final LL, but it is difficult to have any meaningful a priori sign directionality assumptions in the presence of a large number of classes/clusters, such as in *Case study 1*.

The current study aims to build on the increasing literature focusing on the integration of ML and DCM. As illustrated in the case studies presented, there are additional benefits to be achieved by incorporating an ML algorithm into a DCM framework. That approach is able to take the best of both worlds by using ML for identifying patterns in the data more effectively, while also allowing the choice process to be modelled by a DCM, thus providing valuation measures, which are important for policy making. More studies are expected to take these approaches even further as the ML-DCM literature keeps developing.

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Chapter 6

Probabilistic choice set formation incorporating activity spaces into the context of mode and destination choice modelling

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Abstract

Understanding the constraints that individuals face during their spatial choices is important from a policy perspective. Such constraints, however, are often overlooked in the choice set generation process during model development. In order to address that gap, the current study proposes a probabilistic choice set formation based on Manski's framework assuming that the actual choice set of an individual is latent (unobserved). Though latent class models with heterogeneous choice sets have been used previously in the context of mode and route choice, their application in the context of spatial choices have been hindered due to the inherently large choice sets making the problem computationally intractable. To address this issue, we propose to computationally simplify the problem by utilising the geography-derived notions of Activity Spaces to delineate a range of potential choice sets per individual helping us to capture both issues of spatial awareness and time-space constraints. In order to account for the latent nature of the true choice set, we propose a Latent Class Choice Modelling (LCCM) framework to allocate the individuals probabilistically into the different resulting choice sets, with each class having a different choice set and a different set of parameters. Thus the LCCM is able to capture heterogeneity in the choice sets and in the sensitivities, at the same time. The proposed LCCM framework is empirically tested on joint mode and shopping destination choices captured through a GPS smartphone application. It is compared to a base MNL model estimated on the global choice set, an LCCM capturing heterogeneity only in the sensitivities and a LCCM with latent consideration choice sets, similarly to the proposed model, but with generic parameters across classes. Our proposed specification is able to outperform all of the remaining models, while also providing insights on the factors affecting individuals to be constrained in their location choices across space hinting to cases of spatial cognition, the importance of the home and workplace geography and the individual's socio-economic status.

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Such insights can be important for developing more behaviourally realistic models that can be used by planners and policy makers to formulate more effective measures that better relate to the underlying population. Furthermore, the analysis provides insights into the discrepancies that can emerge by accounting for latent consideration sets in willingness-to-pay measures and demand elasticities, which could have significant implications in the effectiveness of policy measures.

1 Introduction

Individuals face constraints during their decision making process. In the context of daily mobility choices, those constraints can refer to either time-space constraints and/or limited spatial awareness, among others. Time-space constraints can arise from the need to participate in specific activities in specific locations and for specific durations, i.e. travel to workplace and stay there for a duration of 8 hours, which limits the ability of the individuals to equally evaluate every possible location for shopping and other discretionary activities before, during or after working hours. On the other hand, spatial awareness or the lack of it could be caused as a result of the regularity of daily mobility patterns, which reinforces travelling within the already familiar geographical space.

Despite being often overlooked, it is important from a policy perspective to uncover those latent constraints from the data for the purpose of proposing more effective policy measures suitable for addressing the needs and intricacies of the underlying population. Furthermore, there is value in understanding the influence of various socio-demographic characteristics in the formation of those constraints or phrase it in a different way, identifying what could be the most likely characteristics of the individuals facing each specific constraint. An example of the derived value from such an analysis, could be the identification of instances of social exclusion (Schönfelder and Axhausen, 2003) or the potential presence of very restrictive space-time constraints that prevent individuals from exploring a wider range of alternatives for their daily choices.

Discrete choice modelling (DCM) has been an important tool for policy making since the seminal work of McFadden (1973) and the development of the Multinomial Logit (MNL) model for understanding individual mobility behaviour. The MNL model has a strong grounding on microeconomic theory postulating that individuals will choose the alternative that maximises their utility for a specific choice task among a set of alternatives, also known as the choice set. Traditionally, a DCM is estimated under the assumption that individuals will consider and equally evaluate all alternatives in the choice set. There have been attempts, however, aiming to relax that assumption acknowledging the fact that not only all alternatives might not be available to all individuals, such as making a car trip for individuals with no car access in their household, but they might also not be considered by everyone, as well, such as making a large distance trip by walking or choosing to go for shopping in a store that is unknown to the individual. Assigning an unrealistic choice set for model estimation is yet another case of model misspecification as noted in Williams and Ortuzar (1982), who emphasised the potential adverse effects arising from that, such as biased estimates and incorrect choice probabilities. Gaudry and Dagenais (1979) demonstrated that accounting for *captive* decision makers (individuals who choose only a specific alternative) will have a significant impact on the estimated market shares. Li et al. (2015) have also showed the potential biased welfare measures that could be caused as a result from a choice set misspecification on simulated data.

Several studies mainly originating from consumer behaviour research have suggested that decision makers utilise heuristic processes to segment the alternatives into a range of cognitive subsets, unobserved to the analyst. According to Punj and Srinivasan (1989), the global choice set, i.e. all alternatives of the case study, such as transport modes for a mode choice model or activity locations for a destination choice model, can be decomposed to two different

subsets, an *awareness* and a *consideration* set (Howard and Sheth, 1969; Wright and Barbour, 1977; Pagliara and Timmermans, 2009; Capurso et al., 2019). Awareness set is a subset of the global choice set, which includes the alternatives the individuals are aware of due to various reasons, such as past experience, familiarity, word of mouth etc. The consideration set is a subset of the awareness set and it is the final set of feasible alternatives that the individuals actually evaluate during their decision making process. In a spatial context, the respective terms of spatial information fields and spatial usage fields have been proposed by Potter (1979). As such, spatial information fields contain the activity locations the individual is aware of (awareness set), regardless if she has ever travelled to those places, while spatial usage fields are a subset of the former containing the locations that have been visited and are actively considered by the individual for conducting her activities (consideration set) (Timmermans et al., 1982). Therefore, there have been studies in the literature suggesting that choice models should be estimated using the consideration set instead of the common practice of simply using the global choice set.

Several approaches have been proposed over the years for defining alternative availability/consideration. A usual approach is the availability to be exogenously defined using deterministic thresholds based on the analyst’s assumptions and the observations in the data, e.g. walking is not considered for trips of distances above the maximum observed walking distance in the data (Calastri et al., 2018; Hasnine et al., 2018; Tsoleridis et al., 2022). A tour-based approach has also been proposed to account for feasible constraints in terms of mode availability, such as the need for a driver to return her car back home at the end of the tour (Tsoleridis et al., 2022). Contrary to that, a behaviourally richer framework was proposed by Manski (1977) suggesting that the probability of individual n choosing alternative i from a consideration choice set C can be decomposed into a probability of choice set C being the actual choice set considered and a probability of choosing alternative i conditional on belonging in the consideration set C from a set of S possible non-empty choice sets, as shown in *Equation 6.1*.

$$P_{in}(C) = \sum_{s=1}^S P_n(i|C_s)P(C_s) \quad (6.1)$$

Manski’s framework requires a complete enumeration of all possible combinations of alternatives forming potential S non-empty choice sets. That number of combinations increases rapidly with the number of alternatives J , as $2^J - 1$, making this approach computationally infeasible for choice contexts with a large number of alternatives, such as in a spatial choice model. In fact, several implementations of Manski’s probabilistic choice set formation have been performed, but the vast majority of them is limited in a mode choice context (Swait and Ben-Akiva, 1987; Ben-Akiva and Boccara, 1995; Calastri et al., 2018; Capurso et al., 2019), which generally offers tractable and well-defined choice sets. To simplify the problem, deterministic availability of alternatives can be initially defined in terms of their feasibility. Examples include, defining car as unavailable for individuals with no car in their household in the context of mode choice or excluding routes involving detours above a certain threshold from the habitual route in the context of route choice. Probabilistic availability can thus be incorporated only to previously defined feasible alternatives to account for the uncertainty of the analyst, such as the maximum distance for walking to be considered as an alternative (Swait and Ben-Akiva, 1986) or the spatio-temporal constraints associated with the route choice (Kaplan and Prato, 2012).

One of the first operational implementations of Manski’s framework was the logit captivity model of Swait and Ben-Akiva (1986), who proposed a probabilistic choice set generation framework to account for captive decision makers on mode choice for commuting trips. That specification presents a simplified version of a probabilistic choice set generation model in which the number of non empty choice sets is restricted to choice sets of only one alternative (captive individuals) and choice sets including all feasible alternatives (individuals free to

choose). That study also laid the foundations for the more general Independent Availability Logit (IAL) model proposed in Swait and Ben-Akiva (1987) assuming that the inclusion of one alternative in the choice set is independent of the remaining alternatives, a necessary assumption to make the specification computationally tractable.

Several attempts were made over the years to approximate Manski's framework, while also relaxing its computational complexity, such as the Implicit Availability/Perception model of Cascetta and Papola (2001) and the Constrained Multinomial Logit (CMNL) model Martinez et al. (2009) incorporating additional terms in the utility function to capture latent constraints. Specifically, the CMNL model includes penalties in the utility function for alternatives exceeding certain attribute thresholds. Despite the authors suggesting that their approach is an approximation of Manski's model, Bierlaire et al. (2010) highlighted some limitations of the CMNL as its inability to produce unbiased estimates on simulated data, contrary to the IAL specification of Swait and Ben-Akiva (1987). Similar conclusions were derived from the study of Li et al. (2015), as well, regarding the comparison of CMNL and IAL models. In the same study, the authors also showed that models capable of uncovering taste heterogeneity, such as MNL models with socio-demographic interactions, mixed Logit or Latent Class Choice Models, will also produce biased estimates and welfare measures, since the choice set formation process is confounded in the sensitivity heterogeneity that is being captured. More specifically, the authors demonstrated -using simulated data- that the IAL specification is the only one capable of producing unbiased estimates in the presence of a latent price threshold.

Consideration of alternatives was traditionally understood by asking additional information to the decision makers (Ben-Akiva and Boccara, 1995; Kaplan and Prato, 2012). A prominent example in the literature is the study of Ben-Akiva and Boccara (1995), in which answers to relevant questions were used as indicators for defining latent variables regarding the consideration of alternatives. Nonetheless, with passively or even semi-passively collected Revealed Preference (RP) data, such as a GPS-based trip diary, only the observed choice is known without having any additional information on the non-chosen alternatives and the reasons for not choosing them. Hence only assumptions can be made about the extent of the considered choice set and the non-chosen alternatives belonging to that. A relevant example can be found in the study of Calastri et al. (2018), where the authors utilised a GPS dataset to specify a Latent Class Choice Model for mode choice with a range of classes adhering to specific combinations of mode alternatives

Contrary to the examples presented so far, a spatial choice model and more specifically a destination choice model of discretionary activities, e.g. shopping, is characterised by large choice sets, which could be comprised of traffic analysis zones or geographic zones (e.g. Middle Super Output Areas - MSOAs), general shopping areas, shopping malls or even specific parcels and stores depending on the level of spatial granularity offered by the utilised dataset and the level of detail required by the analyst. Sampling of alternatives has been proposed as a method suitable for reducing the computational complexity for choice models with large choice sets (Guevara and M. Ben-Akiva, 2013a; Guevara and M. Ben-Akiva, 2013b; Tsoleridis et al., 2021). Besides the computational advantages, however, sampling of alternatives does not account for the latent consideration of alternatives during the decision making process. Therefore, in order to account for the potential presence of latent choice set formation mechanisms in a spatial context, certain simplifications might be necessary to make the problem computationally tractable. To the best of our knowledge, only the study of Thill and Horowitz (1997b) has attempted to develop a probabilistic choice set formation specification for a spatial choice model first using simulated data and then applied on the real-world context of shopping destinations for home-based trips (Thill and Horowitz, 1997a). Their approach relies on the notion that individuals have to make destination choices, while being subject to latent time constraints, therefore the set of destinations under consideration will depend on each individual's time budget. The simplification applied in that study, relative to the IAL specification of Swait and Ben-Akiva (1987), is that individuals are probabilistically allocated into a finite number of exogenously defined time thresholds as concentric circles from

their home locations within which reachable destinations form the respective consideration sets. Their specification which is effectively an LCCM specification –although not stated as such– is able to outperform a base unconstrained MNL model. Nonetheless, it is also worth mentioning that the specification of Thill and Horowitz (1997a) does not account for differences in sensitivities across classes, thus having the possibility of confounding the presence of latent choice set formation constraints with individual unobserved heterogeneity. Furthermore, no additional covariates were used in the allocation of individuals to the specified time thresholds limiting our ability to link latent constraints with specific sociodemographic attributes that could lead to better informed policy measures.

In the current study, we follow a similar approach to Thill and Horowitz (1997a), but we differ our utilised proxy measures of latent constraints by considering the coexistence of spatial awareness/cognition and space-time constraints. The geography-derived notions of Activity Spaces (Hagerstrand, 1970) in the form of detour ellipses (Justen et al., 2013; Leite Mariante et al., 2018; Tsoleridis et al., 2021) and standard deviational ellipses (Brown and Moore, 1970; Horton and Reynolds, 1970; Horton and Reynolds, 1971; Yuill, 1971; Schönfelder and Axhausen, 2003; Schönfelder and Axhausen, 2004; Schönfelder and Axhausen, 2010; Manley, 2016) are utilised to define proxy measures of trip-specific space-time and individual-specific spatial awareness/cognition constraints, respectively. Our proposed specification, is compared against a base MNL model estimated using a choice set of feasible alternatives based on logical checks and deterministic exogenous thresholds and a base LCCM specification estimated again using the same choice set and capturing heterogeneity on the sensitivities across classes. Contrary to that base LCCM, our approach is capturing heterogeneity both in the sensitivities and the consideration choice sets at the same time. More specifically, our proposed specification includes three classes each with its own choice set. The choice set of *class a* includes alternatives within the estimated detour ellipses adhering to trip-specific space-time constraints. The choice set of *class b* includes alternatives, within both the estimated detour ellipses as before, but also within the individual-specific standard deviational ellipses thus capturing additional spatial cognitive constraints of the individuals. Finally, *class c* has the same choice set as the base MNL and the base LCCM models including all feasible alternatives, thus representing individuals that do not face any of the two aforementioned latent constraints. In addition, each of the three classes has a range of class-specific parameters to avoid confounding unobserved heterogeneity among individuals with the presence of latent choice set formation mechanisms, while also sociodemographic attributes are used to assist the allocation of individuals to each class, thus addressing some of the limitations identified in the work of Thill and Horowitz (1997a). An equivalent LCCM specification with different choice sets, but with generic parameters across classes and only constants in the class allocation, is also utilised for comparison purposes and to highlight the discrepancies in the two approaches.

According to the description above, the proposed specification is a similar case to the logit captivity model of Swait and Ben-Akiva (1986), where individuals are either captive to their space-time constraints, their spatial awareness or are free to choose from all the range of available and feasible alternatives being more inclined to explore the space around them. The proposed approach is empirically tested on a joint mode-destination choice model of shopping activities utilising a 2-week GPS trip diary. The model’s objective is to jointly capture individual behaviour regarding the choice of an intermediate shopping location, as well as the modes of the two trip legs travelling to and from that location. The results suggest that our proposed LCCM framework is capable of uncovering significant latent constraints, which also leads to significant model fit improvements compared to the base LCCM specification. More importantly, however, a specification like that is able to shed light into the types of individuals that are more likely to face certain latent constraints during their daily decision making process, thus deriving valuable insights for more effective policy measures able to account for those constraints.

The remainder of the paper is as follows. In the second chapter, a description of the different forms of activity spaces is performed. In the third chapter, the methodological

frameworks of the proposed model specifications are thoroughly explained, while in the following chapter the data used in the practical application is described. In the fifth chapter, the modelling outputs and their interpretation are highlighted. Finally, in the last chapter the conclusions and limitations of the study are summarised and recommendations for future research are suggested.

2 Forms of Activity Spaces

The notions of Activity Spaces (AS) originate from the fields of time-space (Hagerstrand, 1970) and behavioural geography (Brown and Moore, 1970; Horton and Reynolds, 1970; Yuill, 1971) and they have been studied extensively in different heterogeneous research areas since their inception with an emphasis on understanding when and where activity participation occurs and identify potential reachable opportunities given the remaining time budget (Schönfelder and Axhausen, 2004; Schönfelder, 2006; Schönfelder and Axhausen, 2010; Kamruzzaman and Hine, 2012; Lam et al., 2018). They are mainly used as a measure of describing the spatial distribution of visited locations and they incorporate a notion of individual spatial awareness (Manley, 2016) by providing invaluable information about the exposure to specific locations and activities that individuals might perform based on their usual mobility patterns and their time-space constraints. Due to the vast range of studies and application domains, there are several different forms of AS proposed in the literature depending on the aspect under examination in each case and the level of analysis. In a systematic review, Smith et al. (2019) summarised the different AS forms, which among others (such as convex hulls, daily path areas, kernel densities, interpolation etc.), include the following:

- Ellipses formed around two fixed points of a specific trip chain, labelled here as *Detour Ellipses (DEs)*
- Ellipses formed around the observed trips of an individual during a survey period, most commonly known as *Standard Deviatonal Ellipses (SDEs)*

In order to produce generalised results, representative of the sample in our dataset, we refrained from using the observed Activity Spaces of both forms, Detour Ellipses and Standard Deviatonal Ellipses, and used estimated Activity Spaces instead as proxy measures of latent constraints entering our behavioural specifications. To accomplish that, we estimate a range of continuous regression models using specific structural components of the Activity Space as dependent variables.

2.1 Detour Ellipse

The first type of ellipse utilised in this study aims to capture the reachable destinations based on trip and individual characteristics and the location of the following activity. Several approaches have been proposed in the literature to define what is commonly known as Potential Path Areas (PPAs) based on Hagerstrand (1970) work on time-space geography. Those approaches typically take into account the available net time between the fixed activity locations and an average travel speed (Kamruzzaman and Hine, 2012) or real network travel times based on the time of day in more advanced cases (Miller, 1991) to identify the intermediate locations that are potentially reachable within those time budgets (Lam et al., 2018). A slightly different approach is taken in the current study, where we propose the use of Detour Ellipses between fixed locations to capture the intermediate reachable areas. A Detour Ellipse (DE) is a type of an ellipse formed around two fixed locations, the foci of the ellipse, which are also referred to as ‘pegs’. More specifically, a DE is based on the Detour Factor (DF) defined as the ratio of the sum of the distances between O (previous origin)- S (shopping destination) and S (shopping destination)- D (next destination) over the

distance between O - D , as defined in *Equation 6.2* (Justen et al., 2013). In other words, a DF measures the deviation that an individual is willing to make to reach an intermediate shopping location S between the O - D (Leite Mariante et al., 2018) and it serves as a measure of spatial dependence among destinations in a trip/activity chain. It is also clear that $DF \geq 1$ should always hold in cases where O and D are different.

$$DF = \frac{l_{OS} + l_{SD}}{l_{OD}} \quad (6.2)$$

Previous studies have used fixed DFs for intermediate locations to be considered along observed O - D paths (Cascetta and Papola, 2009). Such an example is presented in the study of Newsome et al. (1998), who defined DEs based on the furthest visited intermediate location between fixed home and work locations. That approach, however, fails to take into account the influence of the total OD distance on the resulting DF, as it can be easily understood that longer OD paths will lead to smaller DFs due to the presence of time constraints for reaching both the intermediate and the following location D . That means that the longer the OD path the smaller the time budget available to the individuals to deviate further away from that path. That relation between DF and OD distance has been taken into consideration in Justen et al. (2013), although their approach is limited by the fact that only average values per DF percentile are considered, while trip-specific and sociodemographic attributes that could have an impact on the formation of DEs have not been taken into account.

In the current study, we make a distinction between trip chains with an intermediate shopping location S between an initial origin O and a following destination D , referred to as OSD , and simple tours in which individuals travel for shopping to a location S and then return back to their origin O , referred to as OSO trip chains in the remainder of the paper. The detour factors of OSD trip chains are always greater than 1.0 and they are exactly equal to 1.0 only in the extreme case of choosing a shopping location S directly on top of the OD path. Therefore, the estimated detour factors from that model will need to adhere to that restriction. In order to accomplish that, the dependent variable, in that case the observed detour factors, are transformed accordingly as $y_i - 1$ and are assumed to follow a log-normal distribution to ensure the estimation of strictly positive values, as shown in *Equation 6.3*.

$$\log(y_i - 1) = \Sigma b_{x_i} x_i + \sigma \quad (6.3)$$

where x_i is a vector of mode-specific, trip-specific (including the straight OD distance), locational and sociodemographic explanatory variables and b_{x_i} are the respective parameters to be estimated. The disturbance term for the log-transformed DF is assumed to follow a normal distribution with $N(0, \sigma)$, where σ is the standard deviation that is estimated alongside the rest of the parameters

For OSO trip chains, a different modelling approach was developed by using the straight distance to the shopping location S as the dependent variable and use it to define the estimated radius of a circle from the respective O . In that case as well, in order to ensure only positive estimated values, the dependent variable is assumed to follow a log-normal distribution. As a result, the modelling formulation of *Equation 6.4* is proposed, where y_i is the observed straight OS distance and as previously x_i is a vector of mode-specific, trip-specific, locational and sociodemographic explanatory variables and b_{x_i} is a vector of parameters to be estimated.

$$\log(y_i) = \Sigma b_{x_i} x_i \quad (6.4)$$

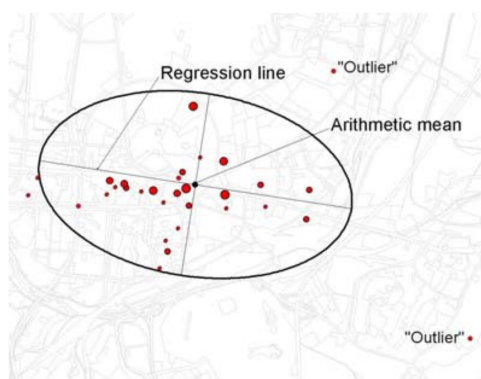


Figure 6.1: Weighted standard deviational ellipse around observed/visited destinations (Schönfelder, 2003)

2.2 Standard Deviational Ellipse

The second type of Activity Space aims to capture the spatial awareness of the participants. The Standard Deviational Ellipse (SDE) is proposed for that purpose, which originates from the fields of behavioural and social geography (Brown and Moore, 1970; Horton and Reynolds, 1970; Yuill, 1971). The SDE captures the spatial dispersion of the visited locations (observed latitude/longitude coordinates) of an individual and has been proposed as a measure of capturing the exposure to opportunities as a consequence of daily activities (Horton and Reynolds, 1971). In that sense, a SDE provides additional information on the individual awareness of certain destinations, that the Detour Ellipse and other forms of Potential Path Areas are not able to provide. Activity spaces formed by SDEs are considered a subset of a larger latent *awareness space* (Brown and Moore, 1970; Patterson and Farber, 2015) or *spatial information field* (Potter, 1979) suggesting that individuals would likely possess spatial knowledge that far exceeds the SDE formed around the observed destinations due to word of mouth and the usually limited durations of surveys.

An SDE is generally considered the two-dimensional equivalence of a standard 95% confidence interval. The mathematical process of defining an SDE, as described in Yuill (1971), involves the calculation of the covariance matrix of the latitude/longitude coordinates and the calculation of the rotation matrix leading to the final definition of the ellipse's perimeter (Tsoleridis et al., 2021). In (Figure 6.1) the main components of an SDE are depicted, such as the ellipse's major axis indicating the axis of major dispersion, which can also be considered as the regression line of latitude/longitude coordinates, the ellipse's orientation capturing the slope of the regression and the sign of the correlation sign among the coordinates and finally the arithmetic mean or else the centroid of the ellipse capturing the centre of gravity of the individual's usual movements (Schönfelder, 2003). Destinations that are outside of an SDE are considered *outliers* relative to the usual movement areas of an individual.

Several measures can be extracted from a SDE that describe the mobility patterns of an individual, such as its shape (minor to major axis ratio), size (area, number of polygons located within etc.), orientation and eccentricity (Yuill, 1971). An ellipse is a generalised form of a circle with one axis (major axis) more elongated than the other (minor axis). In the case of a very small minor axis close to 0, the ellipse resembles a straight line, while in the case of equal axes the ellipse takes the form of a circle. The ratio of minor/major axis, $\frac{b}{a}$, can provide an initial indication of time constraints or spatial exploration. For instance, an ellipse with a small $\frac{b}{a}$ can characterise a person with significant time constraints that does not have the freedom or the willingness to roam around, and the opposite can be said for an ellipse resembling with $\frac{b}{a}$ close to 1.0 resembling a circle.

Temporal factors and individual sociodemographic characteristics can also be taken

into account, such as examining weekday/weekend differences on the stability of SDEs among full-time and parti-time workers (Srivastava and Schoenfelder, 2003; Smith et al., 2019). Time also plays an important role in the evolution of the Activity Spaces providing opportunities to the individuals for more spatial search and exposure to the surrounding area, thus increasing their spatial cognition. SDEs might stabilise after a certain period of time, but significant longitudinal data will be required in order to capture that. Schönfelder (2006) used longitudinal data from traditional trip diaries to study the impact of time on the formation of activity spaces (SDEs). He concludes that, in general, datasets of longer durations (around 6 weeks) than the common ones (1-2 weeks) are necessary for SDEs to reach stability. That finding, however, could be different for emerging data sources, such as GPS trip diaries, which generally offer a more comprehensive depiction of individual mobility behaviour by capturing a higher number of smaller trips during the day.

In order to reconstruct estimated SDEs per individual we need to estimate a range of models referring to several important structural components of an SDE (see *Figure 6.1*). Specifically, we need to estimate the distance $dist_{hc}$ and the angle θ_{hc} between the home location h and the ellipse centroid c , the orientation θ_{sde} and the total area of the ellipse A_{sde} , as well as the shape of the ellipse defined as the ratio between the small and large axis ($\frac{b_{sde}}{a_{sde}}$). Therefore, five continuous models have been developed, in total, to assist with the reconstruction of estimated activity spaces. From the estimated distance $dist_{hc}$ and angle θ_{hc} , the centroid of the estimated confidence ellipse per individual can be defined. Following that, we are using the estimated minor/major axis ratio and the estimated area to define the shape of the ellipse and finally the estimated orientation of the ellipse to complete its mapping over space.

The models for $dist_{hc}$ and A_{sde} are specified as linear regression models with log-normally distributed dependent variables similarly to the *OSO* model previously described in *Equation 6.4*. To estimate the models referring to the angles, i.e. for the angle between home-centroid θ_{hc} and the ellipse orientation θ_{sde} , the predicted values had to be restricted between $0^\circ - 360^\circ$. In order to achieve that, the dependent variables were scaled between 0-1 by dividing them with 360. Then the scaled angles were used as the dependent variables in beta regression models. Beta regression is a type of model suitable for modelling continuous variables with values between 0 and 1 (Ferrari and Cribari-Neto, 2004). A similar approach was followed for the specification of the minor/major axis ratio $\frac{b_{sde}}{a_{sde}}$ model, where the dependent variables should also take values only between 0-1. The mean μ of the dependent variable y can be calculated as $\mu = E(y) = \Sigma b_{x_i} x_i$ and the variance as $Var(y) = \frac{\mu(1-\mu)}{1+\phi}$, where ϕ is a precision parameter, which is inversely proportional to variance (Ferrari and Cribari-Neto, 2004).

3 Methodology

The MNL model has been the main workhorse of DCM and has been applied in numerous studies of behavioural modelling in the fields of transport, environment and health, among others (McFadden, 1973; Domencich and McFadden, 1975; McFadden, 1978; Ben-Akiva and Lerman, 1985; McFadden, 2000). According to that specification, an individual n will choose among a set of alternatives J , the alternative i that provides the highest utility for a specific choice task t . The utility U_{int} is a latent construct comprised of a systematic part V_{int} and a disturbance term ϵ_{int} as $U_{int} = V_{int} + \epsilon_{int}$, assuming an additive disturbance term. Different distributional assumptions regarding the disturbance term will yield different specifications, with the assumption of a Type-I Extreme Value distributed ϵ_{int} leading to an MNL model.

In an MNL model, individual heterogeneity can be captured by specifying interaction terms with socio-demographic attributes as shifts from the base level of specific parameters. More advanced specifications are necessary, however, to account for unobserved heterogeneity, such as mixed Logit (McFadden and Train, 2000) and LCCM (Kamakura and Russell, 1989).

In the mixed Logit model, heterogeneity is captured in a continuous manner by assuming that sensitivities across individuals follow a certain distribution with normal, uniform or log-normal distributions being the most commonly used ones. The mixed Logit has been widely used for the purpose of capturing heterogeneity in the sample and it is considered the most flexible logit specification (McFadden and Train, 2000; McFadden, 2000). Mixed Logit models usually require the use of simulation to estimate the parameters of the specified distributions and a large number of draws is usually needed to reach a certain level of estimation stability, which significantly increases the estimation times. Furthermore, that means that the estimated parameters largely depend on the analyst’s distributional assumptions, which can have adverse effects in the case of behaviourally inaccurate ones. On the other hand, LCCMs capture heterogeneity by assuming that individuals in the sample can be probabilistically allocated into a discrete and finite number of latent classes based on their sociodemographics and their choice behaviour.

Three consideration sets are constructed per individual and choice task after the creation of the mode-specific Detour Ellipses and individual-specific Standard Deviational Ellipses. Individuals can belong to each consideration set with a positive probability, thus acknowledging the latent nature of the true choice set. The probability of individual n belonging to a consideration set C is modelled as a multinomial logit, as shown in Equation 6.5. The hypothesis behind this specification, is that the individuals in the sample are likely to be subject to either time-space constraints for the specific trip chain (class a) or to be constrained due to issues of spatial awareness (class b) or alternatively to be free to consider alternatives from the global choice set (class c) during their choice of mode and shopping location. As such, the proposed LCCM specification allocates individuals probabilistically into three classes, with each class having a different choice set. The choice set of *class a* includes mode-destination alternatives (feasible in terms of mode) that are located within the estimated mode-specific Detour Ellipses, therefore capturing individuals who are *captive* to their time-space constraints. The choice set of *class b* includes alternatives within the merged area of the estimated Detour and Standard Deviational Ellipses, thus capturing individuals *captive* to their spatial awareness. Finally, the choice set of *class c* includes all feasible alternatives in the global choice set per trip.

$$\pi_n(C) = \frac{e^{\delta_c + \gamma_c x_n}}{\sum_{r=1}^C e^{\delta_r + \gamma_r x_n}} \quad (6.5)$$

According to this framework, the probability of choosing an alternative i for individual n is calculated based on the logit function conditional on alternative i belonging to consideration set C and it is 0 otherwise, as shown in Equation 6.6. Finally, the unconditional likelihood of observing a sequence of choices for individual n is calculated by weighting the class-specific conditional probabilities for alternative i with the class membership probabilities $\pi_n(C)$ across G potential classes, i.e. non-empty choice sets, which in that case is limited to 3, as shown in Equation 6.7. The coefficients of both model components are jointly estimated by using Maximum Likelihood Estimation.

$$P_{ni|C} = \begin{cases} \frac{e^{V_{ni}}}{\sum_j e^{V_{nj}}} & , \text{ if } i \in C \\ 0 & , \text{ otherwise} \end{cases} \quad (6.6)$$

$$P_{ni} = \sum_{C \in G} \pi_n(C) P_{ni|C} \quad (6.7)$$

Further complexity can be added to the proposed specification in order to capture additional heterogeneity within each class by specifying a 2-stage LCCM similar to the study

of Song et al. (2019). Nonetheless, that is out of the scope of the current and it is left as an idea for potential future research.

The utility function of the behavioural model follows the size variable specification proposed in Daly (1982) and specifically the one implemented in the joint mode and destination choice model presented in the study of Kristoffersson et al. (2018) combining mode preferences with shopping destination attraction. According to that, the systematic utility V_{md} for mode m and destination d presented in Equation 6.8 is comprised of several parts referring to mode- and destination-specific Level-of-Service (LOS) variables, locational variables capturing the quality of each destination and variables capturing its size, also known as size variables. That size variable specification was proposed to account for the utility of the elemental destinations within the aggregated destination alternatives.

$$V_{md} = \sum_{r \in R} b_r x_{rmd} + \sum_{q \in Q} b_q y_{qd} + \phi \log(S_d) \quad (6.8)$$

The first component includes mode- and destination-specific variables that best describe the trip to destination d with mode m , such as travel time and cost for motorised modes and distance for active travel, as well as ASCs capturing inherent preferences for specific modes/destinations and sociodemographic interactions. With this, x_{rmd} is the r -th LOS variable for mode m and destination d . The second component captures the impact (positive or negative) that certain characteristics could have on the utility of a specific destination, such as available parking space for car users, where y_{qd} is the q -th quality variable for destination d . The final component in Equation 6.8 aims to capture the attraction or the “size” of a destination d , S_d and is specified as a composite logarithmic term as shown in the following Equation 6.9:

$$S_d = a_{1d} + \sum_{r > 1} \exp(\gamma_r) a_{rd} \quad (6.9)$$

where a_{1d} is the attraction attribute used as a base with a γ parameter normalised to 1.0, a_{rd} are the additional attraction attributes of destination d relative to the base attribute, and γ_r are the parameters to be estimated capturing the effect of those attributes on the attraction of the target destination. The γ_r parameters are constrained to be positive by using an exponential transform.

The log-size parameter ϕ is usually kept fixed to 1.0 ensuring that a change in the size of a destination will affect proportionately its utility. Therefore, the choice probabilities will not be affected by the zoning discretisation that usually forms the destination alternatives. Kristoffersson et al. (2018), however, proposed a freely estimated ϕ , which can lead to estimated values different than 1.0, leading to a behavioural interpretation on the formation of destination alternatives. Specifically, in the case of $\phi < 1$, the authors suggest that the model captures significant correlation among the utilities of the elemental alternatives within each aggregate destination alternative.

4 Data

For the practical implementation of the proposed approach, a 2-week GPS-based trip diary captured by a smartphone application is utilised. The GPS trip diary was collected as part of the research project “DECISIONS” conducted by the Institute for Transport Studies, University of Leeds, between October 2016-March 2017. Besides the utilised GPS trip diary, the “DECISIONS” project aimed to capture a range of different aspects of individual behaviour, such as in-home and out-of-home activity participation, energy appliance usage

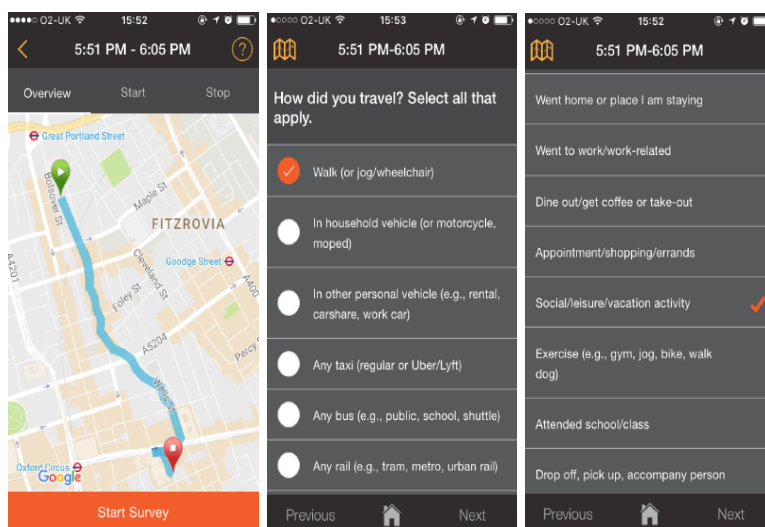


Figure 6.2: User interface of smartphone application used for the trip diary

and the effect of social networks. The GPS trip diary captured the daily trips over the survey period with the use of a smartphone application, which was tracking the traces of the participants. After the end of each trip, the participants had the chance to correct the information of the logged trip and provide additional information regarding the chosen mode and the type of the activity at the destination (trip purpose). A depiction of the application’s interface is presented in *Figure 6.2*. A background household survey was also conducted in order to capture several important sociodemographic attributes of the participants, such as their age, their household composition, the availability of mobility tools (e.g. private vehicles and PT season ticket ownership) and their personal and household income, among others. A more detailed description of the data collected during the “DECISIONS” project and its various sub-modules is provided in Calastri et al. (2020).

The initial GPS trip diary included trips captured throughout the UK, but the vast majority of them were in the region of Yorkshire and more specifically in and around the city of Leeds. Therefore, the final dataset used for the subsequent analysis included only individuals residing within the local authority of Leeds. As previously described, the purpose of the analysis is to understand where the individuals are more likely to travel in order to cover their daily shopping needs and how to travel there and to the following activity location, thus acknowledging the interrelations between mode and destination and among the locations of consecutive activities. As a result, only the shopping trips and their following trips were selected for the subsequent analysis resulting in a final dataset of 1,541 shopping-following trip chains performed by 270 unique individuals. The analysis is conducted at the trip chain level, 66% of which are *OSD* trip chains and the remaining 34% are *OSO* trip chains. Shopping trips are comprised of three subcategories, namely grocery (82%), clothes (12.7%), and other types of shopping (5.3%), mainly for durables. The vast majority of following trips were trips going home (61.5%), while there was a small percentage of 9.3% of a consecutive shopping trip to a different shopping destination. The alternative modes of transport included car, public transport (PT) – as a combination of bus and rail – and walking.

The high spatial resolution of the GPS traces, despite the benefits, it also provides additional challenges for their analysis compared to traditional data sources. Therefore, because each GPS trace is a unique pair of latitude and longitude coordinates, a clustering approach had to be developed to identify unique activity locations. Hierarchical Agglomerative Clustering (HAC) was utilised for that purpose as it does not require any a priori assumptions about the number of the required clusters. HAC, however, required a specific distance threshold to be defined to assign points within that threshold in the same cluster. A distance

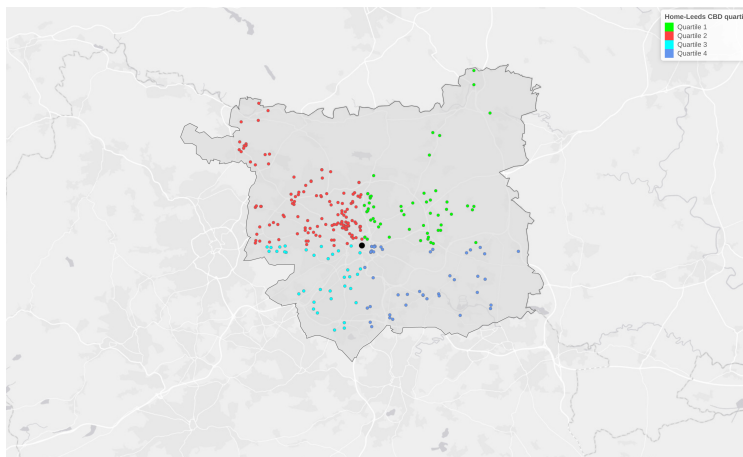


Figure 6.3: Home locations segmented in quartiles relative to their position from Leeds CBD (black circle)

threshold of 200m was chosen to ensure a small distance difference (approximately 100m) of points allocated in the same cluster of an activity location per individual. The implementation of HAC helped us to define unique home and work locations based on the purposes of trips going to those destinations in order to further define daily tours and sub-tours. In cases, where trip purposes were not enough to define home and work locations, additional information on time of day and activity duration was used, such as assigning a work location to a cluster if an individual spends the majority of working hours (09:00-17:00) there. The home locations of the individuals were also segmented according to their position relative to Leeds Central Business District (CBD) into four quartiles, as depicted in *Figure 6.3*. Out of the 270 individuals, 55 (20.4%) live in quartile 1, 136 (50.4%) in quartile 2, 35 (12.9%) in quartile 3 and 35 (16.3%) in quartile 4.

In order to take advantage of the high spatial resolution provided by the GPS data, the definition of shopping destination alternatives was not limited to the usual UK geographical boundaries, but were defined at a more granular level by clustering the observed elemental shopping destinations. HAC was implemented again with a distance threshold of 800 metres among the shopping trip destinations. The cluster centroids defined as the mean of the latitude/longitude coordinates of the points in each cluster were then used to replace the original destination points of each shopping trip belonging to the cluster. The main goal of choosing an appropriate distance threshold was to ensure a small average distance difference between the original destination points of a cluster and its centroid. After trying different distance thresholds between 500m-1,000m, a 800m distance threshold was selected resulting in small average distance differences of around 4-5 minutes of walking (assuming a 5 km/h average walking speed). As a final step, a 400m buffer was defined around each cluster centroid to create the aggregate shopping areas used as destination alternatives in the analysis. This process resulted in the definition of 176 general shopping areas around the region of Yorkshire, capturing 76% of the retail polygons located within the Local Authority of Leeds, as defined in OpenStreetMaps (OSM).

Further steps were necessary in order to enrich the initial dataset with additional information important for behavioural modelling. Initially, the dataset contained only the self-reported travel times/distances for the chosen modes, however, the values of the unchosen mode alternatives were also required to properly define the attributes for all alternatives. For that reason, the Bing maps route API² was utilised to obtain the travel times and distances for all the modes (car, bus/rail, walking) and for trips starting from each initial origin to each shopping cluster and from each shopping cluster to each following destination. For consistency reasons, the travel times/distances of the chosen mode alternatives were recalculated as

²Details can be found here: <https://docs.microsoft.com/en-us/bingmaps/rest-services/routes/>

well to ensure that the data used for estimation would come from the same data generating process. The total number of queries passed to the API was 1,627,296 (1,541 trips \times 176 shopping destinations \times 3 modes \times 2 for the current and the subsequent trip). After that data collection stage, deterministic mode availability was assigned based on logical feasibility checks of the results obtained from the API, such as cases of short distance PT trips for which the API returned only walking segments, or in specific cases where car was the chosen mode and the participant had to return it back home. For that latter case, special attention was given to the stated size of the party that participated in the trip in order to understand whether the participant of the survey was the actual driver. As such, if the individual was the only person in a car trip, then she was assigned as the car driver and all the remaining modes would become unavailable only in the case where the following trip was to return back home. For other trip purposes for the following trip, it is assumed that the individual is free to consider all the available modes. On the contrary, if there were more than 1 people participating in a car trip, then we could not safely assume that the individual was the driver and all the modes would remain available for the following trip, as well.

Information on travel cost was also missing both for chosen and unchosen modes. Car travel cost was computed using the UK's official Transport Appraisal Guidance (WEBTag) specifications for fuel and operating costs (Department for Transport, 2014). Parking cost was also calculated for trips with destinations in central areas/high streets across the region of Yorkshire based on information on hourly or fixed parking costs provided by the respective Local Authorities. Fuel, operating and parking costs were then aggregated to form a total car travel cost used for estimation. For PT, an average distance-based fare was used for bus and rail and a total PT cost was calculated per trip based on the distance of the leg performed by bus or rail. A discount was also applied for trips made by season ticket holders.

Additional locational data were acquired from the Office for National Statistics (ONS) and OpenStreetMaps (OSM) to be used in the modelling specifications as attraction variables for specific shopping destinations. Specifically, the total areas of retail, grocery and durable shopping parcels within each aggregated shopping destination was calculated from OSM together with the total parking areas and the locations of the most popular retailers per shopping type in the UK market. The population around shopping locations was also extracted from the Office of National Statistics (ONS) together with Indices for Multiple Deprivation for 2015³ (Figure 6.4), as well as average house prices and percentages of white residents for 2016-2017 in order to capture instances of spatial inequalities.

The different types of shopping stores among the elemental shopping destinations within an aggregate destination alternative was also acquired using the OSM categorisation. The purpose of that was to capture the impact of shopping store variability using Shannon's entropy (Shannon, 1948; Whittaker, 1949), H_d , measuring the percentage of the area covered by a specific store type $t \in T$ inside a shopping destination d from a total number of N different store types as shown in Equation 6.10. Shannon's entropy is used to examine whether an increased variability in store types makes a shopping destination more likely to be chosen, since that would enable the completion of different shopping activities within the same trip.

$$H_d = - \frac{\sum_{t=1}^T (p_t \ln(p_t))}{\ln N} \quad (6.10)$$

In order to capture agglomeration effects and the impact of neighbouring shopping destinations on the attraction of a target shopping destination, the same information on the aforementioned locational variables was extracted for additional buffers between 400-1,000m, 1,000-2,000m and 2,000-5,000m from each cluster centroid, similar to the study of Kristoffersson et al. (2018).

Finally, the impact of the location of the intermediate shopping destination S , in relation to the straight distance between O and D , was captured by calculating the angles between

³Details can be found here: <https://www.gov.uk/government/statistics/english-indices-of-deprivation-2015>

5. Results

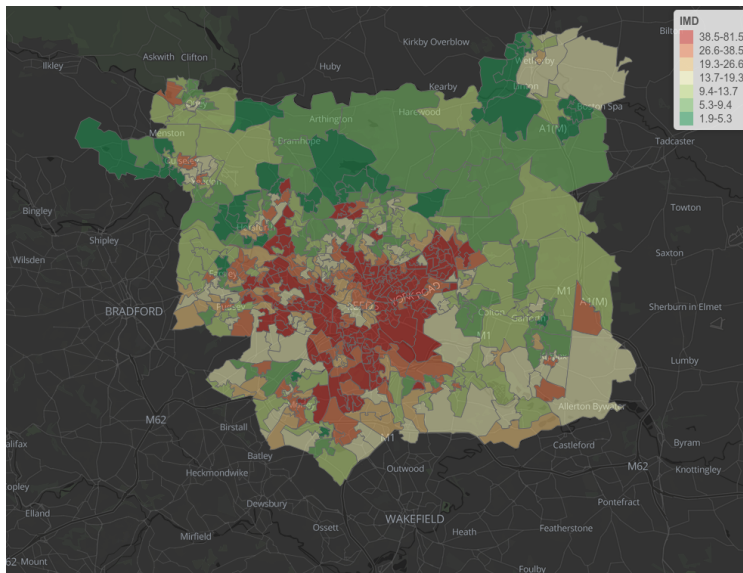


Figure 6.4: Index of Multiple Deprivation for 2015

OS-OD and *SD-OD*. It is assumed that shopping destinations, which require a significant deviation from the straight *OD* path would be less likely to be chosen compared to others that are in the same direction.

5 Results

In the following, the modelling outputs are going to be described starting first with the auxiliary specifications for OSD and OSO trip chains and then the five models for the structural components of the SDE –namely models for the distance and the angle between home locations and the SDE centroid, its orientation, its minor/major axis ratio and its area– before moving on to the main outputs of the proposed LCCM specification.

5.1 Detour Ellipse outputs

The estimates of the Detour Factor and the distance model for the OSD and OSO trip chains, respectively, described in the following were used to re-create estimated Detour Ellipses for both cases (OSD and OSO trip chains). The resulting trip- and mode-specific estimated Detour Ellipses, on average, contain 19.5 shopping locations out of the 176 identified locations within the study area (11.1%).

The Detour Factor model for the OSD trip chains achieves a correlation of 0.72 between observed and estimated detour factors. The estimated parameters of the corresponding model are presented in [Table 6.1](#) along with the robust t-ratios to account for the multiple observations per individual (Daly and Hess, 2010). According to the model, the individuals are willing to take a shorter detour to reach a shopping destination, when the destination for the next activity is further away indicating the time-space constraints the individuals are subject to. Choosing walking for the first shopping trip or also travelling by mode combinations of car-PT, car-walking will result in smaller detours than the base mode combination of car-car. Nonetheless, the opposite is true when travelling by PT in both trip legs with individuals choosing longer detours. Longer detours are also predicted for clothes and durables shopping, when the following activity is for education purposes or the shopping trip is part of a tour with education as its main purpose, for male individuals and for mostly older ages (above 76 years

old). Furthermore, individuals with a household income between £40,000-£50,000 will also tend to take longer detours, while the higher the average income around the individuals' home locations the longer the detours they are willing to choose, as well. Longer detours were also estimated for individuals living in households of mostly above 3 members, those employed in Healthcare, Education, Academia or other types of occupations, when the trip occurs during morning weekend hours and when there are more available parking areas around the shopping location. Contrary to that, smaller detours are estimated for individuals living together with more than four employed individuals possibly due to the increased time requirements to accommodate everyone's daily mobility needs, for part-time workers most likely due to increased housekeeping responsibilities, for shopping trips during night or early morning periods during weekdays and for individuals of the smallest household income band (below £10,000).

Moving on to the model for the estimated distances of the OSO trip chains, a correlation of 0.67 was achieved between observed and predicted distances. The modelling outputs are presented in *Table 6.2*, where it can be seen that mode combinations of car-walking and walking-walking lead to smaller straight distances to reach a shopping destination compared to the base mode combination of car-car. Shopping for durables will lead to larger distances mainly due to the more specialised type of stores, which can be located further away from home locations. Living in households of either 1 or 4 members will lead to smaller distances, while that is also the case for male individuals, when the shopping trip is part of a tour with work or education as its main purpose, when the following activity is for social, other purposes or to return back to work with the latter mostly referring to short shopping trips from work locations during lunch break. Longer distances can be expected for trips during the interpeak or during morning hours for retired people and for engineers, community/social workers, students and those working on management. The model was also able to uncover that younger and older individuals, specifically those between 25-29 and above 76 years old, and those who have not disclosed their income tend to choose longer distances. In addition, participating in shopping activities of longer durations (which is considered as exogenous in that case) will make individuals to also travel for longer distances. Considering shopping duration as endogenous within a discrete-continuous framework, however, would be a more accurate approach, leading to better capturing the trade-offs between shopping duration and distance travelled, which could be an interesting direction for future research. Finally, decreasing marginal utilities/disutilities have been uncovered for a range of locational variables specified in a logarithmic function. Specifically, shopping locations with more retail and parking areas will cause individuals to travel for longer distances to visit them. Individuals living in areas with a higher average income tend to choose longer distances. Finally, an increased shopping store variability (Shannon's entropy) will lead to smaller distances.

5.2 Standard Deviation Ellipse outputs

In the following, the estimates of the five SDE-related sub-models are detailed. Those estimates were used to re-create estimated individual-specific SDEs, which on average contain 73.2 (41.6%) of the shopping locations in the study area.

5.2.1 Home-SDE centroid distance outputs

The estimated distances between home and SDE centroids achieved a correlation of 0.48 with the observed distances. The outputs of the corresponding model are presented in *Table 6.3*. According to those, individuals living in areas other than quartile 3 tend to have an SDE centroid, i.e. the centre of gravity of their usual movements, further away from their home locations. The distance between home and Leeds CBD also has an impact on the home-SDE centroid distance with larger distances leading also to larger home-SDE centroid distances for quartiles 2 and 4. On the contrary, distances between work locations and Leeds CBD

Table 6.1: Modelling outputs of the DF model for *O-S-D* trip chains

Parameters	Estimates	Rob. t-ratios
<i>Constant</i>	-4.7480	-3.62
<i>O-D straight distance (km) (log)</i>	-1.3221	-20.57
<i>Car-PT</i>	-0.4283	-1.46
<i>Car-Walking</i>	-2.1897	-6.60
<i>PT-PT</i>	0.9615	2.31
<i>Walking-Car</i>	-1.4913	-4.24
<i>Walking-PT</i>	-0.6923	-2.59
<i>Walking-Walking</i>	-1.7347	-7.34
<i>Shopping: Clothes - Other</i>	0.5791	3.22
<i>Household size: 3-4 members</i>	0.4599	3.05
<i>Household size: 5 members</i>	-0.9965	-1.46
<i>Household size: 6 members</i>	1.1187	2.58
<i>Other employed household members > 4</i>	-1.8039	-8.44
<i>Part time workers</i>	-0.4286	-2.54
<i>Occupation: Healthcare</i>	1.0691	3.77
<i>Occupation: Education</i>	0.2591	1.46
<i>Occupation: Academia</i>	0.4369	1.74
<i>Occupation: Students</i>	0.6211	1.42
<i>Occupation: Other</i>	0.5894	2.81
<i>Time of day: Weekday night</i>	-0.4682	-1.65
<i>Time of day: Weekday morning</i>	-1.1338	-1.43
<i>Time of day: Weekend morning</i>	0.6974	3.21
<i>Following trip purpose: Groceries</i>	0.3666	1.78
<i>Following trip purpose: Education</i>	2.5978	5.21
<i>Age 25-29</i>	0.3771	1.61
<i>Age 60-65</i>	0.4492	1.50
<i>Age ≥ 76</i>	1.2577	2.96
<i>Parking areas 400m around shopping destination in 1,000m² for car trips</i>	0.0186	6.21
<i>Shannon's entropy 400m around shopping destination (log)</i>	0.3833	2.24
<i>Total passengers in shopping trip >1</i>	0.2520	1.73
<i>Household income <£10,000</i>	-0.6036	-1.53
<i>Household income £40,000-£50,000</i>	0.4140	2.06
<i>Male</i>	0.2854	1.86
<i>Population in 400m around home location in 1,000 people</i>	0.4275	1.56
<i>Average annual income in 400m around home location in £1,000 (log)</i>	1.0374	2.82
<i>Trip part of a tour with main purpose: Education</i>	0.6589	1.44
<i>Sigma</i>	1.9616	33.05

Table 6.2: Modelling outputs of the distance (km) model for *OSO* trip chains

Parameters	Estimates	Rob. t-ratios
<i>Constant</i>	-1.8424	-3.52
<i>Car-Walking</i>	-1.3592	-2.04
<i>Walking-Walking</i>	-1.3846	-13.83
<i>Shopping: Other</i>	0.4366	2.97
<i>Household size: 1 member</i>	-0.1666	-2.29
<i>Household size: 4 members</i>	-0.2578	-2.06
<i>Occupation: Engineering/Community/ Social/Management/Student/Other</i>	0.2336	3.54
<i>Occupation: Retired</i>	0.4607	2.33
<i>Time of day: Interpeak</i>	0.1588	1.87
<i>Time of day: Weekday night</i>	-0.2577	-2.04
<i>Time of day: Weekday morning</i>	1.1395	6.99
<i>Time of day: Weekend morning</i>	0.1459	1.59
<i>Following trip purpose: Other</i>	-0.4919	-1.36
<i>Following trip purpose: Social/Leisure</i>	-0.6376	-3.27
<i>Following trip purpose: Return to Work</i>	-0.1687	-1.45
<i>Age 25-29</i>	0.4385	4.99
<i>Age 30-39</i>	0.1261	1.69
<i>Age 50-59</i>	0.1626	1.71
<i>Age \geq 76</i>	0.2502	1.94
<i>Shannon's entropy 400m around shopping destination (log)</i>	-0.1079	-1.51
<i>Retail areas 400m around shopping destination in 1,000m² (log)</i>	0.1196	4.05
<i>Household income £20,000-£30,000</i>	-0.1305	-1.28
<i>Household income £75,000-£100,000</i>	-0.1872	-1.29
<i>Household income- Not disclosed</i>	0.4409	3.37
<i>Parking areas 400m around shopping destination in 1,000m² for car trips (log)</i>	0.0456	1.38
<i>Gender: Male</i>	-0.1104	-1.64
<i>Total passengers in shopping trip >1</i>	0.0851	1.36
<i>Duration of shopping activity</i>	0.1953	3.53
<i>Marital status: Widowed</i>	-0.6593	-2.95
<i>Trip part of a tour with main purpose: Education/Work</i>	-0.7579	-2.40
<i>Average annual income in 400m around home location in £1,000 (log)</i>	0.5275	3.25
<i>Sigma</i>	0.6150	23.43

Table 6.3: Modelling outputs for the distance of the Standard Deviational Ellipse centroid from the home location ($dist_{hc}$)

Parameters	Estimates	t-ratios
<i>Constant</i>	-12.0510	-1.51
<i>Home location in quartile 2, 4</i>	12.0179	1.51
<i>Home location in quartile 1</i>	18.0662	2.15
<i>Home-Leeds CBD distance in km (quartile 4)</i>	0.1871	1.23
<i>Home-Leeds CBD distance in km (quartile 2)</i>	0.0432	2.39
<i>Work-Leeds CBD distance in km (quartile 2, 3)</i>	-0.1351	-2.63
<i>Household income £30,000-50,000</i>	0.1382	1.55
<i>Household income £75,000-100,000</i>	0.2617	1.58
<i>Occupation: Sales, Maintenance</i>	0.6715	2.51
<i>Occupation: Social</i>	0.2706	1.71
<i>Occupation: Academics, Research</i>	0.3332	1.84
<i>Home-Work distance in km (quartile 1)</i>	0.2583	2.96
<i>Home-Work distance in km (quartiles 2, 3)</i>	0.3372	5.31
<i>Home-Work distance in km (quartile 4)</i>	0.4320	3.13
<i>Married</i>	-0.2224	-2.38
<i>Age 25-29</i>	-0.3202	-2.01
<i>Age >66</i>	0.5669	2.37
<i>Home-York CBD distance in km (quartile 1)</i>	-1.6410	-2.28
<i>Home-York CBD distance in km (quartile 3)</i>	3.3845	1.55
<i>Unemployed (quartile 4)</i>	0.7089	1.91
<i>Sigma</i>	0.6753	23.24

will lead to smaller home-SDE centroid distances for quartiles 2 and 3. The CBD of York also was found to have an impact on the estimated distances. Specifically, larger home-York CBD distances will lead to larger home-SDE centroid distances for individuals in quartile 3, but to smaller distances or those living in quartile 1. An interesting insight also arises by investigating the impact of the distance between home and work locations, where larger distances will lead to larger home-SDE centroid distances, as well, since the individuals are in generally required to travel further away from their home due to the distant work location. Regarding the remaining parameters, individuals of household income between £30,000-50,000 and £75,000-100,000 have higher home-SDE centroid distances, while that also holds for elderly individuals (above 66 years old), for unemployed people and for those working in the sales or maintenance industry, social workers and academics. Smaller distances, however, are expected for married individuals and younger people (between 25-29 years old).

5.2.2 Home-SDE centroid angle outputs

The model regarding the angle between home locations and SDE centroids achieved the highest level of accuracy of the five SDE-related sub-models with a correlation of 0.78. The model outputs are presented in *Table 6.4*. That model, together with the previous one for home-SDE centroid distance, is important for the identification of the coordinates of the estimated SDE centroid, since a point can be defined by its distance and its angle from another known point, in that case the home locations. Nonetheless, it is difficult to extract any meaningful behavioural interpretation from its estimated parameters. It is important to note that angles were measured from the home location to the SDE centroid, since the directionality matters for the size of the calculated angles. The main interpretation that can be extracted from the estimates is that on average the CBD of Leeds acts a strong attraction to the centre of gravity of individuals' usual areas of movement, as captured by the SDE

Table 6.4: Modelling outputs for the angle between the Standard Deviational Ellipse centroid and the home location (θ_{hc})

Parameters	Estimates	t-ratios
<i>Constant</i>	-4.1798	-4.11
<i>Home in quartile 1</i>	3.3350	3.40
<i>Home in quartile 2</i>	40.6517	2.61
<i>Home in quartile 4</i>	2.9321	2.99
<i>Home-Leeds CBD distance in km (linear) (quartile 2)</i>	-1.3490	-2.76
<i>Home-Leeds CBD distance in km (log) (quartile 2)</i>	1.4916	3.50
<i>Work-Leeds CBD distance in km (log) (quartile 2)</i>	-0.2239	-2.41
<i>Population 400m around home location in 1,000 people (log) (quartile 3)</i>	4.1139	2.13
<i>Personal income <£10,000</i>	0.9963	4.20
<i>Occupation: Engineering</i>	0.7541	3.27
<i>Occupation: Maintenance</i>	-1.2733	-1.72
<i>Occupation: Food and serving</i>	1.0490	1.46
<i>Occupation: Business, Education</i>	0.2439	1.68.69
<i>Student</i>	1.1086	3.94
<i>Home-Work distance in km (log) (quartile 2)</i>	-0.3182	-2.53
<i>Age 30-39 and 50-59</i>	-0.3822	-2.87
<i>Age 60-65</i>	-0.9361	-2.93
<i>Home-Work angle (quartile 2)</i>	0.7091	2.48
<i>Home-Work angle (quartile 3)</i>	1.3336	2.35
<i>Home-Wakefield CBD distance in km (quartile 2)</i>	2.4829	2.59
<i>Home-Sheffield CBD distance in km (quartile 2)</i>	-1.4075	-2.50
<i>Precision ϕ</i>	3.3457	12.28

centroid, regardless of the geographic quartiles they reside. Specifically, individuals living in quartile 3 have the smallest home-SDE centroid angle with an average angle of 87.5° . Individuals from quartile 4 and 1 have larger home-SDE centroid angles with average values of 150.9° and 195.7° , respectively. Finally, quartile 2 has the largest angles with an average value of 280.8° . All the above are also captured in the model from the estimated parameters for quartiles 1, 2 and 4 using quartile 3 as the base. It is also interesting to note that angles in quartile 2 are decreasing as home and work locations are further away from Leeds CBD and the distance between home-work locations is increasing. In addition, the neighbouring cities of Wakefield and Sheffield located in the south of Leeds also have an influence on the position of the SDE centroid relative to the home locations in quartile 2 with those increasing as the home-Wakefield CBD distance also increases and are decreasing as the home-Sheffield CBD distance increases. Larger distances between home and work locations also can cause an increase in angles in quartile 3. Population has an influence on the home-SDE centroid angles in quartile 3 with a larger population around home locations leading to increased angles. From the remaining parameters, individuals working in maintenance occupations and those aged between 30-39 or 50-65 years old have smaller angles, while individuals of lower income, engineers, students and those working in the food and serving industry have larger home-SDE centroid angles, all else held equal.

5.2.3 SDE orientation outputs

The modelling specification for the SDE orientation achieved a correlation of 0.43 between observed and predicted values. The estimated parameters are depicted in *Table 6.5*. Similarly to the previously described home-SDE centroid angles, this model also captures the impact

Table 6.5: Modelling outputs for the orientation of the Standard Deviational Ellipse (θ_{sde})

Parameters	Estimates	t-ratios
<i>Constant</i>	0.4372	1.07
<i>Home located in quartile 2</i>	1.7330	3.22
<i>Home located in quartile 1</i>	-0.5826	-1.35
<i>Home-Leeds CBD distance in km (log) (quartile 4)</i>	0.4272	3.69
<i>Population 400m around home in 1,000 people (log) (quartile 1)</i>	1.3999	1.92
<i>Personal income £10,000-30,000</i>	0.2429	1.79
<i>Personal income £40,000-75,000</i>	0.2962	1.32
<i>Personal income £75,000-100,000</i>	-1.0363	-1.66
<i>Unemployed (quartile 3)</i>	-1.0155	-1.60
<i>Average IMD 400m around home (log) (quartile 2)</i>	-0.3718	-2.20
<i>Precision ϕ</i>	2.5125	13.3

of the Leeds CBD to the orientation of the SDE. The values of the SDE orientation range from 0° to 180° , since those angles in that case are measured from the SDE centroid to the top end of the ellipse. Because of that, SDEs for individuals residing in quartiles 1 and 3 have smaller values largely between $0^\circ - 90^\circ$ and average values of 79.2° and 71.1° , respectively, while individuals living in quartiles 2 and 4 have SDEs with orientations between $90^\circ - 180^\circ$ and average values of 109.0° and 111.5° , respectively. That is also captured in the model, with larger orientation angles being predicted for quartile 2 and smaller for quartile 1 (although statistically significant only at the 80% confidence level) relative to the base quartile 3. Orientations in quartile 4 are larger than those in quartile 3, but they were omitted from the final model since they were not statistically significant even at the 50% confidence level. Regarding the remaining parameters, the larger the population around the home location and the distance between home-Leeds CBD the larger the angle orientation of the SDE. Individuals with personal income of £10,000-30,000 and £40,000-75,000 have larger orientations, while the opposite is true for higher personal incomes between £75,000-100,000, unemployed people living in quartile 3 and for those living in more deprived areas in quartile 2.

5.2.4 SDE minor/major axis ratio outputs

The estimated model for the minor/major axis ratio ($\frac{b_{sde}}{a_{sde}}$) of the SDEs achieved a correlation of 0.45 between observed and predicted values and its outputs are presented in *Table 6.6*. Overall, individuals located at quartile 4 have larger $\frac{b_{sde}}{a_{sde}}$ ratios compared to the rest and especially compared to those residing in quartile 2. Those living in quartile 2 also tend to have larger ratios as the variability of shopping store types around their home locations increases. An interesting finding can be observed for the effect of income on the estimated ratios, with an almost monotonically decreasing $\frac{b_{sde}}{a_{sde}}$ ratio as the personal income increases. In addition, as the size of the household increases the $\frac{b_{sde}}{a_{sde}}$ ratio decreases possibly due to increased family commitments, while smaller ratios are also expected for people with no car availability, unmarried, working in Education or in arts, media and the sports industry and being between 18-24 or 40-49 years old.

Table 6.6: Modelling outputs for the minor/major axis ratio of the Standard Deviational Ellipse ($\frac{b_{sde}}{a_{sde}}$)

Parameters	Estimates	t-ratios
<i>Constant</i>	0.2799	1.45
<i>Home located in quartile 4</i>	0.3888	1.55
<i>Home located in quartile 2</i>	-0.4586	-1.20
<i>Home located in quartile 1</i>	0.1548	0.91
<i>Average Shannon's entropy 400m around home (quartile 2)</i>	1.3516	1.72
<i>Angle between home location and Leeds CBD (quartile 2)</i>	-0.0045	-1.49
<i>Personal income £10,000-20,000</i>	-0.3262	-2.18
<i>Personal income £20,000-30,000</i>	-0.5208	-3.52
<i>Personal income £30,000-40,000</i>	-0.2023	-1.33
<i>Personal income £40,000-50,000</i>	-0.6026	-2.84
<i>Personal income £75,000-100,000</i>	-1.0159	-2.11
<i>Occupation: Food and serving</i>	1.2547	2.20
<i>Occupation: Art, sports and media</i>	-1.0400	-1.63
<i>Occupation: Education</i>	-0.3602	-2.41
<i>Household size</i>	-0.0777	-2.50
<i>No car ownership</i>	-0.3759	-3.00
<i>Home-Work distance in km (log) (quartile 4)</i>	-0.2513	-2.27
<i>Non married</i>	-0.3119	-2.80
<i>Age 18-24</i>	-0.2264	-1.46
<i>Age 40-49</i>	-0.2259	-1.79
<i>Precision ϕ</i>	5.9588	12.43

5.2.5 SDE area outputs

The model regarding the SDE area achieved a correlation of 0.42 between the observed and estimated areas and its outputs are presented in *Table 6.7*. In general, individuals residing in quartile 1 have a larger SDE area. Furthermore, distance between home and Leeds CBD is a significant factor influencing the area with higher instances also leading to larger areas. The same also holds for distances between the individuals' work locations and the Leeds CBD, as well as distances between home-work locations (for quartiles 2 and 4), which also positively affects the SDE area with larger distances leading to larger SDE areas, i.e. the visited locations of the individual are more dispersed in space. Male individuals, students, and low income individuals have lower SDE areas, while the opposite is true for retired, divorced and unemployed individuals residing in quartiles 1 and 4. Higher population in buffers of 400m around home locations will lead to larger areas for homes in quartiles 1 and 4, but smaller for quartile 4. Finally, a more diverse set of land uses around home locations (as captured by Shannon's entropy) will lead to lower SDE areas for homes in quartile 2, but the opposite is true for quartile 4 leading to larger areas.

5.3 Latent Class Choice Model outputs

Moving on to the estimation of the behavioural models, it is worth mentioning that they were estimated on choice sets comprised of 1584 alternatives (3 modes for first shopping trip x 176 shopping locations x 3 modes for following trip). The general specification of the models presented includes a range of Alternative Specific Constants (ASCs) as shifts from the base alternative, which in this case is assumed to be travelling by car for both trip legs to destination 1, which refers to the central shopping mall in the city of Leeds (car-car-dest 1). As expected in a case of a model including $J = 1584$ alternatives, it is not possible to estimate $J - 1$ ASCs for numerical and computational reasons. As a result,

Table 6.7: Modelling outputs for the area of the Standard Deviatonal Ellipse (A_{sde})

Parameters	Estimates	t-ratios
<i>Constant</i>	1.9131	3.26
<i>Home-Leeds CBD (quartile 1)</i>	2.7535	3.02
<i>Home-Leeds CBD distance (log) (quartile 1)</i>	0.4817	1.83
<i>Home-Leeds CBD distance (log) (quartile 2)</i>	0.4843	2.12
<i>Home-Leeds CBD distance (log) (quartile 3)</i>	1.0470	3.72
<i>Work-Leeds CBD distance (log)</i>	0.1603	2.34
<i>Population 400m around home location in 1,000 people (log) (quartile 1)</i>	2.0909	3.79
<i>Population 400m around home location in 1,000 people (log) (quartile 3)</i>	1.8691	1.49
<i>Population 400m around home location in 1,000 people (log) (quartile 4)</i>	-1.2987	-1.42
<i>Average Shannon's entropy 400m around home (quartile 1)</i>	-2.0843	-1.57
<i>Average Shannon's entropy 400m around home (quartile 4)</i>	4.1394	3.06
<i>Personal income £10,000-20,000</i>	-0.3074	-1.58
<i>Student</i>	-0.9935	-3.62
<i>Retired</i>	0.6626	1.83
<i>Number of cars</i>	0.4861	3.82
<i>Home-Work distance (log) (quartile 2)</i>	0.4179	2.91
<i>Home-Work distance (log) (quartile 4)</i>	0.7289	3.98
<i>Divorced</i>	1.0171	3.52
<i>Male</i>	-0.4708	-3.01
<i>Unemployed (quartile 1)</i>	0.8565	1.59
<i>Unemployed (quartile 4)</i>	2.2312	3.48
<i>Sigma</i>	1.1722	23.24

we opted to group alternatives based on their general geographical area relative to Leeds Central Business District (CBD), with that grouping comprising of 9 categories, namely Leeds CBD, north-east-south-west of Leeds and north-east-south-west of the remaining region of Yorkshire. The shifts from the base ASC, include interaction effects for specific modes and for specific areas, separately for individuals with and without car ownership in their household, for students and for married individuals. The Level-of-Service (LOS) parameters include travel times for the mechanised modes of car and Public Transport (PT), distance for walking and travel cost for car and PT. Base parameters for the three LOS attributes specifically for the first shopping trip were specified using a Box-Cox transformation for the purpose of capturing the presence of non-linearities in the sensitivities (Box and Cox, 1964). Using that approach, the LOS attributes x are entering the Utility function as $\beta \frac{x^\lambda - 1}{\lambda}$, with β being the base parameter for a specific LOS attribute and λ being an additional estimated parameter capturing the degree of non-linearity. An estimated $\lambda = 1$ indicates a linear specification as the Box-Cox transformation effectively collapses to βx , a $\lambda < 0$ indicates the presence of decreasing marginal disutilities, while in the case of $\lambda = 0$ the Box-Cox specification takes a logarithmic form $\beta \log(x)$. Finally, the flexibility of a Box-Cox transformation allows for the case of $\lambda > 1$ indicating the presence of increasing marginal disutilities, such as instances of increasing discomfort or time restrictions for the remaining time budget as travel time and/or cost increases. Shifts from those base LOS parameters are also specified for the following trip, for specific types of shopping activities, types of tours, trip chains and times of day. Furthermore, interactions with continuous measures of shopping duration are specified for time and walking and of personal income for cost. The remaining specified parameters refer to a measure capturing the angular deviation from the straight OD path that is required to reach the intermediate shopping location, a range of locational variables aiming to capture the preference of car drivers for parking spaces, the preference of individuals living in richer places to go shopping in poorer areas and vice versa, as well as a similar measure for individuals

living in less racially diverse to go shopping to more racially diverse neighbourhoods. In that study, the quartiles of the distribution of house prices around the home location are used to characterise an area as rich (quartile 4) or poor (quartile 1) and the same is done for racial diversity using the distribution of the percentage of white residents to characterise an area as less (quartile 4) or more racially diverse (quartile 1). The additional attraction due to the presence of major retailers per shopping type is also captured, while finally a range of size variables referring to the population around the shopping location, the total retail area per shopping type and the diversity of shopping store types are also included in a composite logarithmic term as described in *Section 3*.

The fit statistics and the estimated parameters of the behavioural models are presented in *Table 6.8* together with the Robust t-ratios to assess their statistical significance. Besides the proposed PCS-LCCM specification, which is able to capture heterogeneity in the choice sets and in the sensitivities, three additional models are presented, a base MNL model, MNL-base, using the global choice set of feasible alternatives, a base LCCM specification, LCCM-base, using the same choice set as MNL-base and capturing unobserved heterogeneity in the sensitivities and a simplified probabilistic choice set formation LCCM (PCS-LCCM-generic) using the same choice set structure across classes as the proposed PCS-LCCM, but with generic parameters across classes and only constants in the class allocation. PCS-LCCM-generic is similar to the specification proposed in the study of Thill and Horowitz (1997a) but using different proxy measures for latent constraints. The inclusion of the PCS-LCCM-generic has the purpose of capturing the impact of confounding unobserved heterogeneity in choice set formation with heterogeneity in sensitivities. That model still provides significant model fit improvements from the MNL-base model with 33.54 LL units with just two additional parameters, namely the two constants in the class allocation model, as depicted in *Table 6.8*. The remaining two models that are able to capture unobserved individual heterogeneity in the sensitivities, namely LCCM-base and PCS-LCCM, provide further improvements over the MNL-base model by 117.9 and 148.1 LL units, respectively, with 52 additional parameters. The proposed PCS-LCCM is also able to outperform the LCCM-base model by 30.18 LL units with the same number of parameters, although a direct comparison of the log-likelihoods of the two models is not a valid approach, since those two are not nested specifications. Nonetheless, the improvements in model fit become evident by examining and comparing the Adjusted ρ^2 , the AIC and BIC statistics (Ben-Akiva and Swait, 1986), all of which are improved for the PCS-LCCM compared to the LCCM-base. The proposed PCS-LCCM model is also able to outperform the PCS-LCCM-generic model by a significant margin, namely by 114.51 LL units with 50 additional parameters. More important, however, are the differences in the estimated shares of the latent classes, with PCS-LCCM-generic allocating individuals by 28.2% to *class a*, 2.9% to *class b* and 68.9% to *class c*. Contrary to that, the PCS-LCCM model estimates a much larger share for *class b*, specifically 29.3% of the sample, and also smaller shares for *class a* and *c*, namely 24.8% and 45.9%, respectively. That serves as an indication of the necessity to capture heterogeneity both in the choice sets and in the sensitivities across the estimated classes, which is an aspect missing in Thill and Horowitz (1997a).

According to the estimated parameters, destination 1 (base) is more likely to be chosen when travelling by a PT or walking due to the parking restrictions in Leeds CBD and due to the increasing promotion of more sustainable modes. The same also holds for the remaining destinations in the city centre, which are also in general less likely to be chosen compared to destination 1. Destinations in the remaining study area further away from the city centre are even less favourable, especially for modes other than car, although shopping locations in local high streets are again more likely to be visited by walking. Mode combinations other than those involving car are also more likely to be chosen for individuals with no car availability in their households. Furthermore, shopping trips including more than 1 passenger are more likely to be performed by car, at least for one of the two legs, due to its convenience. Finally, walking for both legs is more likely to be chosen by students, but less likely by married couples hinting to cases of more constrained time budgets for the latter demographic group

compared to the former.

Regarding the LOS variables of travel time, travel distance and travel cost statistically significant non-linearities were found for PT time, walking distance and travel cost, while only linear sensitivities were found for car time. In general, decreasing travel time and walking distance sensitivities were found as the shopping duration increases, while decreasing cost sensitivities were found as personal income increases, but not for all classes for the LCCM specifications. Finally, travel time for motorised modes and walking distance sensitivities were slightly higher for the following trip relative to the first shopping trip.

The model is also able to uncover interesting insights that could hint to instances of spatial and economic inequality in the area of Leeds. According to the model, all else held equal, individuals living in more affluent areas (highest percentile of house prices) are less likely to visit shopping destinations located in poorer areas (lowest percentile of house prices). In contrast, individuals living in poorer areas do not show any preference difference in visiting richer or equally poor areas to cover their shopping needs. A potential interpretation of the above, relevant for policy makers, could be that a pound earned in the most affluent areas is more likely to be spent, hence distributed, in similarly affluent areas, while a pound earned in the least affluent areas is more likely to be equally distributed across space. Therefore, in the long run, wealth accumulation would favour more the already wealthy areas in Leeds compared to the rest leading to increased spatial inequalities. In a similar way, individuals living in areas with a higher percentage of white residents are less likely to shop in areas at the lowest percentile of white residents. Nonetheless, the same does not hold for individuals living in those areas at the lowest percentile as they are more willing to visit shopping destinations located in areas at the second and third percentile than in areas similar to theirs. As in every other problem in the urban context, there is of course a circular causality to disentangle here, as well (Bettencourt, 2021). According to that, all of the above, could be the result of the agglomeration of higher quality elemental shopping stores or better urban environment in general in richer or white dominated areas, which leads to a reinforcing feedback loop favouring specific areas over others. That is exactly the problem that policy makers could try to alleviate by breaking that loop with the implementation of proper policy measures to provide relevant investment incentives in less affluent areas, as well.

A Box-Cox transformation of parking areas captured significantly positive, but also decreasing sensitivities as the area of parking increases. The presence of major retail attractions per shopping category (clothes, grocery, other) significantly increases the likelihood of visiting the shopping destination for trips of the respective shopping category. With regard to the direction of travel, shopping destinations located in places where the angular deviation between OS and OD is greater than 90° are less likely to be chosen compared to others, conforming to our initial assumptions.

The estimated multiplier ϕ of the logarithm of the composite size variable is significantly lower than 1.0 in all of the models presented. According to Kristoffersson et al. (2018), that hints to instances of significant unobserved correlation among the elemental alternatives within the aggregate shopping destinations used in the choice set. An increased cumulative retail floor area of grocery, clothes and durable stores in a destination acts as a more significant attractor for trips of the respective shopping category than population that was used as the base size variable. Furthermore, the cumulative floor area of grocery stores and an increased store type variability in neighbouring destinations in medium distances (1000-2000 m) will add to the attraction of the shopping destination, when the subsequent trip is also for shopping.

Regarding the estimated sensitivities of PCS-LCCM, *class a* representing individuals with significant space-time constraints has the highest travel time for car/PT and walking distance sensitivity for the first trip to the shopping destination. At the same time, those individuals are half as sensitive for travelling to the following activity location by a motorised mode and equally sensitive for walking there. That indicates that individuals in *class a* are more likely to choose a shopping destination closer to their initial origin to cover their

shopping needs before travelling by car/PT to their next activity. Also worth noting is that the Box-Cox λ for walking distance of *class a* is above 1.0 indicating increasing marginal disutilities as distance increases. In contrast, *class b*, with individuals restricted within their usual area of movement, shows the smallest travel time and walking distance sensitivities for the first trip and the largest for the following one, meaning that they are more likely to choose a shopping destination closer to the destination of the following activity. Contrary to those, *class c* has time and walking distance sensitivities more in line with the estimates of the MNL-base model. All three classes show a decreasing marginal time disutility as the duration of the shopping activity increases. The same does not hold, however, across classes for the sensitivity to walking distance, with class a being the exception showing an increasing marginal disutility. Regarding cost sensitivities, *classes a* and *b* have similar base cost parameters, but *class a* also shows an increasing marginal cost disutility as captured by the Box-Cox λ and a decreasing one as income increases, while *class b* has a linear marginal cost disutility and an increasing one as income decreases. Finally, individuals in *class c* have a much lower and in fact not statistically significant linear base cost sensitivity, but one that increases proportionately to income. Most of the remaining parameters, i.e. angular deviation, locational parameters and size variables, were found to be generic across classes and their estimates are similar with those of the MNL-base and LCCM-base models. The only exception is the parameter capturing how likely is for individuals living in richer areas to go shopping to poorer areas, which has been allowed to differ across classes. According to the estimated PCS-LCCM, individuals in *class a* who live in richer areas have a dispreference to travel to poorer areas for covering their shopping needs, but the opposite is true for individuals in *class b*. Nonetheless, both of those parameters are not statistically significant. Residents of richer areas of *class c*, however, show an even higher and statistically significant dispreference for shopping in areas with lower house prices.

As already mentioned, according to the class allocation model, 24.8% of the sample is allocated to *class a*, therefore it is subject to space-time constraints, 29.3% to *class b* being subject to spatial cognition limitations and the remaining 45.9% is allocated to *class c*, labelled as the *explorers*, since they are willing to move in areas not visited before or at least not captured systematically during the survey period. With regard to the behavioural profiling of the estimated classes, *class a* is more likely to include individuals of higher household income above £65,000 (30.0% - average household income = £54,500), who are in a possession of at least one car (27.3% - average number of cars = 1.0), but also living in higher than average deprived areas (30.6% living in areas with $IMD > 30$ - average $IMD = 23.7$), live in a household of a size above 4 people (31.3% - average household size = 2.0) and be of younger age below 30 years old (27.9%) or older age above 60 years old (33.6% - average age = 39.5). According to the remaining sociodemographic attributes not used in the class allocation model, individuals in *class a* are more likely to be employed in social (28.8%) and legal occupations (42.9%) or be retired (33.9%), cohabiting with their partner (28.5%) and have at least three more employed adults in their household (28.0%). From that profile analysis, it can be concluded that those individuals could face space-time constraints mainly due to their family requirements and the need to accommodate the daily needs of the household members or due to their age. The highly deprived immediate neighbourhood that they reside might not provide the necessary incentives either in terms of infrastructure or general urban environment for them to wander in the space around them and explore new opportunities and amenities in neighbouring areas. As a result, they are more constrained to their pre-defined schedules and time budget constraints. Especially, for the case of the elderly individuals it is important to provide the necessary conditions to avoid cases of social exclusion.

With regard to *class b*, it is also more likely to include individuals of higher household income above £65,000 (39.2% - average household income = £54,000), who live in a household of a size above 4 people (38.1% - average household size = 2.0), but those also have a very low percentage of uniquely visited locations (44.6% have below 20% of uniquely visited locations). According to their remaining sociodemographic attributes, individuals in *class b*

5. Results

are more likely to be employed in the media/sports industry (45.1%) and technical (31.0%) and sales-related (31.6%) occupations, be in a possession of a season ticket for PT (34.6%) and live in a household with at least four more employed adults (38.1%). The behavioural profiling of *class b* indicates that those individuals are more likely to be bounded to their usual areas of movement due to the need to accommodate a significant amount of daily household needs, especially for the case of households with many employed individuals and probably not in a possession of a sufficient amount of private vehicles to accommodate all those individual needs. Contrary to *class a*, however, that increased number of employed individuals in *class b* might also provide the necessary incentives and be the reason behind the increased area of movement of those individuals, who are at least not bounded to their space-time constraints in a similar way as individuals of *class a*. The increased family commitments, however, do constrain their time budgets to not roam outside their familiar space to explore new opportunities and visit new locations. In order to understand the impact of the increased family commitments of individuals allocated into *classes a* and *b*, the ratio of personal to household income is calculated. According to that, the personal income of individuals allocated into *classes a* and *b* is more likely to be only a small percentage of the total household income with 29.3% and 33.3% allocated to *class a* and *b*, respectively, having a personal income of less than 20% of the total household income. Those allocation probabilities to *classes a* and *b* drop almost monotonically as their personal income ratio increases. That means that individuals in those classes are not the top earners in their family, hence are more likely to be involved with in-home activities to support the needs of the household.

Finally, *class c* is more likely to include younger individuals below 30 years old (48.3% - average age = 40.5) of lower household income below £35,000 (55.6% - average household income = £46,000) with no car ownership (54.5%) being alone in their household (67.0%) and visiting unique locations more frequently (51.0% have above 60% of uniquely visited locations). In addition, individuals in *class c* are more likely to be students (49.7%), working in maintenance and repairing occupations (61.8%) or be unemployed (55.1%) and be single with regard to their marital status (49.4%). That behavioural profiling hints to individuals free of the increased family commitments captured in *classes a* and *b* and hence able and willing to explore the space beyond their usual areas of movement.

Table 6.8: Fit statistics and estimated parameters of the modelling specifications

Fit statistics	MNL-base	LCCM	PCS-LCCM-generic	PCS-LCCM
<i>Log-likelihood (0)</i>			-11,045.05	
<i>Log-likelihood (model)</i>	-4,106.186	-3,988.274	-4,072.650	-3,958.099
<i>Adjusted ρ^2</i>	0.6235	0.6295	0.6264	0.6322
<i>AIC</i>	8,316.37	8,184.55	8,253.3	8,124.2
<i>BIC</i>	8,594.06	8,739.93	8,541.67	8,679.58
<i>Number of parameters</i>	52	104	54	104
<i>Number of individuals</i>			270	
<i>Number of observations</i>			1,541	
Parameters	Estimate (Rob. t-rat. 0) (Rob. t-rat. 1.0)			
	MNL-base	LCCM	PCS-LCCM-generic	PCS-LCCM
Households with car ownership (base: car-car/dest 1)				
<i>ASC dest 1 shift Car-PT/Car-Walking</i>	-1.6871 (-2.55)	-1.5334 (-2.25)	-1.5453 (-2.32)	-1.7506 (-2.15)
<i>ASC dest 1 shift PT-PT</i>	1.4219 (3.70)	1.5695 (3.86)	1.4275 (3.71)	1.6282 (4.14)
<i>ASC dest 1 shift Walking-PT/Walking-Walking</i>	2.5854 (9.25)	2.7180 (9.45)	2.6698 (9.40)	3.0955 (7.34)
<i>ASC rest Leeds CBD</i>	-2.2826 (-6.47)	-2.2197 (-6.08)	-2.2339 (-6.46)	-2.1619 (-5.84)
<i>ASC rest Leeds CBD PT-Car/Walking-Car/PT-PT/PT-walking</i>	1.7345 (4.20)	1.7530 (4.33)	1.6992 (4.27)	1.7232 (3.95)
<i>ASC rest Leeds CBD Walking-PT</i>	2.9668 (6.50)	2.9974 (6.49)	2.9381 (6.66)	3.2687 (5.76)
<i>ASC rest Leeds CBD Walking-Walking</i>	3.8365 (9.02)	3.9309 (8.98)	3.8931 (9.20)	4.0709 (8.05)
<i>ASC rest Leeds (no CBD)</i>	-0.6215 (-5.66)	-0.6500 (-5.59)	-0.6525 (-5.71)	-0.5632 (-4.94)
<i>ASC rest Leeds (no CBD) Car-PT/Car-Walking</i>	-2.8230 (-8.53)	-2.8247 (-8.97)	-2.6713 (-8.06)	-3.2396 (-7.29)
<i>ASC rest Leeds (no CBD) PT-Car/PT-PT/PT-walking/Walking-Car/Walking-PT</i>	-1.2653 (-5.59)	-1.4362 (-5.83)	-1.2973 (-5.66)	-1.6280 (-4.96)
<i>ASC rest Leeds (no CBD) Walking-Walking</i>	0.8037 (2.88)	0.8646 (2.99)	0.8828 (3.09)	0.7185 (1.50)

Continued on next page

Chapter 6. Probabilistic choice set formation incorporating activity spaces into the context of mode and destination choice modelling

Table 6.8 – continued from previous page

Parameters	Estimate (Rob. t-rat. 0) (Rob. t-rat. 1.0)			
	MNL-base	LCCM	PCS-LCCM-generic	PCS-LCCM
<i>ASC rest Yorkshire (no Leeds) Car-PT/Car-Walking/PT-Car/PT-PT/PT-Walking/Walking-Car/Walking-PT</i>	-1.7449 (-5.79)	-1.8331 (-5.76)	-1.6678 (-5.54)	-1.9882 (-5.47)
Shifts for households with no car ownership				
<i>Car-PT/Car-Walking/Walking-PT/Walking-Walking</i>	2.4892 (7.18)	2.2060 (7.11)	2.5350 (7.53)	2.7200 (7.01)
<i>PT-PT</i>	4.3207 (10.94)	4.1018 (10.27)	4.2962 (11.37)	4.7209 (9.61)
<i>PT-Walking</i>	3.1890 (7.06)	2.4761 (5.97)	3.2227 (7.29)	3.4159 (4.66)
Shifts for central areas outside Leeds city centre				
<i>Walking-PT/Walking-Walking</i>	2.0958 (3.41)	2.0963 (3.12)	2.1850 (3.66)	2.2892 (3.74)
Shifts for trips with more than 1 passenger				
<i>PT for first/following trip</i>	-1.4224 (-5.57)	-1.3454 (-5.22)	-1.4396 (-5.68)	-1.6195 (-5.33)
<i>Walking for first/following trip</i>	-0.5303 (-3.94)	-0.5217 (-4.25)	-0.5185 (-3.96)	-0.6501 (-4.46)
Shifts for students				
<i>Walking-Walking</i>	1.2361 (3.60)	1.2182 (3.32)	1.2759 (3.79)	1.7160 (3.28)
Shifts for married individuals				
<i>Walking-Walking</i>	-0.5279 (-2.10)	-0.7629 (-3.19)	-0.5077 (-2.01)	-0.6256 (-2.14)
LOS variables				
<i>Travel time car, PT for first trip (mins)</i>	-0.0996 (-11.46)	–	-0.0876 (-10.28)	–
<i>Travel time car, PT for first trip (mins) (class a)</i>	–	-0.0796 (-776.23)	–	-0.2033 (-4.24)
<i>Travel time car, PT for first trip (mins) (class b)</i>	–	-0.1217 (-3.98)	–	-0.0233 (-0.33)
<i>Travel time car, PT for first trip (mins) (class c)</i>	–	-0.1025 (-10.20)	–	-0.0989 (-6.60)
<i>Travel time shift for clothes shopping</i>	0.0371 (3.87)	–	0.0350 (3.75)	–
<i>Travel time shift for clothes shopping (class a)</i>	–	0.0321 (19.86)	–	-0.0752 (-1.07)
<i>Travel time shift for clothes shopping (class b)</i>	–	0.0188 (0.37)	–	0.0242 (0.36)
<i>Travel time shift for clothes shopping (class c)</i>	–	0.0310 (2.28)	–	0.0211 (0.96)
<i>Travel time shift for OSO trip chains</i>	0.0154 (2.44)	–	0.0139 (2.26)	–
<i>Travel time shift for OSO trip chains (class a)</i>	–	0.0542 (130.85)	–	0.1906 (2.24)
<i>Travel time shift for OSO trip chains (class b)</i>	–	-0.0066 (-0.30)	–	-0.0011 (-0.13)
<i>Travel time shift for OSO trip chains (class c)</i>	–	0.0109 (1.49)	–	0.0069 (0.67)
<i>Travel time shift for HWH tours</i>	-0.0477 (-4.55)	–	-0.0438 (-4.37)	–
<i>Travel time shift for HWH tours (class a)</i>	–	-0.0384 (-0.96)	–	0.0155 (0.25)
<i>Travel time shift for HWH tours (class b)</i>	–	-0.1006 (-1.77)	–	-0.0080 (-0.28)
<i>Travel time shift for HWH tours (class c)</i>	–	-0.0339 (-2.74)	–	-0.0639 (-3.57)
<i>Travel time shift for morning/weekend night</i>	-0.0513 (-3.45)	–	-0.0456 (-2.83)	–
<i>Travel time shift for morning/weekend night (class a)</i>	–	-0.0855 (-1.59)	–	-0.0961 (-1.22)
<i>Travel time shift for morning/weekend night (class b)</i>	–	0.0104 (0.28)	–	-0.0019 (-0.09)
<i>Travel time shift for morning/weekend night (class c)</i>	–	-0.0844 (-3.35)	–	-0.0755 (-1.69)
<i>Travel time multiplier for following trip</i>	1.2386 (2.94)	–	1.2813 (3.14)	–
<i>Travel time multiplier for following trip (class a)</i>	–	1.4275 (1.09)	–	0.4945 (-4.51)
<i>Travel time multiplier for following trip (class b)</i>	–	2.0494 (2.21)	–	7.7936 (0.26)
<i>Travel time multiplier for following trip (class c)</i>	–	1.0417 (0.44)	–	1.0793 (0.33)
<i>Shopping duration-travel time elasticity</i>	-0.3261 (-10.85)	–	-0.3540 (-10.71)	–
<i>Shopping duration-travel time elasticity (class a)</i>	–	-0.3522 (-3.68)	–	-0.3005 (-2.48)
<i>Shopping duration-travel time elasticity (class b)</i>	–	-0.2807 (-3.04)	–	-0.4121 (-1.72)
<i>Shopping duration-travel time elasticity (class c)</i>	–	-0.3573 (-9.15)	–	-0.3384 (-5.98)
<i>Box-Cox λ PT travel time</i>	0.7652 (-9.31)	–	0.7748 (-8.60)	–
<i>Box-Cox λ PT travel time (class a)</i>	–	1.3010 (6.57)	–	0.8088 (-1.54)
<i>Box-Cox λ PT travel time (class b)</i>	–	0.6012 (-6.86)	–	0.7093 (-2.87)
<i>Box-Cox λ PT travel time (class c)</i>	–	0.8025 (-6.36)	–	0.7856 (-5.86)
<i>Walking distance for first trip (km)</i>	-1.5930 (-12.60)	–	-1.4470 (-11.67)	–
<i>Walking distance for first trip (km) (class a)</i>	–	-7.4632 (-4.02)	–	-6.5966 (-3.36)
<i>Walking distance for first trip (km) (class b)</i>	–	-1.9114 (-2.80)	–	-0.1913 (-0.15)
<i>Walking distance for first trip (km) (class c)</i>	–	-1.3102 (-8.66)	–	-1.4650 (-5.42)
<i>Walking distance shift for OSO trip chains</i>	0.1981 (1.80)	–	0.2026 (1.88)	–
<i>Walking distance shift for OSO trip chains (class a)</i>	–	-1.2952 (-0.65)	–	2.8216 (1.81)
<i>Walking distance shift for OSO trip chains (class b)</i>	–	0.1782 (0.18)	–	-0.1261 (-0.36)
<i>Walking distance shift for OSO trip chains (class c)</i>	–	0.1886 (1.22)	–	0.2416 (1.18)
<i>Walking distance multiplier for following trip</i>	1.2272 (2.41)	–	1.2660 (2.58)	–
<i>Walking distance multiplier for following trip (class a)</i>	–	0.1448 (-8.04)	–	1.2761 (1.27)
<i>Walking distance multiplier for following trip (class b)</i>	–	1.0851 (0.41)	–	22.2251 (0.13)
<i>Walking distance multiplier for following trip (class c)</i>	–	1.4818 (2.63)	–	0.7755 (-0.83)
<i>Box-Cox λ walking distance</i>	0.7887 (-4.08)	–	0.8219 (-3.21)	–
<i>Box-Cox λ walking distance (class a)</i>	–	1.7529 (1.44)	–	1.8287 (1.76)
<i>Box-Cox λ walking distance (class b)</i>	–	0.8440 (-0.89)	–	2.0684 (0.29)
<i>Box-Cox λ walking distance (class c)</i>	–	0.8353 (-1.98)	–	0.9832 (-0.12)
<i>Shopping duration-walking distance elasticity</i>	-0.1443 (-4.32)	–	-0.1593 (-4.45)	–
<i>Shopping duration-walking distance elasticity (class a)</i>	–	0.1608 (1.13)	–	0.1591 (1.89)
<i>Shopping duration-walking distance elasticity (class b)</i>	–	-0.3807 (-2.13)	–	-0.1580 (-0.91)
<i>Shopping duration-walking distance elasticity (class c)</i>	–	-0.1398 (-3.06)	–	-0.2710 (-4.08)
<i>Travel cost (£)</i>	-0.5887 (-8.44)	–	-0.5165 (-7.46)	–
<i>Travel cost (£) (class a)</i>	–	-2.7637 (-8.71)	–	-0.9448 (-2.38)
<i>Travel cost (£) (class b)</i>	–	-0.6751 (-2.40)	–	-1.1802 (-1.66)
<i>Travel cost (£) (class c)</i>	–	-0.4275 (-5.33)	–	-0.1618 (-1.06)

Continued on next page

5. Results

Table 6.8 – continued from previous page

Parameters	Estimate (Rob. t-rat. 0) (Rob. t-rat. 1.0)			
	MNL-base	LCCM	PCS-LCCM-generic	PCS-LCCM
<i>Box-Cox</i> λ travel cost	0.5900 (-7.43)	–	0.6568 (-6.02)	–
<i>Box-Cox</i> λ travel cost (class a)	–	0.8878 (-0.68)	–	1.2473 (1.83)
<i>Box-Cox</i> λ travel cost (class b)	–	1.0110 (0.03)	–	1.0049 (0.04)
<i>Box-Cox</i> λ travel cost (class c)	–	0.7106 (-3.93)	–	0.7888 (-0.81)
Cost-Personal income elasticity	-0.2862 (-2.91)	–	-0.3112 (-2.72)	–
Cost-Personal income elasticity (class a)	–	0.1863 (1.92)	–	-0.5483 (-2.54)
Cost-Personal income elasticity (class b)	–	0.7297 (1.11)	–	0.5531 (1.21)
Cost-Personal income elasticity (class c)	–	-0.5207 (-3.03)	–	-1.0933 (-1.54)
Direction of travel				
Presence of angle > 90° between O-S and O-D	-0.2621 (-2.22)	-0.2968 (-2.55)	-0.1920 (-1.58)	-0.2424 (-1.87)
Locational variables				
Parking areas (400m buffer)	0.1036 (4.00)	0.1091 (4.34)	0.1057 (4.05)	0.1151 (4.20)
<i>Box-Cox</i> λ for parking areas (400m buffer)	0.4219 (-7.86)	0.4189 (-8.39)	0.4237 (-7.94)	0.4085 (-8.44)
Living in rich areas - shopping in poor areas	-0.6817 (-2.51)	–	-0.7166 (-2.64)	–
Living in rich areas - shopping in poor areas (class a)	–	0.1737 (0.31)	–	-0.8626 (-0.85)
Living in rich areas - shopping in poor areas (class b)	–	0.1674 (0.33)	–	0.5875 (0.70)
Living in rich areas - shopping in poor areas (class c)	–	-1.0518 (-2.71)	–	-2.2892 (-2.62)
Living in areas with high % of whites (quart.4) - shopping in low % whites (quart.1)	-0.3732 (-1.72)	-0.3971 (-1.90)	-0.3664 (-1.68)	-0.2679 (-1.10)
Living in areas with low % of whites (quart.1) - shopping in high % whites (quart.4)	0.2889 (1.07)	0.2830 (0.93)	0.3011 (1.06)	0.4794 (1.61)
Living in areas with low % of whites (quart.1) - shopping in medium % whites (quart.2-3)	0.5348 (2.72)	0.5826 (3.05)	0.5576 (2.76)	0.6755 (2.99)
Major clothes shopping retailers (400m buffer)	1.3288 (6.03)	1.3515 (6.09)	1.3211 (5.94)	1.3672 (5.87)
Major grocery retailers (400m buffer)	0.4576 (4.51)	0.4657 (4.40)	0.4469 (4.33)	0.4180 (3.84)
Major durables retailers (400m buffer)	2.0015 (2.51)	1.9768 (2.59)	2.2064 (2.64)	1.9689 (2.74)
Size variables				
Natural logarithm multiplier ϕ	0.6638 (-3.88)	0.6698 (-3.59)	0.6594 (-3.93)	0.6730 (-3.71)
Population (400m buffer) (base)	1.0000 (–)	1.0000 (–)	1.0000 (–)	1.0000 (–)
Retail areas for clothes (400m buffer) (log.)	0.4515 (0.95)	0.4260 (0.86)	0.4833 (1.00)	0.5543 (1.04)
Retail areas for groceries (400m buffer) (log.)	0.8961 (2.24)	0.8995 (2.15)	0.9113 (2.27)	1.0641 (2.53)
Retail areas for durables (400m buffer) (log.)	0.3905 (0.56)	0.2969 (0.42)	0.3035 (0.44)	0.2744 (0.38)
Shopping store variability when following trip purpose is shopping (1000-2000m buffer) (log.)	2.1171 (1.75)	1.8938 (1.38)	2.0269 (1.58)	1.9265 (1.35)
Retail areas for groceries when following trip purpose is shopping (1000-2000m buffer) (log.)	-0.8628 (-1.08)	-0.9231 (-1.18)	-0.7967 (-1.02)	-0.6079 (-0.80)
Class allocation model				
Constant class a	–	-2.6019 (-1.94)	-0.8920 (-3.97)	-1.9282 (-1.93)
Constant class b	–	-1.9054 (-1.01)	-3.1578 (-0.85)	-0.7224 (-0.65)
Household income class a	–	-0.0326 (-1.74)	–	0.0165 (1.98)
IMD 400m around home class a	–	0.0355 (2.02)	–	0.0281 (2.32)
No car ownership class a	–	-1.6226 (-2.22)	–	-1.2401 (-2.62)
Population 400m around home class a	–	1.0254 (1.73)	–	-0.1348 (-0.31)
Low unique visits class a	–	1.1357 (1.59)	–	0.6834 (1.25)
Household size above 4 members class a	–	0.4062 (0.25)	–	0.9635 (0.70)
Age below 25 years old class a	–	-0.8398 (-0.82)	–	0.6862 (1.20)
Age above 60 years old class a	–	-0.4860 (-0.61)	–	0.6982 (1.24)
Household income class b	–	0.0016 (0.16)	–	0.0095 (1.28)
IMD 400m around home class b	–	0.0102 (0.49)	–	0.0088 (0.63)
No car ownership class b	–	0.9518 (1.23)	–	-0.2809 (-0.36)
Population 400m around home class b	–	-0.1769 (-0.15)	–	-0.3375 (-0.50)
Low unique visits class b	–	1.8876 (2.74)	–	1.4264 (1.66)
Household size above 4 members class b	–	2.1574 (1.42)	–	1.4468 (1.28)
Age below 25 years old class b	–	-0.3860 (-0.34)	–	-0.9790 (-0.71)
Age above 60 years old class b	–	-2.6021 (-0.45)	–	0.0576 (0.06)

Besides the improvements in model fit and the interesting behavioural insights derived from the PCS-LCCM specification, it is also important to note the discrepancies across models in the trade-offs of the individuals as captured by the Values of Travel Time (VTT) estimates, depicted in *Table 6.9*. In general, car VTTs are higher than PT values and VTTs for the first trip leg (shopping trips) are smaller than the ones for the following trips, which also include commuting trips, among others. According to the VTTs across the models examined, the values derived from PCS-LCCM are larger than the VTTs from the remaining models indicating the impact of capturing latent constraints on the VTT estimation. Furthermore, demand elasticities for different scenarios referring to a 1% increase in cost and time for

Table 6.9: Comparison of Values of Travel Time estimates across models (£/hr)

Parameters	MNL-base	LCCM	PCS-LCCM-generic	PCS-LCCM
Shopping trip				
<i>Car</i>	11.38	15.46	11.98	28.13
<i>PT IVT</i>	7.29	9.65	7.51	14.86
Following trip				
<i>Car</i>	13.17	18.52	14.46	30.61
<i>PT IVT</i>	11.01	15.18	11.68	21.63

Table 6.10: Comparison of demand elasticities across models

Parameters	MNL-base	LCCM	PCS-LCCM-generic	PCS-LCCM
Increase car cost by 1%				
<i>Car</i>	-0.122	-0.100	-0.105	-0.089
<i>PT</i>	0.340	0.287	0.300	0.300
<i>Walking</i>	0.180	0.150	0.154	0.121
Increase PT cost by 1%				
<i>Car</i>	0.059	0.056	0.057	0.061
<i>PT</i>	-0.549	-0.516	-0.516	-0.526
<i>Walking</i>	-0.016	-0.016	-0.017	-0.021
Increase car time by 1%				
<i>Car</i>	-0.383	-0.365	-0.348	-0.291
<i>PT</i>	1.187	1.182	1.068	0.938
<i>Walking</i>	0.548	0.517	0.500	0.424
Increase PT IVT by 1%				
<i>Car</i>	0.090	0.087	0.087	0.077
<i>PT</i>	-0.748	-0.747	-0.698	-0.637
<i>Walking</i>	-0.039	-0.030	-0.039	-0.025

car and PT are presented in [Table 6.10](#). From that comparison, it can be concluded that PCS-LCCM leads to generally more modest demand elasticities/cross-elasticities compared to the remaining specifications examined. It is important to note the significant overestimation of demand elasticities resulted from MNL-base in all scenarios examined both for time and cost and across modes. Similar findings were also derived in the study of Basar and Bhat (2004) indicating important policy implications from choice set misspecification.

6 Conclusions

In the current study, we focused on proposing a specification able to capture space-time and spatial awareness constraints in a spatial choice context. The study illustrates that the proposed approach is able to perform better than a range of other specifications used for comparison purposes. Furthermore, the study also demonstrates the impact of capturing latent choice set formation mechanisms in the estimated VTT values and demand elasticities, which can be important measures of analysis from a policy perspective.

The geography-derived notions of Activity Spaces have been utilised in this study to define proxy measures for capturing the aforementioned latent space-time and spatial awareness constraints. Nonetheless, other measures could also be used for that purpose and future studies should continue on that direction to provide more computationally efficient ways of defining latent consideration choice sets in a spatial choice modelling context and its inherent

complexity.

As a limitation of the current, we should acknowledge the limited duration of the survey, which could have significant impacts on the proper estimation of the Standard Deviation Ellipses. In fact we could easily assume that we would end up with larger SDEs as a result of capturing more trips, which seem as less frequent ones with the current utilised dataset. On the other hand, however, we also can not exclude the possibility that the significant spatio-temporal regularities of travel would put more weight to specific locations leading to less variance and noise and more compact SDEs for specific individuals than the current ones.

In any case, the current study proposes an operational implementation of Manski's framework and its IAL version suitable and applicable for a spatial choice context with the necessary simplifications to make the problem computational tractable. The study also demonstrates that Activity Spaces can be incorporated as proxy measures of capturing latent space-time and spatial cognition constraints leading to interesting insights that could inform policy making. The behavioural profiling of the estimated classes of the LCCM can provide invaluable information to policy makers for the purpose of proposing measures more suitable to the constraints of the underlying population, while also being able to identify in time and prevent cases of social exclusion. More research efforts in that direction, however, are necessary to disentangle the inherent complexity behind the formation of latent constraints and choice set elicitation mechanisms.

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Chapter 7

Discussion and conclusions

1 Summary

This thesis has made several contributions on the use of semi-passively collected datasets for behavioural modelling and have made several methodological and applied contributions in an attempt to prove their usefulness. In the introduction a number of research gaps have been identified. This chapter starts by linking the relevant contributions made in each of the previous chapters with the identified research gaps in *Chapter 1*, before drawing final concluding remarks by considering all the work together as a whole.

RG1: Limited use of GPS trip diaries for spatial disaggregate behavioural modelling.

Despite the benefits that GPS data can bring to the study of individual mobility behaviour, the significant pre-processing requirements to make the data usable for behavioural modelling has hindered their wider adoption among researchers and practitioners. In the current thesis, a 2-week GPS trip diary has been utilised as the main dataset for the purpose of increasing the research community's trust into using such forms of datasets by documenting the required steps needed to make the data usable for behavioural modelling and by addressing open research questions in the process. The GPS trip diary was collected as part of the research project "DECISIONS" conducted by the University of Leeds between October 2016-March 2017 and can be characterised as a form of a semi-passive GPS data, where minimum input by the participants is provided at the end of each trip and the data is complemented with a background survey capturing the respondents' sociodemographic attributes. In addition, further steps were performed and documented in the previous chapters for the purpose of enriching the GPS trip diary with additional information, which mostly referred to the non chosen alternatives. Readily available Application Programming Interfaces (APIs) were used for that purpose, namely the Google "Directions" and Bing Maps APIs, for which algorithmic procedures were developed to extract and store the relevant trip- and mode-specific information. The APIs were also used for the re-calculation of times and distances for the chosen alternatives to ensure that information coming from the same data generation process would enter the specifications of the behavioural models. The stated times and distances were used instead as a means of validation of the resulting API-based values. Time of day and day of the week were also important parameters for the queries passed on to the APIs to ensure that individual constraints for specific time periods and days would be adequately represented and captured in the models. Travel cost information also had to be added both for chosen and non chosen alternatives, as well, which was computed separately for car, taxi and public transport modes, i.e. bus and rail. For car, the specifications of WEBTag regarding fuel and operating costs were utilised, while parking costs were also added

based on the destinations visited (e.g. central areas) and the activity durations captured there. An average cost based on area-specific fixed, hourly and distance-based fares was computed for taxi by taking into account the Local Authority within which each trip. Finally, a distance-based fare was computed for bus and rail trips and a discount was applied for season ticket holders. Additional locational data, important for the specification of a spatial model, were acquired from the Office of National Statistics and OpenStreetMaps.

The aforementioned procedure of enriching a GPS trip diary both during the data collection process and after it, resulted in a dataset not only rich in mobility information, but also rich in semantic information, as well, with the latter being a common limitation in emerging datasets hindering their wider use for behavioural modelling. The specifications presented in the thesis were able to prove that such a dataset can lead to behaviourally intuitive estimates with expected signs (Chapters 2-6), realistic individual trade-offs and willingness-to-pay measures (Chapters 3 and 5) and demand elasticities (Chapter 4), while the increased granularity and panel sizes provide the necessary leverage for capturing additional unobserved heterogeneity (Chapters 3, 5, 6) and tackle issues of choice set formation (Chapters 2, 6). Analysing individuals choices in the spatial context, has been a core focus of the current thesis due to its inherent complexity. The multitude of open research questions in the field of spatial choice modelling has provided the ideal environment to explore the potential benefits of GPS trip diaries and identify their limitations.

RG2: Lack of a systematic comparison between estimates derived from GPS and other traditional data sources.

Despite the fact that it is understood in the transport research community that new emerging semi-passively collected data sources can provide significant benefits over traditional sources, there is still not an attempt to document those comparisons in a systematic way. Accumulated knowledge from studies over the years has identified several limitations of traditional Revealed Preference (RP) data from pen-and-paper trip diaries, such as travel time and cost misreporting and omission of smaller duration trips. Consequently, researchers and practitioners have put more trust in Stated Preference (SP) data, which have become the dominant data source for Values of Travel Time (VTT) estimation with RP data being used in limited scale to provide meaningful attributes for pivoting the SP designs around them. Significant efforts have also been conducted to account for the presence of hypothetical bias and its adverse effects with the state-of-the-art approaches being implemented in the latest national VTT studies in various European countries. Despite the methodological improvements in SP designs the fact remains that transport appraisal and hence decisions on future investment largely depend on responses to hypothetical scenarios. That inertia to already established methods and approaches hinders the adoption or at least the experimentation with new emerging data sources for VTT estimation and how those estimates would compare with official SP-based ones. Voices of concern pointing to the need of reconsidering the use of new emerging RP data have been raised since almost a decade ago (Daly et al., 2014), but still no additional relevant studies can be found in the literature. The current thesis provides such a comparison in Chapter 3 by estimating VTT values from a behavioural model following the methodology of the latest UK study (Batley et al., 2019). Chapter 6 also provides an indirect comparison between two LCCM models, one estimated on a GPS trip diary and the second on a traditional trip diary. The comparison is performed on the basis of the ease of capturing unobserved heterogeneity even in the case of smaller sample sizes. Overall, the aim behind addressing RG2 is to steer the research community towards the direction of increasingly considering the new types of RP datasets at least as complementary data to traditional trip diaries and SP surveys, especially if they can achieve the same level of accuracy with smaller sample sizes, although more studies are necessary to establish that finding.

RG3: Current literature focusing on contrasting Machine Learning and Discrete Choice Modelling rather than combining the two approaches.

Machine Learning (ML) approaches have inadvertently entered the field of transport

research as a response to the need of analysing data of increasing complexity, such as the case of new emerging datasets. The necessity of comparing and contrasting ML algorithms with already established econometrics techniques, such as Discrete Choice Modelling (DCM), could be justified in the initial stages of their introduction to the field, to identify their merits and limitations. Nonetheless, it is worth mentioning that the focus of the literature solely in their comparison has the potential negative consequence of missing the benefits that can potentially arise from their integration. In the current thesis, ML-DCM have been effectively combined by using ML approaches both during pre-processing (Chapters 2-6) and as an integral part of a behavioural model (Chapter 5). More specifically, due to the unique nature of each GPS trace in the initial trip diary, a clustering algorithm had to be implemented in order to define unique activity locations and general shopping areas, thus moving into a finer spatial resolution and taking advantage of the granularity of GPS data. That step forms the basis for the subsequent analysis in the thesis. In addition to that, an ML approach is also proposed in Chapter 5 as an integral part of a behavioural model, namely a Latent Class Choice Model (LCCM). In that integrated ML-DCM framework, a deterministic clustering algorithm effectively takes the part of the class allocation model of a traditional LCCM specification by transforming it into a probabilistic one, while a choice model at the lower model is used to capture individual choice behaviour. Both model components are estimated jointly, thus the clustering algorithm is being adjusted based on feedback from the choice model, until convergence is reached for both. The proposed approach is able to take advantage of the best of both worlds by utilising an ML algorithm for pattern recognition and a DCM for understanding choice behaviour, without compromising the microeconomic interpretability of the modelling outputs at the same time.

2 Objectives and contributions

Several approaches have been proposed throughout the thesis for the purpose of meeting the objectives defined in Chapter 1, which are described in the following.

M1: Provide a more detailed representation of individual mode and location choices for discretionary activities (addressing RG1 and RG3).

Objective M1 has been met in Chapters 2, 4, 5 and 6, in which issues of reducing large choice sets, accounting for spatial correlation and uncovering unobserved heterogeneity and latent constraints, all common in spatial choice modelling, have been addressed. Integral parts of those studies are the finer definitions of shopping location alternatives in the form of general shopping areas instead of limiting the analysis to common UK geographical areas (e.g. MSOA zones) and the attempt to capture the impact of the following activity, as well, to the choice of the intermediate shopping location. The definition of shopping areas was performed by clustering elemental observed shopping destinations using a Hierarchical Agglomerative Clustering (HAC) algorithm with a 800m distance threshold -after trying a range of different thresholds- which led to the creation of distinct shopping clusters within the same geographical boundaries further enabling the capture of heterogeneity in choices among individuals. It is worth mentioning that this approach would not have been possible with traditional trip diaries, which usually provide a more coarse spatial resolution. Furthermore, by including the influence of the following activity type and its location (considered fixed) allows to better capture the detour or the deviation the individuals are willing to make from the straight path between the previous origin O and the following destination D in order to reach an intermediate shopping location S , which can depend on the chosen modes for the two legs, trip-specific and individual-specific characteristics. In addition, capturing travel time and walking distance sensitivities for both trip legs allows the analyst to understand where the shopping activity will occur within the range between O and D , i.e. closer to the previous origin or to the following destination. The results largely indicate that individuals tend to have a higher travel time and walking distance sensitivities for the following trip

meaning that they are more likely to choose an intermediate shopping destination closer to the destination of the following activity, all else held equal. Further discrepancies, however, can emerge when accounting for unobserved heterogeneity in the sample, such as in the model presented in Chapter 6, where different segments of the sample show opposite sensitivities regarding the shopping and the following trip. Additional interesting insights emerge when accounting for the individuals' surrounding living environment and how that might affect their decisions to go shopping to specific locations, e.g. individuals living in richer areas being less likely to go shopping to poorer areas. The more detailed representation of individual mode and shopping location choices led to a number of interesting policy insights, similar to the aforementioned ones, which otherwise would most likely remain hidden within aggregated zonal alternatives.

M2: Examine concepts around choice set formation in a spatial context (addressing RG1).

Objective M2 has been met in Chapters 2 and 6. In both chapters, concepts from time-space and behavioural Geography were implemented to provide proxy measures of space-time and spatial cognition constraints to aid the process of two different approaches around choice set generation, namely the formation of sampled choice sets and the formation of latent consideration sets. In Chapter 2, Detour Ellipses (DEs) and Standard Deviational Ellipse (SDEs) are created to provide strata for importance sampling, where after selecting the chosen alternative, alternatives within the smaller DEs are sampled with a higher probability than those within SDEs. Finally, alternatives from the remaining space are also sampled, albeit with a lower probability from the other two strata, to complete the pre-defined choice set sizes. As such, all alternatives have a non-zero probability of being included, thus the DEs and SDEs act as soft constraints acknowledging the uncertainty in their estimation. Furthermore, the inclusion of alternatives from all strata in the sampled choice set has the purpose of providing the necessary balance between relevant and irrelevant alternatives and to help the behavioural model to capture meaningful trade-offs from the observed choices. The proposed sampling protocol is compared with random sampling and a range of other importance sampling protocols incorporating different combinations of the utilised forms of Activity Spaces. The outputs indicate that stratified importance sampling, besides needing an additional sampling correction term to be included in the utility function, in all cases they offer a more efficient alternative approach to random sampling. The proposed protocol incorporating both forms of Activity Spaces also outperforms the remaining importance sampling protocols, since the additional stratum defined by the SDE provides an additional pool of alternatives to sample from, which are more relevant to the individual than the remaining ones from the global choice set. Activity Spaces of the same form are utilised again in Chapter 6, but this time for the purpose of providing proxy measures of space-time and spatial cognition constraints and uncovering latent choice set formation mechanisms. To achieve that, an LCCM is specified, where each class has a different choice set, while class-specific LOS parameters were also specified to account for potential confounding between choice set constraints and individual heterogeneity. According to that specification, classes a and b adhere to different forms of latent constraints, namely space-time and spatial cognition respectively, while class c represents individuals that are free to roam and explore the space around them. The proposed model provides significant improvements in terms of model compared to an LCCM, where only heterogeneity in sensitivities is captured without accounting for the presence of latent consideration sets. The behavioural interpretation of the estimated classes indicates to the presence of significant housekeeping responsibilities for individuals who live in large households with many members and are not the top earners in their household, which leaves them limited time to explore more opportunities in the surrounding space. On the contrary, single individuals and those with generally more time available, such as students, are more likely to belong to class c and hence be in a position to better explore opportunities in the urban environment. Insights like that captured from models accounting for the potential presence of latent constraints in the choice set formation can lead to better informed policy

measures addressing the needs of individuals in a more efficient way.

M3: Propose an efficient framework for capturing spatial correlation among locations by treating space as continuous (addressing RG1).

Objective M3 has been met in Chapter 4, where a Cross Nested Logit (CNL) model was proposed with the ability to account for spatial correlation among locations both for a destination choice model (conditional on the mode) and a joint mode and destination choice model. The proposed framework is based on the first Law of Geography postulating that “*everything is related to everything else, but near things are more related than distant ones*” (Tobler, 1970) and it aims to capture correlation among locations based on spatial proximity, while acknowledging the continuous nature of space instead of discretising it into disjoint nests, such as the case of the most commonly used Nested Logit (NL) model. More specifically, the main principle behind the proposed approach is to define a nesting structure, where the number of nests equal the number of destination alternatives in the choice set and each destination is allocated to every nest with a non-zero allocation probability parameterised as a function of its distance from every destination-nest. The allocation probabilities follow a distance decay function indicating a higher allocation of an destination alternative to its own nest, with the allocation probabilities decreasing with distance. The methodology developed is first applied on a destination choice model conditional on mode, where its benefits over previously proposed approaches in the literature are clearly illustrated. A demand elasticity analysis at the individual level illustrates the benefits of the proposed approach to capture more realistic substitution patterns. The core methodology is then further extended to accommodate joint choice dimensions of mode and destination choices, where it is illustrated how the proposed model is able to capture correlation across both choice dimensions and across all destination at the same time. A demand elasticity analysis in that case also highlights the important implications on the effectiveness of policy measures, if spatial correlation among locations is left uncaptured.

M4: Explore potential benefits arising from the integration of Machine Learning and Choice Modelling (addressing RG3).

Objective M4 has been met throughout the studies presented in the thesis and more explicitly in Chapter 5. More specifically, as previously mentioned an Hierarchical Agglomerative Clustering was used during the initial stages of pre-processing to handle the unique pairs of latitude-longitude coordinates of the observed visited destinations and to define unique activity locations per individual. That has allowed the identification of home-work locations (also based on the time and duration of visit), the creation of daily tours starting and finishing at the home locations and finally the identification of tour-based feasibility constraints for the definition of mode availability. HAC was also used to define general shopping areas forming the location alternatives in the choice sets of the corresponding models developed providing the additional benefit of analysing individual shopping behaviour in a finer spatial resolution. Besides that, in Chapter 5, a probabilistic adaptation of the deterministic K-Means clustering algorithm was developed to effectively take the role of a class allocation model in an LCCM framework allocating individuals probabilistically into latent classes. The transformation to a probabilistic K-Means algorithm is achieved by considering the distance of every data point -in that case the sociodemographic covariates- from the cluster centroids, which are randomly assigned in the first iteration. As such, the data points instead of being deterministically allocated to their closest centroid, they are instead allocated with a non-zero probability to every centroid, but still with a higher probability to their closest one (similar to the distance decay approach for the allocation probabilities in Chapter 4). After the allocation of individuals into latent clusters, a cluster-specific choice model is estimated to understand individual choice behaviour. Therefore, a framework like that can take advantage of the best of worlds, with ML and DCM components being responsible for tasks where they excel, respectively. More importantly, however, that integrated framework still provides the necessary microeconomic interpretability in the final model outputs, which can further be used

for policy-oriented post-processing analysis, such as deriving willingness-to-pay measures and demand elasticities. The proposed framework was applied in separate models of mode and destination choices and in two different datasets, namely the GPS trip diary that was used throughout this thesis and a pen-and-paper trip diary. In all cases examined, the proposed approach performed at least the same, if not better, from a traditional econometric LCCM specification in terms of model fit. The most important benefit, however, becomes evident by examining the behavioural profiling of the estimated latent classes/clusters, which in almost all cases was more behaviourally intuitive for the ML-DCM integrated framework than the econometric LCCM hinting to the improved pattern recognition abilities of ML, even with a simple clustering algorithm, such as K-Means. The same framework can also be extended to include more advanced deterministic clustering algorithms, which can be turned into probabilistic ones in a similar manner.

A1: Focus on the practical applicability of proposed modelling frameworks by reducing their computational cost (addressing RG1).

Objective A1 was met in Chapters 2, 4 and 6. In Chapter 2, an efficient stratified importance sampling protocol was proposed by incorporating different forms of Activity Spaces reaching a higher level of sampling accuracy and stability for the same choice set size compared to random sampling and other forms of importance sampling, as well. The outcomes of that study could potentially lead practitioners to step away or at least reconsider the use of random sampling for reducing choice set sizes, as the higher probability of including irrelevant alternatives will inevitably lead to the need of sampling a larger number of alternatives, thus unnecessarily increasing the computational cost. The inclusion of an additional layer encompassing spatial awareness, compared to the existing importance sampling protocols in the literature (Leite Mariante et al., 2018), helps to add a further structure upon space to sample alternatives located within that space with a higher probability compared to the remaining space. In Chapter 4, the CNL specification developed, which is able to capture spatial correlation across location alternatives by treating space as continuous, is computationally more efficient than the equivalent Paired Combinatorial Logit (PCL) (Sener et al., 2011) and Error Component (EC) (Weiss and Habib, 2017) models, currently proposed in the literature. For a destination choice model, conditional on mode, the CNL model is able to outperform the PCL specification, while also being computationally significantly faster (by a factor of more than 10). Furthermore, the proposed CNL model is able to scale better in joint models of mode and destination choices being able to handle larger choice sets, while at the same capturing correlation simultaneously among all choice dimensions, contrary to the more widely-used Nested Logit model, where correlation is captured only along $C-1$ choice dimensions, where C is the number of choice dimensions in the joint model. Finally, in Chapter 6 an attempt of incorporating a probabilistic choice set formation framework for a spatial choice model has been proposed with the necessary simplifications to make it computationally tractable in the spatial context. The proposed framework is based on Manski’s two-stage probabilistic choice set formation model (Manski, 1977) and specifically on its Independent Availability Logit (IAL) version proposed in Swait and Ben-Akiva (1987). The incorporation of mode- and trip-specific Detour Ellipses and individual-specific Standard Deviation Ellipses helps to avoid the need to evaluate the inclusion probabilities of each mode-destination alternatives separately in the choice set. The proposed framework, instead, assumes that alternatives within those spaces will have the same probability of being included in the consideration set, which significantly increases the computational efficiency, but at the same time still capturing significant and behaviourally intuitive latent constraints, which can be important from a policy perspective. Those three studies also clearly demonstrate the potential policy implications resulting from utilising simpler modelling frameworks ignoring cases of including more irrelevant alternatives in sampled choice sets, not accounting for spatial correlation and not capturing the impact of latent constraints in the consideration sets.

A2: Provide a systematic comparison of behavioural models and their respective

estimates utilising GPS trip diaries and traditional data sources (addressing RG2).

Objective A2 has been achieved in Chapters 3 and 5. Specifically, in Chapter 3 the Values of Travel Time (VTT) estimates obtained from the utilised GPS trip diary were compared against the official VTT estimates currently used in transport appraisal in the UK and are based on the latest nation-wide Stated Preference (SP) survey of 2014. For the purpose of offering a systematic review, the study follows as closely as possible the methodology developed in the latest UK VTT study reported in Batley et al. (2019), and Hess et al. (2017) and the validity of the resulting GPS-based VTT estimates was assessed based on their statistical difference from the official SP-based values. The negligible insignificant differences provide the necessary empirical evidence for the transport research community to increase its trust again on Revealed Preference data, which over the years fell out of favour compared to SP data due to the inherent limitations of traditional trip diaries. In addition to that, in Chapter 5 an indirect comparison between GPS and traditional trip diaries is also performed based on estimated LCCM specifications estimated on each dataset and the ease of capturing unobserved heterogeneity in the former. More specifically, the increased number of trips per individual on the GPS trip diary provides a data structure that can lead to the identification of more latent classes in the sample and with more covariates in the class allocation model, thus providing more value for policy making. The two aforementioned case studies provide initial evidence on the validity of GPS trip diaries for policy making, however, it is worth mentioning that additional similar studies are necessary to derive more concrete conclusions. Nonetheless, the two studies presented in the thesis provide an initial point of departure for future studies.

3 Outlook

In the current thesis, several topics relevant to incorporating GPS trip diaries for addressing research questions in spatial choice modelling and have been analysed. In addition to the aforementioned objectives and contributions, each chapter and its relevant study proposes several avenues for future research. In the following, those potential research questions are summarised with respect to the aforementioned research gaps.

The importance sampling protocol proposed in Chapter 2, despite the increase in efficiency relative to existing approaches, it does not answer the question of finding the most efficient combination of relevant and irrelevant alternatives in the sampled choice set, since both are needed for the model to identify meaningful trade-offs. Future studies could try to formulate sampling of alternatives as a case of an optimisation problem to better capture the right choice set size. Finally, it should be mentioned that observed Standard Deviation Ellipses were used to form one of the strata for sampling. A more generalised approach was followed in Chapter 6, instead, were the structural parameters of the observed Standard Deviation Ellipses were used as dependent variables for a range of linear regression models in order to re-create estimated Standard Deviation Ellipses.

The comparison of GPS-based and SP-based VTT estimates presented in Chapter 3 successfully illustrates the validity of current RP data enhanced by GPS-based data collection methods to capture behaviourally realistic time and cost trade-offs. The methodology developed aims to follow as closely as possible the official approach of the SP-based VTT study (Batley et al., 2019), however, certain discrepancies could not be avoided. The main limitation of that study is the generally smaller sample size of the GPS trip diary compared with the official SP survey. That limitation was further enhanced with the exclusion of London-based trips both in the estimation, as well as in the application datasets. The decision to exclude London trips was on the basis of having only a limited number of trips from London in the estimation data, which would lead to higher estimation errors for parameters regarding London-specific transport modes, such as the underground. In addition, the GPS dataset

includes mostly urban trips with a small range of trip distances. Nonetheless, the estimates were applied to larger distances in the application data to provide a more direct comparison with the distance-segmented VTT values in the official study. All three of the aforementioned limitations have an impact on the standard errors of the GPS-based VTTs, which are evident in the study. Parameters regarding the weather and the slope of the network, which could have an impact on the choice of active modes, such as cycling and walking, were not taken into account in the model. Finally, the inherent problem of choice set generation and the latent nature of the consideration choice set in RP dataset was not taken into account and alternative availability was deterministically defined based on feasibility checks and exogenous thresholds. Future studies should aim to account for the latent nature of consideration sets, as well as capture the impact of weather and slope on the estimation of willingness-to-pay measures and whether their discrepancies from the official VTTs increase or not.

The CNL specification in Chapter 4 presented a novel approach to capture spatial correlation in a continuous way among location alternatives and it showed that it can scale better in the case of larger choice sets, while being able to be easily extended to accommodate joint choice dimensions. Correlation was captured based solely on spatial proximity staying true to the first Law of Geography. Spatial proximity was defined based on straight distances among destinations, however other continuous variables could also be used, such as travel times and network distances, while time of day could also have an impact with different time periods during the day and different congestion levels having an effect on the perceived similarities among destinations. Further parameters could also influence individuals to perceive certain alternatives as more similar than others, besides spatial proximity, which would require a further investigation. Spatial proximity might be an efficient proxy measure to capture spatial proximity, but it can be easily understood that it is not the only factor.

The integrated ML-DCM framework presented in Chapter 5 is able to provide model fit improvements, as well as estimated latent clusters with a more intuitive behavioural profiling compared to the ones resulting from a traditional LCCM specification. The methodology developed, however, is subject to certain limitations most important of which is the random assignment of the initial cluster centroids during the first iteration, which can have a significant impact on the overall convergence of the model. That limitation can be sufficiently mitigated in models with two latent clusters, where assumptions about the sign directionality of specific covariates can help the estimation process. Nonetheless, the same does not hold for models with a higher number of latent clusters. The value of the proposed method, however, lies in its flexibility since it could be easily adapted to accommodate more advanced clustering algorithms, as well.

Finally, the probabilistic choice set formation framework developed in Chapter 6 provides a computationally more efficient approach suitable for the complexity of a spatial choice model uncovering space-time and spatial cognition latent constraints. A limitation quickly identified is the small duration of the survey and the GPS tracking of daily mobility behaviour (2 weeks), which can have a significant impact on the captured visited locations and hence on the estimated Standard Deviation Ellipses. The impact of the survey duration is not clear, however, as a higher duration could lead to more locations being visited in areas that are currently considered outside of the SDE, but it could also lead to put a higher weight to already visited locations in cases of higher spatio-temporal regularities reducing the variation/noise. Furthermore, that study illustrates that the utilised spaces can effectively act as proxies to help uncover latent constraints affecting the formation of consideration sets, however they are likely not the only choice set formation mechanisms affecting the respondents' decision making process. More similar studies are hence necessary to uncover latent spatial constraints utilising different proxy measures.

Overall, the work presented in this thesis demonstrates that semi-passively collected datasets are suitable to be used in behavioural modelling, while also having the potential of addressing current research issues much more rigorously than traditional data sources. At the same time, new avenues for future research are opening due to the high granularity of

GPS data and the large panels of individual mobility behaviour that can be collected from such trip diaries. More studies are necessary to increase the trust of the research community and the industry into utilising them on an everyday basis and using them as the base for new policy initiatives. The future research avenues presented in this section will continue to take advantage of GPS data and all the benefits they can provide in the field of disaggregate behavioural modelling. Those can be further enhanced by other forms of emerging datasets, such as mobile phone, smart-card or location-based social media data, which may lack in their spatio-temporal resolution compared to GPS data, but they can offer significantly larger sample sizes of mobility behaviour captured through multiple years. In any case, the abundance and the variability of new data sources will continue to challenge well-established methods and modelling frameworks, but through that new opportunities can emerge for the transport research community to provide answers to new research questions never posed before, always with the overall purpose of proposing better informed policy initiatives that more efficiently address the needs and the underlying behaviour of the targeted population.

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