The q-spread dimension and the maximum diversity of square grid metric spaces

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Abstract

The main aim of this thesis is to compute the growth rate of the q-spread and the maximum diversity for several square grids at various scales, then explain some of their characteristic mathematical features.

On one hand, we compute the growth rate of the q-spread of three different square grids at various scaling. For large n and very small scales as well as reasonably big scales, the growth rate of the q-spread of these squares are similar. This occurs because when the scale factor is small, we can heuristically map the points of the square grid to the solid square, and we numerically determine that the q-spread is seen to be very close to some quadratic equation. While, if the scale factor is big, we can approximate the q-spread of these squares to the q-spread of finite subset of points in the middle of these squares and we show that the q-spread of the square grid over some positive function approaches zero as a scale factor goes to infinity.

On the other hand, we compute the subsets of points for several square grids that admit a maximum magnitude with non-negative weightings at various scales which is the maximum diversity, and we see that the magnitude which has non-negative weighting for 4×4 and 5×5 square grids is the magnitude of orbits and union of orbits this implies the maximum diversity occurred for orbits or unions of such orbits. Therefore, we conjecture that maximum diversity always comes from orbits and union of orbits. Motivated by this, we prove that when the scale factor is very small, the magnitude of the orbit that contains the four corner points in the $n \times n$ square grid is bigger than the magnitude of any other orbit of the symmetry group. Also, we show that the set which contains the union of the four corner points and any other orbit has negative weighting. Furthermore, we look at the behaviour of the weights for the points in the middle row of the 201×201 square grid metric space at various scaling. We see that for very small scale and for the scale bigger than 0.6, the weighting of the points in the middle row of the space has non-negative weights, whereas different oscillations happens between the above scalings.

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I thought when I finished my Master's thesis, that I knew a lot about mathematics. The truth is, I knew nothing compared to the teaching system here in the Britain. Undertaking a PhD has been a life-changing experience for me, and I would like to take this opportunity to express my sincere appreciation to those who have contributed to this thesis and supported me in one way or another during this journey.

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Chapter 1

Introduction

In most mathematical topics there is a canonical notion of sizes, such as, sets having cardinality, vector spaces having dimension, probability spaces having entropy, and topological spaces having Euler characteristics. Leinster [29] added a new item to this already extensive list by noting that metric spaces have a magnitude for more details see Chapter 2. This chapter has three sections. The first section explains how a metric space can be viewed as an enriched category and where the magnitude of a metric space originally comes from. The second section provides a brief literature review of the magnitude. In the last section, an overview of the structure of this thesis is given.

§ 1.1 Where does magnitude come from

Consider C is a finite category whose objects are putting in some order $a_1, a_2, \ldots, a_n$. Let the matrix Z be an $n \times n$ matrix whose (i, j)-entry is the cardinality of the set of the morphisms from a_i to a_j denoted by $\#\,\mathrm{Hom}(a_i, a_j)$. A function $\omega : C \to \mathbb{R}$ with

$$\sum_{a_j \in C} \#\,\mathrm{Hom}(a_i, a_j)\omega_{a_j} = 1$$

for all $a_i \in C$ is called a **weighting** on C. If the category C has at least one weighting, then it has **the Euler characteristic** which is defined by Leinster [30] as

$$\chi(C) = \sum_{a_i} \omega_{a_i}.$$

This concept of Euler characteristic can be naturally generalized from categories to enriched categories. For example, given a category of vector spaces over a field K. This is a monoidal category with the product $\otimes$ is the usual tenser product $\otimes_K$ and unit K. So we can have a category enriched of vector spaces (with only finitely many objects $a_1, a_2, \cdots, a_n$), then the simple change in the above expression is $\#\,\mathrm{Hom}(a_i, a_j)$ to $\dim(\mathrm{Hom}(a_i, a_j))$.

In general, given the monoidal category $(V, \otimes, I)$, a notion of size of a category enriched in V is a function

$$|.| : (ob(V), \otimes, I) \to (k, ., 1),$$

with the property that $|X| = |Y|$ whenever $X \cong Y$ and satisfying the multiplication axioms $|X \otimes Y| = |X|.|Y|$ and $|I| = 1$, where k is a ring, $X, Y \in V$ and I is the unit object of V.

Now, the set of all non-negative real numbers $[0, \infty]$ is an ordered set under $\geq$ which consequently becomes a category, whose objects are elements of $[0, \infty]$, and for any $a, b \in [0, \infty]$ there is one morphism $a \to b$ if $a \gneqq b$ and zero otherwise. This is a monoidal category with tensor product $+$ and unit 0. So we can now define an enriched category over $[0, \infty]$.

The $[0, \infty]$-category A consists of

- A class of objects $a, b, c, \ldots,$
- For all $a, b \in ob(A)$, $Hom_A(a, b) \in [0, \infty]$,
- For all $a, b, c \in ob(A)$, $Hom_A(a, b) + Hom_A(b, c) \geq Hom_A(a, c)$,
- For all $a \in ob(A)$, $0 \geq Hom_A(a, a) \in [0, \infty]$.

An $[0, \infty]$-category is generalized metric space, we write $Hom_A(a, b) = d(a, b)$, as first pointed out by Lawvere [28].

The notion of size of a finite metric space is a size function

$$|.| : (ob([0, \infty]), +, 0) \to (k, ., 1),$$

satisfy $|X + Y| = |X|.|Y|$ and $|0| = 1$ called **magnitude**.

Two examples of enriched categories are metric spaces and categories

$$\text{(categories)} \subset \text{(enriched categories)} \supset \text{(metric spaces)}$$

The comparison between categories and metric spaces is given in table 1.1. We specialize the definition of Euler characteristics to metric spaces after generalizing from ordinary to enriched categories.

Category	Metric space
Has objects.	Has points.
For any two objects there is maps between them.	For any two points there is the distance between them.
For any three objects there is an operation of composition	For any three points there is a triangle inequality.

Table 1.1: The comparison between categories and metric spaces.

§ 1.2 A brief history of magnitude

The concept of the Euler characteristic of a finite category is defined in [30] by Leinster, who demonstrated its compatibility with various concepts of size in mathematics, including the Euler characteristics of topological space, graphs and posets. This concept of the Euler characteristic can be easily generalized from categories to enriched categories and then to metric spaces, which were given in an internet posting [29] by Leinster. This internet post contains the basic ideas of the paper [32], which was written by Leinster and includes all the basic motivation and background; most of the papers on magnitude that written after have already built on it. Magnitude was extended to the compact infinite metric spaces by Leinster and Willerton in several ways in ([32], [39], [55] and [57]), which were shown to be equivalent for positive definite spaces by Meckes in [41]. Also, Meckes [40] gave several ways of interpreting the magnitude of compact metric spaces, one of which used a notion of a potential function, and another using the notion of weight distribution.

Magnitude turns out to be related to various fields of mathematics including differential geometric, diversity, graph theory and homology.

With regard to geometric information, Leinster and Willerton [39] studied the asymptotics of the magnitude of subsets of Euclidean space, and gave a conjecture related to intrinsic volumes. More evidence of the conjecture heuristic and computer calculations as defined by Willerton [55]. Barceló and Carbery [4] gave a procedure for the explicit calculation of the formula for the magnitude of odd-dimensional balls in Euclidean space using a potential function that led to the Leinster and Willerton conjecture [39] in the case of balls in dimension three, but the magnitude of higher dimensional balls does not satisfy the principle of inclusion-exclusion. Starting from these ideas [4], Gimperlein and Goffeng [10] gave a geometric origin of the magnitude and obtained an asymptotic variant of the Leinster and Willerton conjecture [39], together with an asymptotic variant of the principle of inclusion-exclusion. Inspired by [4], Willerton [58] gave an algorithm to evaluate the magnitude of odd-dimensional balls in Euclidean space using weight distributions. An explanation for how these explicit formula for the magnitude of balls in odd dimensions led to the conjecture given in [59] by Willerton, who [57] also found the connection between magnitude and intrinsic volumes of Riemannian manifolds. Meckes [42] gave the bounded version of the magnitude of a convex body in Euclidean space in terms of its intrinsic volumes. Leinster and Willerton [39] investigated the concept of dimension linked to magnitude. Meckes [40] showed that the magnitude of dimension and the Minkowski dimension are equal in Euclidean space.

In [52], magnitude originally appeared in the context of biodiversity, where it was described as the "effective number of points" in metric spaces. Leinster and Cobbold [35] presented a one-parameter family of diversity measures, taking into account both the difference and the similarities between species. Leinster [31] described the connections between the maximum diversity and the magnitude of metric spaces. The main results in [36] previously appeared in [31], but the proofs that Leinster and Meckes presented in [36] are significantly simpler. An infinite family of diversity measures were defined in [35] and [31]. Meckes [40] introduced the maximum diversity of infinite metric space to be the maximum value of its diversity of order 2. Using this definition, Leinster and Roff [38] described the connections between maximum diversity and Minkowski dimension. Inspired by the Leinster-Cobbold diversity measures, Willerton [56] defined the concept of the spread of a finite metric space, which is connected to the magnitude of a metric space.

In graph theory, Leinster [33] introduced the magnitude of a graph as an integer power series related to a graph, as motivated by the magnitude of metric space. A survey of the theory of magnitude, from its category theory to its relationships with this geometric information, was given by Leinster and Mecks in [37], who also gave the maximum diversity of the graphs in [36].

Hepworth and Willerton [18] introduced a magnitude homology for graphs, and the magnitude homology of several graphs is accordingly computed in [[18] and [14]]. Leinster and Shulman [37] extended magnitude homology to metric spaces and enriched categories, which was developed in [25], [24], [47], [17], [12], [13], [3].

§ 1.3 Thesis outline

This thesis is organized as follows.

Chapter 2 recalls the basic definitions and characteristics which are used in this work.

Chapter 3 discusses the notion of the q-spread dimension of a metric space which is defined in the Definition 3.0.1 as the growth rate of the q-spread as the metric space is scaled. We compute the q-spread of different grid squares 60×60, 110×110 and 160×160 as shown in Figure 3.1 and we see that when the scaling factor increases, these q-spread dimensions are identical and independent to their number of points. This gives the notion of a scale-dependent dimension. Mathematically, we prove why this happens in Theorem 3.1.3. Also, we plotted the 0-spread dimension, 1-spread dimension and 2-spread dimension of a 160×160 grid square metric spaces together at various scales as represented in Figure 3.7, we can see that when the scale factor is very small, these three types of dimensions are identical. Computationally, we explain why this happens in Section 3.2.

The maximum diversity was first proved by Leinster [31] to be the maximum magnitude of the subsets of the metric space with non-negative weighting. In Section 4.1 of Chapter 4, we determine the magnitude for the all subsets of a 3×3 grid square metric space and we show that the magnitude of the subsets which have 3 points or less of the 3×3 metric space admits non-negative weightings, then we compute the magnitude of the subsets which have more than three points that have non-negative weightings at different scaling and record the maximum magnitude. From this, we get the following conjecture, the maximum magnitude with a non-negative weighting always comes from symmetric subsets and union of symmetric subsets. In Section 4, we compute the magnitude of the orbits which partitioned the $3 \times 3, \ldots,$ 10×10 grid squares and the unions of these orbits that have non-negative weighting and record the maximum magnitude at various scales which is the maximum diversity. Then we prove in Section 4.3 that at very small scaling the magnitude of the four corner points orbit of the $n \times n$ grid square is greater than the magnitude of any other orbit. Furthermore, we show that the set that consists of the union of the four corner points and any other orbit have negative weighting. At the end of this chapter, we numerically calculate the weighting for the points of the middle row for the 201×201 grid square and looking to their behavior at various scales.

In Chapter 5, we mathematically determine 0-spread of the disk and we see numerically that, if the disk is scale by a factor $\tau > 0$, then the 0-spread is close to some quadratic equation of τ. Also, we compute the 0-spread dimension and the magnitude dimension of various cases of rectangular grid metric spaces.

Appendix A contains the Maple code to compute the q-spread, the q-spread dimension, the approximate q-spread, the approximate q-spread dimension and the Matlab code to compute the heuristic q-spread, for $q = 0, 1, 2$.

The first section of Appendix B give the Maple code that deals with finding the magnitude of the subsets of $n \times n$ square grid metric space that admits non-negative weightings by checking all subsets of space. Whilst, the second section give the Maple code that deals with evaluating the magnitude of the subsets of $n \times n$ square grid metric space that admits non-negative weightings by checking only the orbits and the union of orbits of space. The final section contains the Python code to evaluate the weighting of points in the middle row of a 201×201 metric space using the conjugate gradient method.

Appendix C contains the Matlab code to compute the 0-spread of the disk at different scaling, also it contains the Maple code to compute the 0-spread of various rectangular grid and the Python code to compute the magnitude and the magnitude dimension of different rectangular grid at various scaling.

Chapter 2

Background

This chapter has seven sections. Section one gives a brief review of group actions. Section two presents some basic aspects of the magnitude of finite metric space: this includes many classes of metric spaces that are positive definite and describes some classes of finite metric spaces for which the magnitude exists. Section three explains the diversity measures that take into account the relative abundance and ignore species similarity, then explains the diversity measures that take both factors into account. It also gives some properties of the Leinster-Cobbold diversity of order q. Section four provides the definition of the q-spread of finite metric spaces and gives some of their associated properties. Section five describes conditions under which the magnitude and the maximum diversity are identical. Section six gives the relations between magnitude and q-spread of finite metric space. The last section describes how to solve the linear system of equations $Ax = b$ using the Krylov subspace method.

§ 2.1 Some basic definitions and results of group actions

In this section we recall some definitions and describe some results of the group actions (See[7], [23] and [51]).

Definition 2.1.1. For any set X, a **partition** of X is a collection of disjoint non-empty subsets of the set X whose union is X.

Definition 2.1.2. A relation on a set X which is reflexive, symmetric and transitive is an **equivalence relation**.

Definition 2.1.3. For a set X and an equivalence relation $\sim$ on X, an **equivalence class** of an element a in X with respect to $\sim$ is a set $\{b \in X : a \sim b\}$.

Definition 2.1.4. Let G be a group and X be a non-empty set. We say that G **acts** on X, if there is a function $G \times X \to X; (g, x) \to g * x$ which satisfies the following axioms:

- for all $x \in X$ and the identity $e \in G$, $e * x = x$,
- for all $g, h \in G$ and all $x \in X$, $g * (h * x) = (gh) * x$.

Definition 2.1.5. For a metric spaces X, Y, a map $f : X \to Y$ is an **isometry** if it is preserves distances between any pair of points,

$$d(f(x), f(y)) = d(x, y),$$

for any $x, y \in X$.

Definition 2.1.6. Let G be a group acting on a non-empty set X,

- the **orbit** of any element x in X is the set $\{g * x\}$ and denoted by $\mathrm{orb}(x)$,
- the **stabilizer** of x in X is the set of all elements g in G such that $g * x = x$ which written $\mathrm{stab}(x)$,
- G is called **transitive** if for each x, y in X and for some g in G $g * x = y$.

Theorem 2.1.7. *If G is a group that acts on a non-empty set X and $\mathrm{orb}(x)$ is the orbit of x in X, then the relation $\sim$ defined as $x \sim y$ if and only if $g * x = y$ for some g in G is an equivalence relation and each orbit is an equivalence class under $\sim$.*

Proposition 2.1.8. *If G is a group which acts on a set X, then the distinct orbits that partition X.*

Definition 2.1.9. Let Y be a subset of a set X and let G be a group that acts on Y. Then Y is **invariant** under G if $\{g * y : y \in Y \text{ and } g \in G\} = Y$.

Theorem 2.1.10. *Let G be a finite group which acts on a set X, for any x in X we have*

$$\#\mathrm{orb}(x) = \frac{\#G}{\#\mathrm{stab}(x)},$$

where $\#$ is a number of elements in X.

This means that every orbit is an invariant subset of X on which a group acts transitively.

§ 2.2 The magnitude of finite metric spaces

This section has three subsections. In the first subsection, we recall the definition of magnitude of finite metric spaces and we give several examples. In the second subsection, we define the magnitude function and we give some associated properties and examples. In the last subsection, we deal with the class of positive definite finite metric spaces which have a magnitude that admits positive weightings.

2.2.1 Basic definition

Here we define the magnitude of finite metric spaces in terms of weightings and we give some elementary examples.

Definition 2.2.1. (See [39]) Let A be a finite metric space. Define a matrix Z with entries $Z_{ab} = e^{-d(a,b)}$ for all $a, b \in A$. A **weighting** on A is an assignment of a number $w_a \in \mathbb{R}$ for each point $a \in A$ such that weight equation 2.1 is satisfied. For each point $a \in A$ we have

$$\sum_{b \in A} e^{-d(a,b)} w_b = 1. \tag{2.1}$$

If a weighting w exists, then we can define the **magnitude** of A as

$$|A| = \sum_{a \in A} w_a,$$

for any weighting w, and is independent of the weighting chosen.

If a metric space has more than one weightings, then its magnitude is independent of the choice of weighting as can be seen in the following example. See also Lemma 2.5.6 below.

Example 2.2.2. If a matrix Z of a metric space A is $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, then we can obtain a weighting $w = \begin{pmatrix} w_a \\ w_b \end{pmatrix}$ by solving the following expression.

$$Zw = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} w_a \\ w_b \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$w_a + w_b = 1.$$

We need to find w_a and w_b that satisfied the above equation. Now if $w_a = \frac{1}{2}$, then $w_b = \frac{1}{2}$. Again if $w_a = -2$, then $w_b = 3$. In both cases the magnitude of A is equal to 1.

However, if a matrix Z is invertible, then a metric space A has a magnitude and there is a unique weighting w given by w_a is the sum of entries in the ath row in the inverse of Z and the magnitude is equal to the sum of all entries of Z^{-1}. Here are some examples(see [32]).

Example 2.2.3. If we have empty space or one point-space, then:

1. $|\emptyset| = 0$,
2. $|*| = 1$.

Example 2.2.4. Let A be the space consisting of two points a distance d apart. Then we can obtain w by solving the following expression.

$$Zw = \begin{pmatrix} 1 & e^{-d} \\ e^{-d} & 1 \end{pmatrix} \begin{pmatrix} w_a \\ w_b \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$e^{-d} w_a + w_b = 1.$$

$$w_a + e^{-d} w_b = 1.$$

and we get $|A| = \frac{2}{1+e^{-d}}$ which is equal to $1 + \tanh(\frac{d}{2})$.

In particular, If $d = \infty$, then $Z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $|A| = 2$.

Example 2.2.5. In general, if the distance between any two distinct points in a metric space A is ∞, then Z is the identity matrix, each point has weighting 1 and the magnitude of A is given by $|A| = \#A$. Therefore, we can see the magnitude as the effect number of points.

2.2.2 The magnitude function

The magnitude function and some of its characteristic are given here (See [32]).

Definition 2.2.6. If A is a metric space and $t > 0$, then tA denotes the metric space with the same points as A and $d_{tA}(a, b) = td_A(a, b)$.

Definition 2.2.7. The **magnitude function** of a metric space A is the partially defined function $t \mapsto |tA|$, defined for all $t > 0$ such that tA has magnitude.

Example 2.2.8. In the two point metric space, the magnitude function is defined everywhere as shown in Figure 2.1.

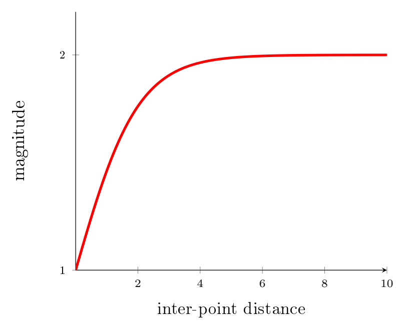


Figure 2.1: The magnitude function of two points space.

Theorem 2.2.9. *If A is a finite metric space, then the following hold.*

1. *For $t \gg 0$, the magnitude function of tA is increasing.*

2. *For $t \gg 0$, there is a unique, positive weighting on tA.*

3. $|tA| \to \#A$ *as* $t \to \infty$.

Definition 2.2.10. (See [32]) If we have an undirected graph G and $t \in (0, \infty]$, then there is a metric space tG whose points are vertices and whose distance are minimal path lengths, a single edge having length t.

Example 2.2.11. (See [32]) [Warning example] Let A be the 5-point space given by the shortest-path metric on the bipartite graph $K_{3,2}$. The magnitude of tA is:

$$|tA| = \frac{7e^{-t} - 5}{2e^{-3t} + 2e^{-2t} - e^{-t} - 1}.$$

We can see in Figure 2.2 it is true that the magnitude function satisfies $|tA| > \#A$ for some t, also it satisfies $|tA| < 0$ for some t and $|tA|$ is undefined at $t = \log \sqrt{2}$.

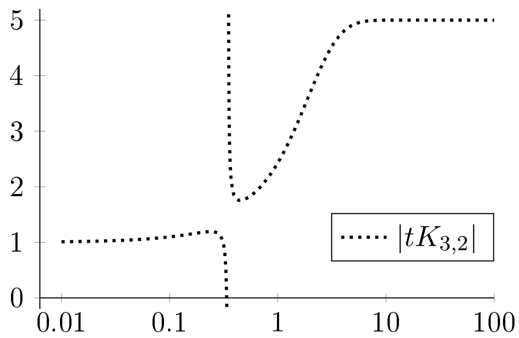


Figure 2.2: Magnitude function of $K_{3,2}$

We can see in Example 2.2.11 that the magnitude of a finite metric space may be undefined or negative.

We now describe some classes of finite metric spaces for which the magnitude exists (See [32] and [39]).

Definition 2.2.12. A metric space is **homogeneous** if its isometry group acts transitively on points.

Theorem 2.2.13. *If a finite metric space A is homogeneous, then there is a weighting w for which all the points have the same weights and we define a weight on each point by*

$$w_b = \frac{1}{\sum_{a \in A} e^{-d(a,b)}},$$

for any $b \in A$*. Therefore, its magnitude is give by*

$$|A| = \frac{\#A}{\sum_{a \in A} e^{-d(a,b)}}.$$

We can see from the following example that the magnitude of a space can be smaller than the magnitude of one of its subspace.

Example 2.2.14. Let $tK_{n,n}$ be a graph. If a similarity between points is equal to $e^{-d_{ij}}$ for all $i, j \in tK_{n,n}$, then by Theorem 2.2.13, the magnitude of $tK_{n,n}$ on $2n$-vertices is

$$|tK_{n,n}| = \frac{2n}{1 + ne^{-t} + (n-1)e^{-2t}}.$$

So, the average similarity between its points is

$$\frac{(n-1)e^{-2t} + ne^{-t} + 1}{2n} = \frac{(\frac{n-1}{n})e^{-2t} + e^{-t} + \frac{1}{n}}{2}.$$

When n is big, so the similarity between points is approximately

$$\frac{1}{2}(e^{-t} + e^{-2t}).$$

While, the magnitude of the complete graph K_n on n-vertices is given by

$$|tK_n| = \frac{n}{1 + (n-1)e^{-t}}.$$

So, the average similarity between the points of $2tK_n$ is

$$\frac{1 + (n-1)e^{-2t}}{n} = \frac{1}{n} + \frac{n-1}{n}e^{-2t}.$$

For big n, its average similarity is approximately e^{-2t}.

Since $e^{-t} > e^{-2t}$, the average similarity between points of $tK_{n,n}$ is greater than that of its subspace $2tK_n$. One over that average similarity is the magnitude which implies that

$$|tK_{n,n}| < |2tK_n|.$$

There is a space for which $\lim_{t \longrightarrow 0} |tA| \neq 1$, as we can see in the following example.

Example 2.2.15. If we have a graph $K_{3,3}$ with vertices a_1, a_2, a_3, b_1, b_2, b_3 and three new edges adjoined from b_i to b_j whenever $1 \leq i < j \leq 3$, then

$$W = \begin{bmatrix} -\frac{e^{-t}-1}{4\,e^{-2\,t}e^{-t}-9\,(e^{-t})^2+2\,e^{-2\,t}+2\,e^{-t}+1} \\ -\frac{e^{-t}-1}{4\,e^{-2\,t}e^{-t}-9\,(e^{-t})^2+2\,e^{-2\,t}+2\,e^{-t}+1} \\ -\frac{e^{-t}-1}{4\,e^{-2\,t}e^{-t}-9\,(e^{-t})^2+2\,e^{-2\,t}+2\,e^{-t}+1} \\ \frac{2\,e^{-2\,t}-3\,e^{-t}+1}{4\,e^{-2\,t}e^{-t}-9\,(e^{-t})^2+2\,e^{-2\,t}+2\,e^{-t}+1} \\ \frac{2\,e^{-2\,t}-3\,e^{-t}+1}{4\,e^{-2\,t}e^{-t}-9\,(e^{-t})^2+2\,e^{-2\,t}+2\,e^{-t}+1} \\ \frac{2\,e^{-2\,t}-3\,e^{-t}+1}{4\,e^{-2\,t}e^{-t}-9\,(e^{-t})^2+2\,e^{-2\,t}+2\,e^{-t}+1} \end{bmatrix}$$

and

$$|tA| = \frac{6}{1+4e^{-t}} \quad \to \quad \frac{6}{5}, \qquad \text{as} \qquad t \quad \to \quad 0$$

.

2.2.3 Positive definite spaces

Here, we describe another class of finite metric spaces which have magnitude (See [32], [39] and [41]).

Definition 2.2.16. A symmetric matrix Z which satisfies this condition $\nu^\tau Z \nu > 0$, for each non-zero column vector ν where ν^τ denote the transpose of ν is called **positive definite matrix**.

Definition 2.2.17. (See [2]) A **principal sub-matrix** P of a matrix A can be found by selecting a subset of rows and the same subset of columns.

Proposition 2.2.18. *(See [54]) The following properties of a positive definite matrix are true*

1. *If a matrix Z is positive definite, then Z is invertible.*
2. *Every principal sub-matrix of a positive definite matrix is positive definite.*
3. *A matrix Z is positive definite if and only if*

$$|Z_{ii}| \geq \sum_{i \neq j} |Z_{ij}| \qquad \textit{for all } i.$$

The prove of the following theorem can be found in [32], here we will be proved by a different way.

Theorem 2.2.19. *If the distance between each pairs of distinct points in a finite metric space A with n points is greater than $\log(n-1)$, then A has a well defined magnitude.*

Proof. As 0 and 1-point spaces have magnitude 0 and 1 respectively. we will assume that $n \geq 2$ and Z be an $n \times n$ matrix with $Z_{xx} = 1$ for each $x \in A$. We have $d(x, y) > \log(n-1)$, for every $x, \in A$ this implies $-d(x,\, y) < -\log(n-1)$ and then $e^{-d(x,\, y)} < 1/(n-1)$. so we get $Z_{xy} < 1/(n-1)$. Now by third part of Proposition 2.2.18, a matrix Z is positive definite and by the first property of Proposition 2.2.18, a matrix Z is invertible. Therefore, a space A have a magnitude. □

Definition 2.2.20. If a matrix Z of a finite metric space A is positive definite, then A is **positive definite**.

In general, a positive definite metric space has a magnitude with unique weighting.

Theorem 2.2.21. *(See [32]) Consider A is a positive definite metric space with n-points. Then*

$$|A| = \sup_{\nu \neq 0} \frac{(\sum_{i \in A} \nu_i)^2}{\nu^\tau Z \nu},$$

where the supremum is over non-zero column vector $\nu \in \mathbb{R}^n$ and ν^τ denotes the transpose of ν. A vector ν the supremum is attained exactly when it is a non-zero scalar multiple of the unique weighting on A.

Proof. Let Z be a positive definite matrix of A. We have the Cauchy-Schwarz inequality

$$(\nu^\tau Z \nu) \cdot (\omega^\tau Z \omega) \geq (\nu^\tau Z \omega)^2 \qquad \Leftrightarrow \qquad (\omega^\tau Z \omega) \geq \frac{(\nu^\tau Z \omega)^2}{\nu^\tau Z \nu},$$

for all $\nu, \omega \in \mathbb{R}^n$. Now if we take ω to be a weighting on A, then

$$|A| = \sum_i \omega_i = \sum_{i,j} \omega_i Z_{ij} \omega_j = \omega^T Z \omega.$$

Also we have $\nu^\tau Z \omega = \sum_{i,j} \nu_i Z_{ij} \omega_j = \sum_i \nu_i$. So we get

$$|A| \geq \frac{(\sum_{i \in A} \nu_i)^2}{\nu^\tau Z \nu}.$$

Suppose that $\nu_i = c\omega_i$ for a constant $c \neq 0$, then

$$\frac{(\sum_{i \in A} \omega_i)^2}{\omega^\tau Z \omega} = \frac{|A|^2}{|A|} = |A|.$$

Therefore $|A| \leq \sup_{\nu \neq 0} \frac{(\sum_{i \in A} \nu_i)^2}{\nu^\tau Z \nu}$. Hence $|A| = \sup_{\nu \neq 0} \frac{(\sum_{i \in A} \nu_i)^2}{\nu^\tau Z \nu}$. □

Corollary 2.2.22. *(See [32]) If B is a subspace of a positive definite metric space A, then B is also positive definite and $|B| < |A|$.*

Definition 2.2.23. (See [48]) A finite metric space A is **ultrametric space** if it satisfies the following condition

$$\max\{d(a,b), d(b,c)\} \geq d(a,c),$$

for all $a, b, c \in A$. For example the discrete metric which is defined as the distance from a point to itself equal zero while the distance between any two distinct points equal one is an ultrametric.

Here we list some classes of metric space that are positive definite, or positive definite with positive weighting.

Theorem 2.2.24. *(See [32], [39] and [41]) The following statements are true*

1. *Each finite subspace of $\mathbb{R}$ is positive definite with positive weighting.*
2. *Each finite subspace of L_p^N is positive definite where L_p^N is $\mathbb{R}^N$ with the metric induced by $\|x\|_p = (\sum_i |x_i|^p)^{\frac{1}{p}}$.*
3. *Each space with 3 or fewer points is positive definite with positive weighting.*
4. *Each space with 4 points is positive definite.*
5. *Each finite metric space A such that the distance between any disjoint points is greater than $\log(\#A - 1)$ is positive definite with positive weighting.*
6. *Each finite ultrametric space is positive definite with positive weighting.*

Every homogeneous space has a positive weighting. But by Theorem 2.2.13, Example 2.2.14 and Corollary 2.2.22, it need not be positive definite.

§ 2.3 Measures of diversity

Diversity is one of the most ecological features of a community and refers to the number and variety of a group of the population that occur together. The simplest measure of diversity is the number of species that can be found in a certain location, which indicates the **species richness**. In fact, various indexes have been used to measure diversity [21] that take into account the number of species present (richness) as well as the relative abundance of each species (evenness), such as Simpson's index, the Shannon index and the Berger-Parker index. However, it is not only the relative abundances of species that reflects this realistic measure of diversity but also the similarity between species pairs, as measured by a coefficient in the range from 0 to 1, where 0 and 1 indicate total dissimilarity and complete identity of the species, respectively.

This section has three subsections. The first subsection considers a natural family of diversity measures by taking into account the relative abundances whilst ignoring similarities between species, and then by taking both factors into account simultaneously in the second subsection. The last subsection explains where Leinster-Cobbold diversities come from.

2.3.1 Ignoring species similarity

In 1973, Hill [21] described a set of diversity numbers of various orders. Assume that a community of organism contains S species that occurs with the particular set of relative abundances $p = \{p_1, p_2, \ldots, p_S\}$; where $p_i \geq 0$ for $i = 1, 2, \ldots, S$ and $p_1 + p_2 + \ldots + p_S = 1$. The diversity number D of order q varies in the interval $[0, \infty]$ and can be obtained from the following formula

$$D^q(p) = (\sum_{i=1}^{S} {p_i}^q)^{\frac{1}{1-q}}, \tag{2.2}$$

where D^q is the qth order of diversity, which is the effective species number. The most common ways of measuring diversity are as follows.

1. Species richness. Easily seen when $q = 0$ in Equation (2.2) to give S, where S is the total number of species in the community.

2. Exponential Shannon diversity index. When $q = 1$, the value of Equation (2.2) is undefined. In 1961, Renyi [49] defined the Renyi entropy of a sample of relative abundance p such that $\sum_{i=1}^{S} p_i = 1$ and
$$\frac{1}{1-q} \log(\sum_{i=1}^{S} {p_i}^q),$$
which is equal to the logarithm of Equation 2.2. So, using L'Hopital's theorem, we can get
$$\lim_{q \to 1} \frac{1}{1-q} \log(\sum_{i=1}^{S} {p_i}^q) = -\sum_{i=1}^{S} p_i \log(p_i).$$
This can also be written as
$$\log(\prod_{i=1}^{S} {p_i}^{p_i})^{-1}.$$
The exponential of above equation is given by
$$e^{\log(\prod_{i=1}^{S} {p_i}^{p_i})^{-1}} = (\prod_{i=1}^{S} {p_i}^{p_i})^{-1},$$

which is the exponential Shannon diversity that is $\lim_{q\to 1} D^q(p)$.

3. Simpson's reciprocal diversity index. This can be observed by setting $q = 2$ in Equation (2.2) to obtain

$$(\sum_{i=1}^{S} {p_i}^2)^{-1}.$$

4. Berger-Parker diversity index. This index is obtained as the reciprocal of the relative abundance of the commonest species.

$$(\max_i p_i)^{-1}.$$

Now in the following proposition we will show that $D^q(p)$ as $q \to \infty$ is equal to $(\max_i p_i)^{-1}$

Proposition 2.3.1. *Assume that* $p_1, p_2, \ldots, p_S$ *are positive numbers such that* $\sum_{i=1}^{S} p_i = 1$ *and let* $D^q(p) = (\sum_{i=1}^{S} {p_i}^q)^{\frac{1}{1-q}}$. *Then*

$$D^\infty(p) := \lim_{q\to\infty} D^q(p) = (\max_i p_i)^{-1}.$$

Proof. Consider $p_{\max} = \max\{p_1, p_2, \ldots, p_S\}$. Then we can write

$$D^q(p) = (p_{\max})^{\frac{q}{1-q}} \left(\sum_{i=1}^{S} \left(\frac{p_i}{p_{\max}} \right)^q \right)^{\frac{1}{1-q}}.$$

Now the sum is bounded above because each term is at most one and there are S terms. The sum is also bounded below because each $p_i \geq 0$. We have for $q > 1$

$$0 \geq \log \left(\left(\sum_{i=1}^{S} \left(\frac{p_i}{p_{\max}} \right)^q \right)^{\frac{1}{1-q}} \right) = \frac{1}{1-q} \log \left(\sum_{i=1}^{S} \left(\frac{p_i}{p_{\max}} \right)^q \right) \geq \frac{\log S}{1-q}.$$

which tends to zero as q tends to infinity to get

$$D^\infty(p) = \lim_{q\to\infty} (p_{\max})^{\frac{q}{1-q}} e^0 = (p_{\max})^{-1}.$$

□

From above, the diversity of order q is

$$D^q(p) = \begin{cases} \left(\sum_{i=1}^{S} {p_i}^q \right)^{\frac{1}{1-q}} & \text{if } q \neq 1, \\ \prod_{i=1}^{S} p_i^{-p_i} & \text{if } q = 1, \\ \frac{1}{\max_i p_i} & \text{if } q = \infty. \end{cases}$$

The value of parameter q is between 0 and ∞ and it is indicates how much significance is attached to species abundance. For example at $q = 0$, $D^0(p)$ is the number of species, at $q = 1$, $D^1(p)$ is the exponential Shannon index, at $q = 2$, $D^2(p)$ is the inverse Simpson index, and at $q = \infty$, $D^\infty(p)$ is the Berger-Parker index. It can be seen that for small q, D^q considers both rare and common species equally. However, for large q, D^q considers only common species and rare species are ignored. All four measures have the property that if we have S species all with equal relative proportions, then $D^q(p) = S$. This gives the maximum value for a population with S species.

Now, given two communities A and B of three species, namely

$$\{30\% \text{ dogs}, 40\% \text{ cats}, 30\% \text{ foxes}\} \quad \text{and} \quad \{30\% \text{ cats}, 40\% \text{ dogs}, 30\% \text{ wolves}\}$$

Using the above measure of diversity, these species will have the same diversity. We can address this by taking into account the similarity between species.

2.3.2 Incorporating species similarity

The Hill numbers were extended by Leinster and Cobbold in [35] to take into account analogous species. There are various ways to measure cross-species similarity; the genetic approach [45], such as via DNA, is possibly the most popular. The refined model can be used as follows. Leinster and Cobbold [35] consider the community to be divided into S species, and they also have a measure of the analogy between each possible pair of species. Let this measure be a real number between 0 and 1, where 0 is a total dissimilarity between species and 1 represents identical species as can be describe in the following definition.

Definition 2.3.2. (See [35]) A similarity matrix Z for a finite set A on S points $\{a_1, \ldots, a_S\}$ is an $S \times S$ matrix Z with entries Z_{ij} in the range 0–1, where 0 and 1 indicate total dissimilarity and identity, respectively, between a_i and a_j.

Definition 2.3.3. (See [35]) Let A be a community of S species with similarity matrix Z and relative abundances $p = \{p_1, \ldots, p_S\}$; thus, $p_i > 0$ and $\sum_{i=1}^{S} p_i = 1$. Then for $0 \leq q \leq \infty$, the **Leinster-Cobbold diversity** of order q is given by

$$^qD^Z(p) = \begin{cases} \left(\sum\limits_{i:p_i>0} p_i (Zp)_i^{q-1} \right)^{\frac{1}{1-q}} & \text{if } q \neq 1, \\ \prod\limits_{i:p_i>0} (Zp)_i^{-p_i} & \text{if } q = 1, \\ \frac{1}{\max\limits_{i:p_i>0} (Zp)_i} & \text{if } q = \infty, \end{cases}$$

where $(Zp)_i = \sum_j Z_{ij} p_j$ for all $i = \{1, \ldots, S\}$.

The Hill numbers can be found as the Leinster-Cobbold diversities of the identity similarity matrix. This means that different species are assumed to be totally dissimilar. Willerton [56] used the Leinster-Cobbold diversity to obtain a concept of the size of finite metric space by providing the space with a canonical relative abundance, which gives rise to the q-spread.

2.3.3 Generalized measure diversity and their connection to the spread of a finite metric space

Inspired by the measure of Leinster and Cobbold diversity, the concept of the spread of finite metric spaces $A = \{a_1, a_2, \ldots, a_S\}$ is defined, which is linked to the magnitude of finite metric spaces (See [31] and [35]). To measure the similarity between each pair of species, we consider the measure to be a real number between 0 and 1, where 0 is to be the total dissimilarity and 1 the identical species denoting Z_{ij} as the similarity between ith and jth species (see Definition 2.3.2).

The similarities to be measured genetically are usually expressed as percentages, which provide similarity coefficients Z_{ij} on a scale of 0 and 1 directly; however, there are cases where a measure of inter-species distance $d(a_i, a_j)$ is given by a scale of 0 to ∞. The transformation $Z_{ij} = e^{-d(a_i, a_j)}$, or more generally by $Z_{ij} = e^{-td(a_i, a_j)}$ for some positive number t, can be used to convert distance $d(a_i, a_j)$ into similarities Z_{ij}. Further, any metric d on a set A gives rise to a similarity matrix by defining $Z_{ij} = e^{-d(a_i, a_j)}$, thus nearby points are assumed to be near identical and distant points are assumed to be dissimilar.

We will describe the way to measure the diversity of the community in a step wise manner.

The S-dimensional column vector Zp can represent the similarities from the $S \times S$ matrix Z and the relative abundances. Therefore, the ith entry of the S-dimensional column vector Zp will take the form

$$(Zp)_i = \sum_j Z_{ij} p_j,$$

which is the expected similarity between a randomly chosen individual and the ith species, and indeed the ordinariness of the ith species within the community is measured by this.

The average ordinariness of an individual from the community is

$$\sum_{i=1}^{S} p_i (Zp)_i.$$

This quantity is large when many of the population is concentrated into a few very similar species. Therefore, average ordinariness can be considered in the sense of the concentration and its inverse related to diversity. The relation between the diversity of the community and the concentration is

$$\frac{1}{\sum_{i=1}^{S} p_i (Zp)_i},$$

which is the diversity of order 2.

Different notions of averages give diversities of different orders, $q \neq 2$. The **weighted mean** for any weights $p = \{p_1, p_2, \ldots, p_S\}$ add up to 1, which is $\sum_{i=1}^{S} p_i x_i$ where $x_i \in \mathbb{R}$. Also, for each $t > 0$ we have a different kind of average: first, every x_i is transformed to x_i^t; next we take the weighted mean, and finally we apply the inverse transformation. This is the referred to as the **power mean** $(\sum_{i=1}^{S} p_i x_i^t)^{\frac{1}{t}}$. Taking $t = q - 1$ and $x_i = (Zp)_i$ gives

$$(\sum_{i=1}^{S} p_i (Zp)_i^{q-1})^{\frac{1}{q-1}},$$

which is a measure of the ordinariness of the community with its reciprocal

$${}^{q}D^{Z}(p) = (\sum_{i=1}^{S} p_i (Zp)_i^{q-1})^{\frac{1}{1-q}},$$

that is the diversity of the community with order q. For further details (see Subsection 2.3.2).

One of the several characteristics of the diversity measures ${}^{q}D^{Z}(p)$ is given in the following proposition.

Proposition 2.3.4. *Let p belongs to the set of relative abundance vectors for S species $P_S = \{(p_1, \ldots, p_S) \in \mathbb{R}^{\mathbb{S}} | p_i \geq 0, \sum_{i=1}^{S} p_i = 1\}$ and let Z be an $S \times S$ similarity matrix. Then ${}^{q}D^{Z}(p)$ is decreasing as a function of q.*

Furthermore, the diversity measure is constant, if the similarity matrix is an identity matrix and there is a uniform relative abundance $p \in \{\frac{1}{S}, \ldots, \frac{1}{S}\}$, then ${}^{q}D^{Z}(p) = S$ for all q.

The following lemma states other characteristics of the diversity measure

Lemma 2.3.5. *(See [35]) Let $p \in \{(p_1, \ldots, p_S) \in \mathbb{R}^{\mathbb{S}} | p_i \geq 0, \sum_{i=1}^{S} p_i = 1\}$ and let Z be an $S \times S$ similarity matrix. Then, the following statements are true.*

- *For $q \in [0, \infty)$, ${}^{q}D^{Z}(p)$ is continuous in q,*
- $\lim_{q \to 0} {}^{q}D^{Z}(p) = {}^{0}D^{Z}(p)$,
- $\lim_{q \to \infty} {}^{q}D^{Z}(p) = {}^{\infty}D^{Z}(p)$.

Proof. To proof (See the Appendix in [35], Propositions A_1 and A_2). □

For the case when there are no varying similarities between species, we will have the similarity coefficients Z_{ij} which would be 0 if $i \neq j$ and 1 if $i = j$. This makes the matrix Z an identity matrix I, and $(Zp)_i = p_i$, we will get naive diversity $D^q(p)$ which called the **Hill number** of order q (see Subsection 2.3.1) for further details.

We use the Leinster-Cobbold diversity measures to obtain measures of the size of finite metric space A by providing the space with a canonical uniform probability measure $P_S(x) = \frac{1}{S}$ for all $x \in A$, named the q**-spread**.

§ 2.4 q-spread of finite metric spaces

The concept of the q-spread of finite metric space has been defined by Willerton [56], as motivated by the Leinster-Cobbold measures of biodiversity [35].

Definition 2.4.1. (See [56]) Given a finite metric space A with S points and a metric d, the q-spread $E_q(A)$ is defined for $0 \leq q \leq \infty$ by

$$E_q(A) \;=\; {}^qD^Z\left(\frac{1}{S}, \ldots, \frac{1}{S}\right).$$

Explicit formulas, derived from Definition 2.4.1, are as follows.

$$E_q(A) = \begin{cases} \sum\limits_{i=1}^{S} \frac{1}{\sum\limits_{j=1}^{S} Z_{ij}} & \text{if} \quad q = 0, \\ S. \prod\limits_{i=1}^{S} \left(\frac{1}{\sum\limits_{j=1}^{S} Z_{ij}} \right)^{\frac{1}{S}} & \text{if} \quad q = 1, \\ \frac{S^2}{\sum\limits_{i,j=1}^{S} Z_{ij}} & \text{if} \quad q = 2, \\ \frac{S}{\max\limits_{i=1,\ldots,S} \sum\limits_{j=1}^{S} Z_{ij}} & \text{if} \quad q = \infty. \end{cases} \tag{2.3}$$

By Proposition 2.3.4, we have $E_q(A) \geq E_{q'}(A)$ whenever, $0 \leq q \leq q' \leq \infty$. Willerton [56] generally concentrated on the greatest of these values, $E_0(A)$ called the 0-spread, which is the analogue of the 'number of species' in an ecology.

The following theorem provided the basic properties of the q-spread

Theorem 2.4.2. *(See [56]) If a finite metric space A with S points is scaled up by a factor $t > 0$, then*

- $1 \leq E_q(tA) \leq S$,

- *$E_q(tA)$ is increasing in t,*
- *$E_q(tA) \to 1$ as $t \to 0$,*
- *$E_q(tA) \to \#A$ as $t \to \infty$.*

In Section 2.3.3, the concept of diversity measures is defined as the idea of the generalized mean. Here we give a description of the q-spread in those terms.

If $A = \{a_1, a_2, \ldots, a_S\}$ is a metric space, then we can defined a **reciprocal mean similarity** as

$$\rho_i = \frac{\#A}{\sum\limits_{j=1}^{S} e^{-d(a_i, a_j)}},$$

for every $a_i \in A$. Now we have ρ_i, for $i = 1, \ldots, S$, then we can think of its as a measure of how different the metric space A is from the point a_i. When all the points are close to a_i, then ρ_i being nearly 1. However, when all of the points are far from a_i, so ρ_i being nearly $\#A$. A measure of the whole space A can be get by taking an average of these reciprocal mean similarities. There are many several averages we can take.

Consider s is a non-zero real number, and $x = \{x_1, x_2, \ldots, x_n\}$ are positive real numbers. The **generalized means** with respect to x is

$$\mu^s(x) = \left(\frac{1}{n} \sum_{i=1}^{n} x_i^s \right)^{\frac{1}{s}}.$$

Which includes many standard means: μ^2 is the quadratic mean, μ^1 is the arithmetic mean, μ^{-1} is the harmonic mean, the μ^∞ and μ^0 can be find as a limit when $s = 0, \infty$ to be the maximum and the geometric mean respectively.

The q**-spread** of the finite metric space is defined as μ^{1-q} with respect to the reciprocal mean similarity ρ, for $1 \leq q \leq \infty$.

$$E_q(A) = \mu^{1-q}(\rho).$$

When the points of A are near to each other, the q-spread being close to 1, and when the points of A are far to each other, the q-spread being close to S.

$$1 \leq E_q(A) \leq S.$$

§ 2.5 Comparisons between magnitude and maximum diversity

The maximum diversity is found to be the maximum of the magnitudes of the subsets of the metric space with non-negative weighting, in which we say that a metric space has a non-negative weighting if there is a weighting for a space such that all of the weights are non-negative.

In this section, we need to answer the following question.

Assume that $p \in \{(p_1, \ldots, p_S) \in \mathbb{R}^{\mathbb{S}} | p_i \geq 0, \sum_{i=1}^{S} p_i = 1\}$ and Z is an $S \times S$ similarity matrix. When $q \in [0, \infty]$, for which relative abundance p is ${}^qD^Z(p)$ maximal?

To solve the maximum diversity problem, we will first give some definitions and some results (see [31] and [36]).

Definition 2.5.1. (See [31]) A **weight distribution** for a similarity matrix Z is a relative abundance p such that $(Zp)_1 = (Zp)_2 = \ldots = (Zp)_S$.

Lemma 2.5.2. *(See [31]) Let A be a finite metric space. Then we have*

1. *If A admits non-negative weighting, then $|A| > 0$,*
2. *If w is a non-negative weighting on A, then $\frac{w}{|A|}$ is a weight distribution for A,*
3. *When A admits a weight distribution, A admits a weight and $|A| > 0$*
4. *If p is a weight distribution for A, then $(Zp)_i = \dfrac{1}{|A|}$.*

Proof. 1. Let A be a metric space with S points. Then by Definition 2.2.1, the magnitude of A is $|A| = \sum_{i=1}^{S} w_i$. By assumption $w_i \geq 0$, for $i = 1, \ldots, S$. Since $S \geq 1$ and the 0-vector is not a weighting, $w_i > 0$, for some i, implies that $|A| > 0$.

2. Consider $\underline{w}$ is a non-negative weighting, so

$$Z\underline{w} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix},$$

so, $(Z\underline{w})_i = 1$, for $i = 1, 2, \ldots, S$. Define $p = \frac{\underline{w}}{|A|}$, then p is a relative abundance as

$$\sum_{i=1}^{S} p_i = \sum_{i=1}^{S} \frac{w_i}{\sum\limits_{j=1}^{S} w_j} = \frac{\sum_{i=1}^{S} w_i}{\sum_{j=1}^{S} w_j} = \frac{|A|}{|A|} = 1.$$

And also,

$$(Zp)_i = \big(Z\frac{\underline{w}}{\sum_{j=1}^{S} w_j}\big)_i = \frac{1}{\sum_{j=1}^{S} w_j}(Z\underline{w})_i = \frac{1}{\sum_{j=1}^{S} w_j} = \frac{1}{|A|},$$

for all i, so p is a weight distribution.

The last two cases follow from the previous case. □

Lemma 2.5.3. *(See [31]) Let A be a finite metric space and p be a weight distribution for A. Then, ${}^qD^Z(p) = |A|$ for all $q \in [0, \infty]$.*

Proof.

$$^qD^Z(p) = \left(\sum_{i=1}^{S} p_i (Zp)_i^{q-1} \right)^{\frac{1}{1-q}}.$$

By the first part of Lemma 2.3.5, ${}^qD^Z(p)$ is continuous. Therefore, it is enough to prove this for $q \neq 1, \infty$. In this case, using the third part of Lemma 2.5.2 we get

$$^qD^Z(p) = \left(|A|^{1-q} \right)^{\frac{1}{1-q}} = |A|.$$

□

Definition 2.5.4. (See [36]) Given a similarity matrix Z, a relative abundance p in $\{1, 2, \ldots, S\}$ is **invariant** when ${}^qD^Z(p) = {}^{q'}D^Z(p)$ for each $q, q' \in [0, \infty]$.

Definition 2.5.5. (See [32]) A weighting on a matrix P is a column vector w such that

$$Pw = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

and a coweighting on P is a row vector v such that

$$vP = [1, \ldots, 1].$$

If w is a weighting and v a coweighting on P then

$$\sum_{a \in P} w_a = [1, \ldots, 1]w = vPw = \sum_{a \in P} v_a.$$

When P admits both a weighting and a coweighting, we then can define its magnitude to be $\sum_{a \in P} w_a = \sum_{a \in P} v_a$ for any weighting w and coweighting v. However, when the matrix P is invertible, P has exactly one weighting and its magnitude is the sum of all the entries of P^{-1}.

In a special case we can see the independence as follows.

Lemma 2.5.6. *(See [34]) Consider a matrix P and its transpose P^T each have at least one weighting. Then $\sum_i w_i$ is independent of the weighting chosen w on P.*

Proof. Let w and $\bar{w}$ be two weighting on P and let v be a weighting on P^T. Then

$$\sum_i w_i = (1, \ldots, 1)w = (P^T v)^T w = v^T P w = v^T \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} = \sum_i v_i.$$

We can similarly show that $\sum_i \bar{w}_i = \sum_i v_i$. So $\sum_i w_i = \sum_i \bar{w}_i$. □

The measures have the property that if $p_i = 0$, for some $i \in \{1, 2, \ldots, S\}$ the diversity is the same as if they had not been mentioned at all. To express this, we introduce a number of notations

Let Z be a $S \times S$ similarity matrix and a subset $B \subseteq \{1, 2, \ldots, S\}$, consider Z_B is the matrix Z restricted to B, so that

$$(Z_B)_{ij} = Z_{ij}\{i, j \in B\}.$$

If B has m elements, then Z_B is an $m \times m$ matrix.

Lemma 2.5.7. *(See [31]) For a similarity matrix Z, let $B \subseteq \{1, 2, \ldots, S\}$, and let p' be a relative abundance on B. If p is a relative abundance achieved by extending p' by zero, then ${}^qD^{Z_B}(p') = {}^qD^Z(p)$ for each $q \in [0, \infty]$. In general, p' is invariant if, and only if, p is similarly invariant.*

We can see by Lemma 2.5.3, that each weight distribution is invariant, and by Lemma 2.5.7 each weight distribution extended by zero is also invariant.

Now if we have a similarity matrix Z, $B \subseteq \{1, 2, \ldots, S\}$ and a non-negative weighting w on Z_B, consider p' be the weight distribution on B given by

$$p' = \frac{w}{|Z_B|},$$

where $|Z_B|$ is a magnitude of Z_B. Thereafter extending by zero to $\{1, 2, \ldots, S\}$. We get, for any similarity matrix there is at least one invariant distribution because if we consider B is one element subset, then Z_B has a unique non-negative weighting $w = \{1\}$ which gives the invariant distribution $p' = (0, \ldots, 0, 1, 0, \ldots, 0)$.

Proposition 2.5.8. *(See [36]) Given an $S \times S$ similarity matrix Z and $p \in \{(p_1, \ldots, p_S) \in \mathbb{R}^{\mathbb{S}} | p_i \geq 0, \sum_{i=1}^{S} p_i = 1\}$. Then the following statements are equivalent.*

1. *p is invariant,*

2. *$(Zp)_i = (Zp)_j$, for each i, j such that $p_i, p_j > 0$,*

3. *p is the extension by zero of a weight distribution on a $\emptyset \neq B \subseteq \{1, 2, \ldots, S\}$,*

4. *p is equal to a weight distribution p' with respect to B, for some $\emptyset \neq B \subseteq \{1, 2, \ldots, S\}$ that have non-negative weighting. Furthermore, ${}^qD^Z(p') = |Z_B|$.*

Let us now define the maximizing distribution

Definition 2.5.9. (See [36]) If Z is a similarity matrix and $q \in [0, \infty]$, a relative abundance p is **q-maximized** if ${}^qD^Z(p) \geq {}^qD^Z(\tilde{p})$ for each relative abundance $\tilde{p}$. A relative abundance is **maximized** if it is q-maximizing for each q.

We will now explain some of the results of a maximizing distribution.

Lemma 2.5.10. *(See [Lemma 2.11, [31]]) Given a similarity matrix Z and an invariant distribution p that maximizes ${}^0D^Z$, then it is also maximizes ${}^qD^Z$.*

Proposition 2.5.11. *(See [31]) Every similarity matrix has a maximizing distribution, and every maximizing distribution is invariant.*

Proof. See the proof of Proposition 3.7 in the [31]. □

The solution to the maximum diversity problem is given by the following theorem.

Theorem 2.5.12. *(See [36]) If Z is s similarity matrix, then*

1. *For all $q \in [0, \infty]$*
$$\sup_{\forall p} {}^qD^Z(p) = \max_B |Z_B|,$$
where the maximum is over all subsets $B \subseteq \{1, 2, \ldots, S\}$ such that Z_B admits non-negative weighting.

2. *The maximizing distributions are $p' = \frac{w}{|Z_B|}$, where w is a non-negative weighting on a subset B subsets of $\{1, 2, \ldots, S\}$, such that $|Z_B|$ is the maximum.*

In particular, there exists a maximizing distribution, and the maximum diversity of order q is the same for all $q \in [0, \infty]$.

Proof. 1. Let's take p to run only through the invariant relative abundances, by Proposition 2.5.11, $\sup_p^q D^Z(p)$ is constant. By Proposition 2.5.8, p is equal to a weight distribution p' with respect to B for some non-negative weighting w on some non-empty subsets B of $\{1, 2, \ldots, S\}$, which means $\sup_p {}^qD^Z(p) = \max\limits_{w,p'} {}^qD^Z(p')$. By Lemma

2.5.7, ${}^qD^Z(p') = {}^qD^{Z_B}(p')$ and by Lemma 2.5.3, ${}^qD^Z(p') = |Z_B|$. Therefore,

$$\sup_{\forall p} {}^qD^Z(p) = \max_B |Z_B|,$$

for each non-empty subset $B \subseteq \{1, 2, \ldots, S\}$ such as Z_B has non-negative weighting.

2. By Proposition 2.5.11, every maximizing distribution is invariant, and for Proposition 2.5.8, we get the result.

□

Corollary 2.5.13. *(See [Corollary 4.1, [31]]) If Z is a similarity matrix and $q \in [0, \infty]$, then an invariant distribution is q-maximizing if and only if it is maximizing.*

Definition 2.5.14. (See [36]) The **maximum diversity** of a similarity matrix Z is $D_{\max} = \sup_{\forall p} {}^qD^Z(p)$, which is independent of the value $q \in [0, \infty]$.

If a similarity matrix is positive definite, then the solution of the maximum diversity problem turns out to be simple.

Theorem 2.5.15. *(See [31]) If a similarity matrix Z is positive definite with a unique non-negative weighting w, then $D_{\max} = |Z|$. Moreover, $\frac{w}{|Z|}$ is a unique maximizing distribution, where $|Z|$ is a magnitude of Z.*

§ 2.6 Comparisons between magnitude and 0-spread

The magnitude is an upper bound for the 0-spread, for the positive definite metric spaces, as can be seen in the following results.

The following result is a trivial corollary of Definitions 2.4.1 and 2.5.14

Corollary 2.6.1. *(See [56]) The 0-spread of finite metric space A is bounded above by the maximum diversity of A.*

$$E_0(A) \leq D_{\max}(A).$$

Theorem 2.6.2. *(See [56]) If A is a positive definite metric space, then the maximum diversity of A is bounded above by the magnitude of A.*

$$D_{\max}(A) \leq |A|.$$

Hence, by Corollary 2.6.1 and Theorem 2.6.2, we get that magnitude is an upper bound for the 0-spread of the positive definite metric space

$$E_0(A) \leq D_{\max}(A) \leq |A|.$$

Note that, there is metric space that magnitude is not always an upper bound for the 0-spread. In Example 2.2.11, we find the magnitude of the five-point space at various scaling $t > 0$, and we see that its magnitude is undefined at $t = \log(\sqrt{2})$. However, the 0-spread of the $K_{3,2}$ space is defined for all different values of $t > 0$, as can be seen in Figure 2.3. The following theorem

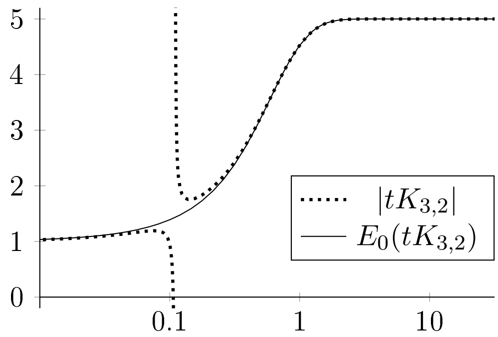


Figure 2.3: The magnitude and the spread of $K_{3,2}$ metric space.

shows that for homogeneous metric spaces, the magnitude and the q-spread are identical,

Theorem 2.6.3. *(See [56]) If a finite metric space is homogeneous, then its magnitude and its q-spread are equal.*

Proof. Let $A = \{a_1, a_2, \ldots, a_n\}$ be a finite metric space. Since A is homogeneous space, then by Theorem 2.2.13 the magnitude of A is

$$|A| = \frac{\#A}{\sum\limits_{j=1}^{n} e^{-d(a_i,\, a_j)}},$$

for each $a_i \in A$. On the other hand, each point in A has the identical reciprocal mean similarity $\rho_i = \frac{\#A}{\sum\limits_{j=1}^{n} e^{-d(a_i,\, a_j)}}$, for $i = 1, 2, \ldots, n$. We define the q-spread as a power mean $\mu^{1-q}(\rho)$. While $\mu^{1-q}(\rho)$ of n copies of ρ is just ρ. Therefore,

$$|A| = \rho = E_q(A).$$

□

§ 2.7 Iterative solution of large systems of equations

One of the most problematic aspects of numerical analysis is finding a feasible method to solve a system of linear algebraic equations

$$Ax = b, \tag{2.4}$$

where A is a non-singular $n \times n$ matrix, b is a real column n-vector and x is an unknown n-vector. There are two main classes of numerical schemes for solving these systems.

- Direct Methods: These can be used to solve a linear system with a finite number of steps, and determine the exact solution. One example is Gaussian elimination.

- Iteration Methods: These are most commonly used to solve a large linear system, giving a sequence of approximate solutions starting from an initial guess.

In particular, the systems of linear equations (2.4) can be solved iteratively, using matrix-vector multiplications, where the first approximation to a solution x_1 belongs to the span of b

$$x_1 \in \text{span}\{b\},$$

after which computing Ab and some linear combination of b and Ab can be taken as the second approximate solution x_2

$$x_2 \in \text{span}\{b, Ab\},$$

so that this process continues until at step k it satisfies

$$x_k \in \text{span}\{b, Ab, \ldots, A^{k-1}b\}, \tag{2.5}$$

for $k = 1, 2, \ldots$. The subspace on the right in the expression (2.5) is called a **Krylov subspace** for A with respect to b and is denoted $K_k(A, b)$.

We use this method to find the weights of the points in the middle row of the 201×201 metric space in Section 4.4 and to find the magnitude dimension of different types of rectangular grid metric spaces in Section 5.3. This section consists of two subsections: the first subsection, we describe the Krylov subspace methods for solving linear systems and in the second subsection, we present the conjugate gradient method based on the Krylov subspace.

2.7.1 Krylov subspace methods

Here we will describe the Krylov subspace methods for solving linear systems. This subspace was first introduced in 1931 [27] by Krylov. He gave a sequence of subspace, which is fundamental for most practical numerical techniques that are commonly used in such applications as the conjugate gradient method.

Let us begin with the following definitions and results.

Definition 2.7.1. (See [9]) The **characteristic polynomial** of an $n \times n$ matrix A is a polynomial of degree n which is given as $p_A(\lambda) = \det(\lambda I_{n\times n} - A) = \lambda^n + c_{n-1}\lambda^{n-1} + \cdots + c_1\lambda + c_0$, where $I_{n\times n}$ is the $n \times n$ identity matrix.

Theorem 2.7.2. *[9, Cayley-Hamilton p. 225] If $p_A(\lambda) = \lambda^n + c_{n-1}\lambda^{n-1} + \cdots + c_1\lambda + c_0$ is the characteristic polynomial of A, then $p_A(A) = 0$.*

The following results are the corollaries of the Cayley-Hamilton theorem.

Corollary 2.7.3. *If A is an $n \times n$ matrix and $S = span\{I, A, A^2, \dots\}$, then $S = span\{I, A, A^2, \dots, A^{n-1}\}$ and $\dim(S) \leq n$.*

Corollary 2.7.4. *If an $n \times n$ matrix A is invertible and has characteristic polynomial $\lambda^n + c_{n-1}\lambda^{n-1} + \cdots + c_1\lambda + c_0$, then*

$$A^{-1} = -c_0^{-1}(A^{n-1} + c_{n-1}A^{n-2} + \cdots + c_2 A + c_1). \tag{2.6}$$

Before we explain the Krylov subspace, let us first give the following definitions

Definition 2.7.5. (See [50]) A **monic polynomial** is a polynomial whose coefficient of the highest degree is equal to one.

Definition 2.7.6. (See [20]) A **minimal polynomial** of a square matrix A is the monic, nonzero polynomial ρ of minimal degree such that $\rho(A) = 0$.

Definition 2.7.7. (See [15]) The Krylov sequence generated by a matrix $A \in \mathbb{R}^{n\times n}$ and a vector $v \in \mathbb{R}^n$ is given as

$$v,\, Av,\, A^2v,\, \dots .$$

Since all $Av^i \in \mathbb{R}^n$, so the $(n+1)$-element subset $v, Av, \dots, A^{n-1}v, A^n v$ is linearly dependent. Therefore there exists a unique $d \leq n$, such that $v, Av, \dots, A^{d-1}v, A^d v$ is linearly dependent but $v, Av, \dots, A^{d-1}v$ is linearly independent. In the case that $A^d v$ is the zero vector, that linear independence implies that $\alpha_0 = \alpha_1 = \cdots = \alpha_{d-1}$ or $A^d v$ is non-zero linear combination of the vectors $v, Av, \dots, A^{d-1}v$.

Definition 2.7.8. (See [43]) The **minimal polynomial of a vector** v **with respect to a matrix** A denoted $\rho_{A,v}$ is the monic polynomial of minimal degree such that $\rho_{A,v}(A)v = 0$. Its degree is called the grade of v with respect to A.

Definition 2.7.9. (See [15]) Given an $n \times n$ non-singular matrix A and a non-zero n-vector v, then the jth **Krylov subspace** generated by A from v is denoted by $K_j(A, v)$ and is given as

$$K_j(A, v) = \text{span}\{v, Av, \dots, A^{j-1}v\}.$$

The next characterization determines the dimension of the Krylov subspace.

Proposition 2.7.10. *(See [11]) The Krylov subspace is of dimension j if and only if the degree of the minimal polynomial of v with respect to A is not less than j.*

In fact, the following proposition states that the Krylov subspace is non-decreasing.

Proposition 2.7.11. *(See [11]) If d is the degree of a minimal polynomial of v, then K_d of degree d is invariant under A and $K_d = K_j$, for all $j > d$.*

From above, it is clearly to see that $K_1 \subseteq K_2 \subseteq \cdots \subseteq K_d = K_j$, for all $j > d$. And at each step, the Krylov subspace dimension increases at most by one.

Also, for any non-singular matrix A, there exist a minimal polynomial and so by Corollary 2.7.4, we can evaluate A^{-1} using the minimal polynomial. Consequently, the solution for the system of linear equations $x = A^{-1}b$ lies in the Krylov subspace, as can be seen in the following theorem.

Theorem 2.7.12. *(See [22]) If the degree of a minimal polynomial is d, then the solution to $Ax = b$ lies within the Krylov subspace of degree d.*

In general, the basic idea of the Krylov subspace iterative algorithm is to compute a sequence of low-dimensional subspaces in which an approximation to a solution x_k, starting from initial approximate x_0 approaches the exact solution, namely

$$x_k \in x_0 + K_k(A, r_0),$$

where $r_0 = b - Ax_0$ is an initial residual.

There are several approaches for choosing a good x_k in krylov subspace of degree k. Some of them are listed below:

- The conjugate gradient method in which the residual $r_k = b - Ax_k$ is orthogonal to the Krylov subspace of A leading to the conjugate gradients.
- GMRES and MINRES which minimize the residual.
- SYMMLQ which minimizes the norm of the error,
- The biconjugate gradient method in which the residual $r_k = b - Ax_k$ is orthogonal to the Krylov subspace of the transpose of A.

Next, we will describe the first of the above methods of the Krylov subspace solver that satisfies the following condition: The k^{th} approximation x_k is uniquely evaluated by

$$\begin{aligned} &x_k \in x_0 + K_k(A, r_0), \\ &b - Ax_k \perp K_k(A, r_0). \end{aligned}$$

Which is intended to solve the systems of linear equations.

2.7.2 Conjugate gradient method

The conjugate gradient iteration was invented in 1950 [19] by Hestenes and Stiefel. This method is used to find the solution n-vector x of linear system equations (2.4). Fletcher and Reeves in 1964 [8] introduced the idea that the solution to these linear equations is equivalent to minimizing a quadratic equation.

We begin with some elementary definitions from [44].

Definition 2.7.13. The **inner product** $\langle , \rangle$ of two vectors $x = [x_1, \ldots, x_n]$ and $y = [y_1, \ldots, y_n]$ in $\mathbb{R}^{\ltimes}$ is given by

$$\langle x, y \rangle = x^T y = \sum_{i=1}^{n} x_i y_i,$$

where x^T is the transpose of x. Recall that,

$$\langle x, x \rangle = \|x\|^2 = \sum_{i=1}^{n} x_i^2.$$

Definition 2.7.14. We say that the vector x is **orthogonal** to the vector y if $\langle x, y \rangle = 0$ and we denote it by $x \perp y$.

Definition 2.7.15. A set of vectors $\{x_1, x_2, \ldots, x_n\}$ is an **orthogonal set** if $x_i \perp x_j$, for all $i \neq j$.

Definition 2.7.16. A vector x is **orthogonal to the linear subspace** $S \subset \mathbb{R}$ if $x \perp z$, whenever $z \in S$.

Definition 2.7.17. A vector x is **A-orthogonal** to a vector y or **conjugate** to y with respect to A if $\langle x, y \rangle_A = x^T A y = 0$.

Definition 2.7.18. A matrix A is called **symmetric** if $A = A^T$ and that it is **positive definite** if $x^T A x > 0$, for all non-zero vector x, where A^T, x^T are the transposes of A and x, respectively.

The conjugate gradient method name is derived from the case that a sequence of orthogonal or conjugate vectors is generated. The residuals and iterates are these vectors. Also, from the gradient of some quadratic form, the minimization of this form is equivalent for the solution of the system of linear equations. The conjugate gradient method is an effective technique when the matrix A is symmetric and positive definite.

The quadratic form

Here, we will look at the conjugate gradient technique as a method for solving a system of linear equations by minimizing a quadratic equation $\phi : \mathbb{R}^n \to \mathbb{R}$, which is given by.

$$\phi(x) = \frac{1}{2}x^T Ax - x^T b, \tag{2.7}$$

where A is an $n \times n$ symmetric positive definite matrix with coefficients a_{ij}, for $1 \leq i, j \leq n$ and x, b are n-vectors.

We first recall some elementary definitions

Definition 2.7.19. (See [5]) An assignment of a vector to any element in a subset of space is **vector field**.

Definition 2.7.20. (See [5]) An element of a field that used to define a vector space is called a **scalar**.

Definition 2.7.21. (See [5]) Consider A to be an $n \times n$ matrix and x, b n-vectors. Then, the scalar of the product

$$\alpha = x^T Ax \quad \text{is} \quad \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_i x_j.$$

Definition 2.7.22. (See [46]) Given a vector $(x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$, $\triangledown$ can be described in terms of partial derivative operators as

$$\triangledown = \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_n}\right].$$

Definition 2.7.23. (See [46]) The $\triangledown$ operator acts on a scalar from $\psi(x)$ produces a vector field

$$\triangledown\psi = \left[\frac{\partial \psi}{\partial x_1}, \frac{\partial \psi}{\partial x_2}, \ldots, \frac{\partial \psi}{\partial x_n}\right]^T, \tag{2.8}$$

is called a **gradient**.

Proposition 2.7.24. *(See [16]) The following statements are true*

$$\frac{\partial x_i}{\partial x_l} = \begin{cases} 1, & \text{if } i = l, \\ 0, & \text{if } i \neq l, \end{cases}$$

and

$$\frac{\partial (x_i x_j)}{\partial x_l} = \begin{cases} 2x_i, & \text{if } i = j = l, \\ x_i, & \text{if } j = l \text{ and } i \neq l, \\ x_j, & \text{if } i = l \text{ and } j \neq l, \\ 0, & \text{otherwise.} \end{cases}$$

Proposition 2.7.25. *(See [8]) Consider A is an $n \times n$ matrix and x, b are n-vectors and defined a quadratic equation $\phi : \mathbb{R}^n \to \mathbb{R}$, as $\phi(x) = \frac{1}{2}x^T Ax - x^T b$. Then, $\nabla\phi = \frac{1}{2}(A + A^T)x - b$.*

Proof. Since the scalar resulting from the product

$$z = b^T x \quad \text{is} \quad \sum_{i=1}^{n} b_i x_i,$$

and the scalar of the product

$$\alpha = x^T Ax \quad \text{is} \quad \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij} x_i x_j.$$

Using Proposition 2.7.24, we get

$$\frac{\partial z}{\partial x_l} = \frac{\partial\left(\sum_{i=1}^{n} b_i x_i\right)}{\partial x_l} = \sum_{i=1}^{n} b_i \frac{\partial x_i}{\partial x_l} = b_i,$$

so,

$$\nabla z = b. \tag{2.9}$$

Also,

$$\begin{aligned}
\frac{\partial \alpha}{\partial x_l} &= \frac{\partial\left(\sum_{i,j=1}^{n} a_{ij} x_i x_j\right)}{\partial x_l} \\
&= \frac{\partial\left(a_{ll}x_l^2 + \sum_{i\neq l} a_{il} x_i x_l + \sum_{j\neq l} a_{lj} x_l x_j + \sum_{i\neq l, j\neq l} a_{ij} x_i x_j\right)}{\partial x_l}, \\
&= a_{ll}\frac{\partial x_l^2}{\partial x_l} + \sum_{i\neq l} a_{il}\frac{\partial x_i x_l}{\partial x_l} + \sum_{j\neq l} a_{lj}\frac{\partial x_l x_j}{\partial x_l} + \sum_{i\neq l, j\neq l} a_{ij}\frac{\partial x_i x_j}{\partial x_l}, \\
&= 2a_{ll}x_l + \sum_{i\neq l} a_{il} x_i + \sum_{j\neq l} a_{lj} x_j + 0 \\
&= \sum_{i=1}^{n} a_{il} x_i + \sum_{j=1}^{n} a_{lj} x_j,
\end{aligned}$$

for $l = 1, 2, \ldots, n$, this implies that

$$\nabla\alpha = (A + A^T)x. \tag{2.10}$$

By formulae (2.10) and (2.9) we get

$$\nabla\phi = \frac{1}{2}(A + A^T)x - b. \tag{2.11}$$

□

At the minimize of the formula (2.7), a solution of the gradient of function equal to zero. By Proposition 2.7.25 we get

$$\nabla\phi = \frac{1}{2}(A + A^T)x - b = 0.$$

Since A is a symmetric matrix, then $Ax - b = 0$. This is true if and only if $Ax = b$. This means that x minimizes $\phi(x)$ and is also a solution for $Ax = b$, which means it is minimize the error.

Definition 2.7.26. (See [8]) The **error vector** is a difference between an actual value and an estimated value.

We will show in the following lemma that the error vector $||x - x^*||$ for x in Krylov subspace is minimized with respect to A-norm $||x - x^*||_A$ by x which minimizes $\phi(x)$, where $x^* = A^{-1}b$ is a solution of linear system (2.4).

Lemma 2.7.27. *(See [26]) Suppose x_k minimizes the quadratic equation ϕ over the Krylov subspace $x_0 + K_k(A, r_0)$, then x_k minimizes $||x - x^*||_A = ||r_k||_{A^{-1}}$ over $x_0 + K_k(A, r_0)$, where $r_k = b - Ax_k$.*

Proof. Let $x^* = A^{-1}b$, so we can define $\|x - x^*\|_A = (x - x^*)^T A(x - x^*)$, and note that

$$\begin{aligned}
(x - x^*)^T A(x - x^*) &= x^T Ax - x^T Ax^* - x^{*T} Ax + x^{*T} Ax^* \\
&= x^T Ax - x^T Ax^* - x^T A^T x^* + x^{*T} Ax^* \\
&= x^T Ax - 2x^T Ax^* + x^{*T} Ax^* \\
&= x^T Ax - 2x^T b + x^{*T} Ax^* \\
&= 2\phi(x) + x^{*T} Ax^*.
\end{aligned}$$

Since $x^{*T} Ax^*$ is independent to x, so that minimizing $\phi(x)$ is equivalent to minimizing $\|x - x^*\|_A$.

Again, we have

$$\begin{aligned}
\|x - x^*\|_A^2 &= (x - x^*)^T A(x - x^*) \\
&= \big(A(x - x^*)\big)^T A^{-1}\big(A(x - x^*)\big) \\
&= \|b - Ax\|_{A^{-1}}^2.
\end{aligned}$$

□

Next we will explain the uniqueness of the solution

Definition 2.7.28. (See [60]) Let x be a real n-vector, the second order derivative of a function ψ of x is known as **Hessian matrix**, and is defined as

$$H = \frac{\partial^2\psi}{\partial x \partial x^T} = \begin{bmatrix} \frac{\partial\psi}{\partial x_1 \partial x_1} & \frac{\partial\psi}{\partial x_1 \partial x_2} & \cdots & \frac{\partial\psi}{\partial x_1 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial\psi}{\partial x_n \partial x_1} & \frac{\partial\psi}{\partial x_n \partial x_2} & \cdots & \frac{\partial\psi}{\partial x_n \partial x_n} \end{bmatrix}$$

Since the second derivative of Equation (2.7) using the above matrix is

$$\frac{\partial^2 \phi}{\partial x \partial x^T} = A,$$

and A is positive definite, the solution of the formula ϕ is unique as seen in the following lemma.

Lemma 2.7.29. *(See [Minimizing function, [1]]) If $\phi : \mathbb{R}^n \to \mathbb{R}$ is a function and $\nabla \phi(x) = 0$, with positive definite Hessian, then x is the unique minimum of ϕ.*

The conjugate gradient algorithm

Consider a sequence of non-zero A-conjugate search direction $\{d_0, d_1, \dots, d_{k-1}\}$, for $k \geq 1$. These conjugate vectors with respect to the symmetric positive definite A are linearly independent.

Proposition 2.7.30. *(See [19]) Consider A is positive definite, and a set of non-zero vectors $\{d_0, d_1, \dots, d_{k-1}\}$, for $k \geq 1$ are A-conjugate. Then these vectors are linearly independent.*

Proof. If $\{d_i\}_{i=0}^{k-1}$ are linearly dependent, then for $j = 0, \dots, k-1$ there exist $\alpha_j \in \mathbb{R}$, not all zero such that

$$\sum_{j=0}^{k-1} \alpha_j d_j = 0.$$

Multiply the above formula by A, we get

$$\sum_{j=0}^{k-1} \alpha_j A d_j = 0.$$

Multiply the above equation by d_0^T

$$\sum_{j=0}^{k-1} \alpha_j d_0^T A d_j = \alpha_0 d_0^T A d_0 = 0.$$

But A is positive definite, $d_0^T A d_0 > 0$, so $\alpha_0 = 0$. Which is contradiction. $\square$

(See [19]) This implies that the sequence $\{d_j\}_{j=0}^{k-1}$ are linearly dependent, so the search direction d_k can be written as

$$d_k = \alpha_0 d_0 + \alpha_1 d_1 + \cdots + \alpha_{k-1} d_{k-1},$$

and thus d_k belongs to same subspace in $\mathbb{R}$.

The following theorems observation indicate that how to compute the coefficients $\{\alpha_j\}_{j=0}^{k-1}$, for an integer $k \geq 0$ which minimizes the quadratic formula (2.7).

Theorem 2.7.31. *(See [46, Conjugate direction algorithm])*
Suppose that $\{d_0, d_1, \ldots, d_{k-1}\}$*, for an integer* $k \geq 0$ *is a sequence of non-zero orthogonal vectors with respect to* A*. Then the set of iterates* $\{x_1, \ldots, x_k\}$ *generated by*

$$x_i = x_{i-1} + \alpha_{i-1} d_{i-1},$$

with

$$\alpha_{i-1} = \arg\min\{\phi(x_{i-1} + \alpha d_{i-1}) : \alpha \in \mathbb{R}\},$$

for $i = 1, 2, \ldots, k$*. Which is converges to the solution of a linear equations after* k *steps, where* x_0 *is an initial iterate and* $d_0 = b - Ax_0$*.*

Theorem 2.7.32. *(See [Expanding subspace theorem, [6]])*
Suppose that $\{d_0, d_1, \ldots, d_{k-1}\}$*, for an integer* $k \geq 0$ *is a set of non-zero orthogonal search directions with respect to* A*. Then for* $i = 1, 2, \ldots, k$*, the sequence generated by*

$$x_i = x_{i-1} + \alpha_{i-1} d_{i-1},$$

with

$$\alpha_{i-1} = \frac{d_{i-1}^T r_{i-1}}{d_{i-1}^T A d_{i-1}}, \tag{2.12}$$

having the property that ϕ *reaches it minimum value on the subspace* $x_0 + span\{d_0, \ldots, d_{k-1}\}$ *at* x_k*.*

Now, consider the following equation

$$x_i = x_{i-1} + \alpha_{i-1} d_{i-1}, \tag{2.13}$$

for $i = 1, 2, \ldots, k$. Multiplying Equation (2.13) by $-A$ and then adding b to both sides, we will get the residual r_i

$$r_i = r_{i-1} - \alpha_{i-1} A d_{i-1},$$

with $r_0 = b - Ax_0$.

In addition, we can choose the search direction d_i for $i = 1, 2, \ldots, k$, by composing the residual at the present point with that of a previous direction as it is stated in the following theorem.

Theorem 2.7.33. *(See [26]) Let* A *be a symmetric positive definite and consider* $r_{i-1} \neq 0$*. Then for* $i = 1, 2, \ldots, k$ *and an integer* $k \geq 0$*, we have*

$$d_i = r_{i-1} + \beta_{i-1} d_{i-1}, \tag{2.14}$$

with $d_0 = r_0 = b - Ax_0$*.*

We can find the value of β in Formula (2.14), by multiply both sides of the Formula 2.14 by $d_{i-1}^T A$ for $i = 1, \ldots, k$ to be

$$d_{i-1}^T A d_i = d_{i-1}^T A r_{i-1} + \beta_{i-1} d_{i-1}^T A d_{i-1},$$

by A-orthogonality of d_i and d_{i-1} for $i = 1, 2, \ldots, k$, we have

$$d_{i-1}^T A d_i = 0.$$

Thus we obtain

$$\beta_{i-1} = -\frac{d_{i-1}^T A r_{i-1}}{d_{i-1}^T A d_{i-1}}. \tag{2.15}$$

There are different equations of α_{i-1}, β_{i-1} that appear in Expressions (2.12) and (2.15) respectively. They are the common implementation of the conjugate gradient method, as modified in the next result.

Lemma 2.7.34. *(See [26]) Let A be symmetric positive definite matrix. Then*

$$\alpha_{i-1} = \frac{r_{i-1}^T r_{i-1}}{d_{i-1}^T A d_{i-1}},$$

and

$$\beta_{i-1} = \frac{r_i^T r_i}{r_{i-1}^T r_{i-1}},$$

for $i = 1, \ldots, k$ and an integer $k \geq 0$.

Putting all above relations together, we obtain the next algorithm

Algorithm 1 conjugate gradient

(See [26])

Ensure: a matrix A and a unit vector b
Ensure: x_0 an initial approximation

```
r_0 = b - A x_0
d_0 = r_0
for i = 1, 2, ... until r_i = 0 do
    α_{i-1} = r_{i-1}^T r_{i-1} / d_{i-1}^T A d_{i-1}
    x_i = x_{i-1} + α_{i-1} d_{i-1}
    r_i = r_{i-1} - α_{i-1} A d_{i-1}
    if r_i ≠ 0 then
        β_{i-1} = r_i^T r_i / r_{i-1}^T r_{i-1}
        d_i = r_{i-1} + β_{i-1} d_{i-1}
    end if
end for
```

Chapter 3

The q-spread dimensions of grid square metric spaces

The concept of the q-spread of finite metric space has been defined in Definition 2.4.1.

If all the points of A are very close together, $Z_{ij} \approx 1$, and accordingly all the formula give $E_q(A) \approx 1$, which makes sense because A looks like one point. However, if all the points of A are widely separated, so its points look like a collection of disconnects points, then all give $E_q(A) \approx \#A$. These can be seen as good measures of the size of finite metric space A, then we can define the concept of the q-spread dimension for $q \in \{0, 1, 2, \infty\}$.

Definition 3.0.1. (See [56]) The q-spread dimension of metric space A is the growth rate of the q-spread of tA at $t = 1$, as defined by

$$\dim_q(A) = \frac{d\log(E_q(tA))}{d\log(t)}\Big|_{t=1}.$$

We have used the formal definition of the chain rule to calculate this derivative, this gives us the following equation

$$\dim_q(A) = \frac{t}{E_q(tA)}.\frac{d(E_q(tA))}{dt}\Big|_{t=1}.$$

Note that the q-spread dimension of the metric space tA is then

$$\dim_q(tA) = \frac{d\log(E_q(sA))}{d\log(s)}\Big|_{s=t}.$$

This chapter consists of two sections. Both sections discuss the growth rate of the q-spread at different scalings, which can be considered as a size-dependent dimension of the metric space. In the first section, we prove Theorem 3.1.3, which shows that for the large scale, the q-spread dimension is independent of the number of points of the square grid. In second section, the heuristic q-spread dimension is numerically calculated; this is viewed as being very close to some quadratic function $at^2 + bt + c$ where a, b, c are positive constants, that represents a best-fit for a large space and small scales.

§ 3.1 q-spread dimension for finite square grid metric spaces

We will first define the concept of the 0-spread dimension for square grid metric space as the growth rate of the 0-spread of the space. This concept of dimension is scale-dependent.

The **square grid metric space** A with an even number n of points per side is the $n \times n$ matrix of points called $p_1, \ldots, p_{n^2}$, where $p_i \in A$ is a pair of numbers (x, y) and $x, y \in \{1, 2, \ldots, n\}$, such that $p_1 = (1, 1)$, $p_2 = (2, 1), \ldots, p_{n^2} = (n, n)$. For $t > 0$, the 0-spread of tA with side length $t(n-1)$ is defined by the Definition 2.4.1 as

$$E_0(tA) = \sum_{i=1}^{n^2} \frac{1}{\sum\limits_{j=1}^{n^2} e^{-td(p_i, p_j)}},$$

where the distance between the points $d(p_i, p_j)$ is the usual distance in Euclidean space and the square grid is scaled by a factor t. This 0-spread is a measure of the size of the grid square, so an associated dimension can be defined as the growth rate of the size.

In particular, the 0-spread dimension $\dim_0(A)$ of the metric space A by the Definition 3.0.1 is given by

$$\frac{d\log(E_0(tA))}{d\log(t)}\Big|_{t=1} = \frac{t}{E_0(tA)} . \frac{d(E_0(tA))}{dt}\Big|_{t=1} .$$

It is informative to look at the 0-spread dimension as an $n \times n$ square grid A being scaled by factor $t > 0$. We used a number of computer calculations, as performed using Maple (see Appendix A), to partition the metric space A into four subsets under the action of a subgroup of order four of the symmetry group of the square. Let A_1 be one of these subsets, then we can evaluate

$$\sum_{p_i \in A_1} \frac{1}{\sum\limits_{p_j \in A} e^{-td(p_i, p_j)}},$$

and multiply the above result by four to get the 0-spread of tA. We repeat this process for various scale factors t, after that we save the 0-spread of square grid with its scaling factor to obtain a list of pairs of points. Then we approximate the logarithmic derivative by finding the gradient, which is equal to the change in 0-spread between two data points divided by the change in scale factor t between the corresponding two data points, then plotting the result (see Appendix A.1.1). For instance, we found the 0-spread dimension of grid squares with 60×60, 110×110 and 160×160 points, as represented in Figure 3.1. We can see that this concept of the 0-spread dimension changes according to the factor t. When the scale factor of the square grid is very small, the square points appear to be just a single point, which is of dimension zero. When the scale is increased, it appears to be more like a true square with a dimension of just under two; however, as the scale is increased further, distinct points become apparent and the dimension drops back to zero.

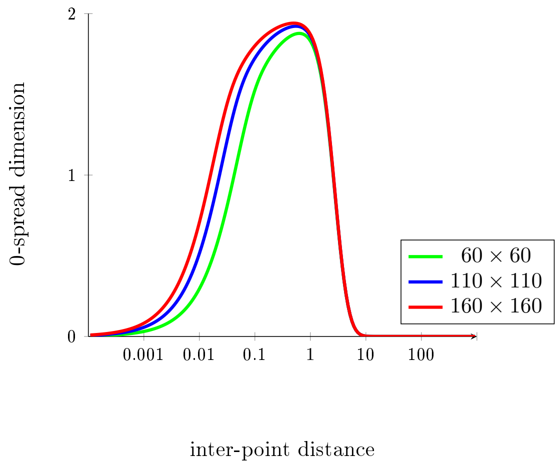


Figure 3.1: The 0-spread dimensions of various square grids.

Furthermore, the 0-spread dimensions of those squares are similar, and approximately independent of the number of points, for $t > 1$.

To find out why this happens, we first considering a point $p = (\frac{n}{2} + 1, \frac{n}{2} + 1)$ to be the bottom left-hand corner of the first quadrant of the grid square (see Figure 3.3), and let X be a subset of these square grids of 10×10 points of the square grids such that tX contains the square with a side-length t, so $p \in X$ as can be seen in Figure 3.3. Since $t \gg 0$, then the impact of a point on other points reduces exponentially with distance, the points in tA only know what is going on locally. therefore, the weight of the points in tX are reasonable constants.

$$\frac{1}{\sum\limits_{p_j \in A} e^{-td(p,p_j)}} \sim \frac{1}{\sum\limits_{p_j \in X} e^{-td(p,p_j)}},$$

for $p \in A$. An **estimate of the 0-spread** of A scaled by a factor t denoted by $F_0(tA,\, p)$ and defined as

$$F_0(tA,\, p) = \frac{\#A}{\sum\limits_{p_j \in X} e^{-td(p,\, p_j)}}. \tag{3.1}$$

Then, we divided the 0-spread for three metric spaces 60×60, 110×110, 160×160 and estimate of the 0-spread by their corresponding numbers of points. After that, we used Maple code (see A.1.2) to plotting them together, as shown in Figure 3.2.

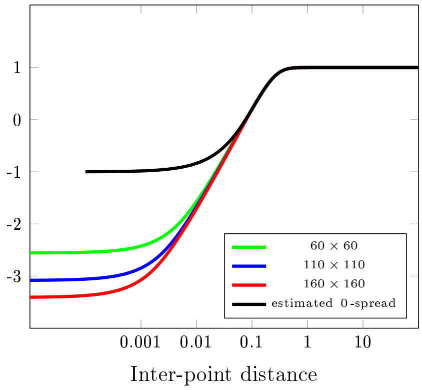


Figure 3.2: The 0-spread of various square grids and the estimate 0-spread that defined in Formula (3.1) divided by their number of points.

From above figure, we see that the 0-spread of the three metric spaces and the estimate 0-spread divided by their number of points are approximately the same, and independent of the number of points, when the inter-point distance of the square grid is greater than one.

In general, if the large square grid scaled by a factor bigger than one, then the estimate 0-spread of square grid with respect to p over the 0-spread of square grid is small as shown in the next proposition.

Proposition 3.1.1. *For any large number n, if an $n \times n$ square grid of lattice points is scaled by a factor $t > 1$, then*

$$\frac{F_0(tA, p)}{E_0(tA)} \to \delta \qquad as \qquad t \to \infty,$$

where $\frac{1}{4} \leq \delta \leq 1$.

Proof. Given a large $n \times n$ grid square metric space A, the 0-spread of A scaled by a factor $t > 0$ is

$$E_0(tA) = \sum_{\hat{p} \in A} \frac{1}{\sum_{\bar{p} \in A} e^{-td(\hat{p}, \bar{p})}}.$$

Now if a point p is an upper right-hand corner of the middle square of side length t of square grid scaled by factor t, then the estimate of the 0-spread with respect to p of square grid A scaled by a factor $t > 0$ is

$$F_0(tA,\, p) = \frac{\#A}{\sum_{\bar{p}\in A} e^{-td(p,\bar{p})}}.$$

If the value of $F_0(tA,\, p)$ is divided by the value of $E_0(tA)$, we get the average over p of $1/\sum_{\bar{p}\in A} e^{-td(p,\bar{p})}$ divided by the average over $\hat{p}$ of $1/\sum_{\bar{p}\in A} e^{-td(\hat{p},\bar{p})}$ to be

$$\begin{aligned}\frac{F_0(tA,\, p)}{E_0(tA)} &= \frac{\#A/\sum_{\bar{p}\in A} e^{-td(p,\bar{p})}}{\sum_{\hat{p}\in A}(1/\sum_{\bar{p}\in A} e^{-td(\hat{p},\bar{p})})} = \frac{1/\sum_{\bar{p}\in A} e^{-td(p,\bar{p})}}{\frac{\sum_{\hat{p}\in A}(1/\sum_{\bar{p}\in A} e^{-td(\hat{p},\bar{p})})}{\#A}}\\ &\approx \frac{1/\sum_{\bar{p}\in A} e^{-td(p,\bar{p})}}{1/\sum_{\bar{p}\in A} e^{-td(\hat{p},\bar{p})}} = \frac{\sum_{\bar{p}\in A} e^{-td(\hat{p},\bar{p})}}{\sum_{\bar{p}\in A} e^{-td(p,\bar{p})}}.\end{aligned}$$

Now the proof is dependent on the position of the point $\hat{p}$ in the grid square.

Case 1. Let $\hat{p}$ be the point on the boundary or nearest point to the boundary (less than ten units). Since n is large, t is big and impact of a point on the other points decays exponentially with distance. so, the point only know what happening around it. Therefore, it is clearly to see that

$$\sum_{\bar{p}\in A} e^{-td(\hat{p},\bar{p})} \approx \frac{1}{4}\sum_{\bar{p}\in A} e^{-td(p,\bar{p})},$$

this implies

$$\frac{F_0(tA,\;\, p)}{E_0(tA)} \to \frac{1}{4} \qquad \text{as} \qquad t\to\infty.$$

Case 2. Let $\hat{p}$ be a point far at least ten units away from the boundary. Let $\hat{X}$ be a subset of square grid A of 10×10 points such that $\hat{p}$ is in the square of side length one in $\hat{X}$. Since the scale factor of the large square grid is big, and effect of a point on other points decays exponentially with distance, so the points in $\hat{X}$ only know what is happening locally. Then we get

$$\sum_{\bar{p}\in A} e^{-td(\hat{p},\;\bar{p})} \approx \sum_{\bar{p}\in A} e^{-td(p,\,\bar{p})},$$

which implies that

$$\frac{F_0(tA,\;\, p)}{E_0(tA)} \to 1 \qquad \text{as} \qquad t\to\infty.$$

□

The following lemma relates to the incomplete Gamma function. This result is important to proving the theorem which follows, as can be explained by the fact that when the measures of the distance of points t grow larger, the dimension becomes independent of the number of points for the square grid.

Lemma 3.1.2. *For a non-negative integer n and t, $k > 0$, we have*

$$\int_{r=k}^{\infty} e^{-tr} r^n \, dr = \frac{e^{-kt}}{t^{n+1}} \sum_{i=0}^{n} \frac{n\,!}{i\,!} t^i k^i.$$

Proof. We proceed the proof by induction on n. The base case being the known case $n = 0$, that

$$\int_{r=k}^{\infty} e^{-tr} \, dr = \frac{-1}{t} e^{-tr} \Big|_{r=k}^{\infty} = \frac{e^{-kt}}{t^1} \frac{0\,!}{0\,!} t^0 k^0.$$

Assume the statement is true for some n

$$\int_{r=k}^{\infty} e^{-tr} r^n \, dr = \frac{e^{-tk}}{t^{n+1}} \sum_{i=0}^{n} \frac{n\,!}{i\,!} t^i k^i.$$

We need to show that it is true for $n + 1$. Now evaluating

$$\int_{r=k}^{\infty} e^{-tr} r^{n+1} \, dr,$$

we integrate by parts

$$\begin{aligned}
\int_{r=k}^{\infty} e^{-tr} r^{n+1} \, dr &= \frac{-r^{n+1}}{t} e^{-tr} \Big|_{r=k}^{\infty} + \frac{(n+1)}{t} \int_{r=k}^{\infty} e^{-tr} r^n \, dr \\
&= \frac{k^{n+1}}{t} e^{-tk} + \frac{(n+1)}{t} \int_{r=k}^{\infty} e^{-tr} r^n \, dr,
\end{aligned}$$

By the induction assumption

$$\begin{aligned}
&= \frac{k^{n+1}}{t} e^{-tk} + \frac{(n+1)e^{-kt}}{t^{n+2}} \sum_{i=0}^{n} \frac{n\,!}{i\,!} t^i k^i \\
&= \frac{e^{-kt}}{t^{n+2}} \big(k^{n+1} t^{n+1} + \sum_{i=0}^{n} \frac{(n+1)n\,!}{i\,!} t^i k^i \big) \\
&= \frac{e^{-kt}}{t^{n+2}} \sum_{i=0}^{n+1} \frac{(n+1)\,!}{i\,!} t^i k^i.
\end{aligned}$$

So we have a base case when $n = 0$, and we have shown that if the statement is true for any n this implies that it is also true for $n+1$. This completes the proof. $\square$

Theorem 3.1.3. *There is some positive function χ of t such that for any large and even number n, an $n \times n$ grid square A with a unit distance between adjacent points is scaled by a factor $t \gg 0$. Then*

$$\frac{\dim_0(tA)}{\chi(t)} \to 1 \qquad as \qquad t \to \infty.$$

Proof. Given a large $n \times n$ grid square A, the 0-spread of A as scaled by a positive factor t is

$$E_0(tA) = \sum_{p \in A} \frac{1}{\sum_{p' \in A} e^{-td(p,p')}}$$

We divide this by the number of points in A

$$\frac{E_0(tA)}{\#A} = \frac{1}{\#A} \sum_{p \in A} \frac{1}{\sum_{p' \in A} e^{-td(p,p')}},$$

to get the average over p of

$$\frac{1}{\sum_{p' \in A} e^{-td(p,p')}}.$$

Let p be a point far from the boundary. We select a point p to be a upper right-hand corner of the middle square of side length t (see Figure 3.3). If the scale of the distance between points t is sufficiently large, then the points are far away from each other, so we shall prove that

$$\sum_{p' \in A} e^{-td(p,p')} \tag{3.2}$$

depends mainly on the distance from the nearest point. Define X to be the sub-grid square of a size 10×10 which contains the point p as seen in Figure 3.3. We then split Expression (3.2) into the sum of two parts

$$\sum_{p' \in A} e^{-td(p,p')} = \sum_{p' \in X} e^{-td(p,p')} + \sum_{p' \in A \setminus X} e^{-td(p,p')}.$$

Since n is even, the points in the grid square A can be divided into four identical quadrants by symmetry. Without loss of generality, we can assume that p the bottom left-hand corner point of the first quadrant is translated to the origin. Writing $d(0, p') = |p'|$, we obtain

$$\sum_{p' \in D} e^{-td(p,p')} = \sum_{p' \in D} e^{-t|p'|},$$

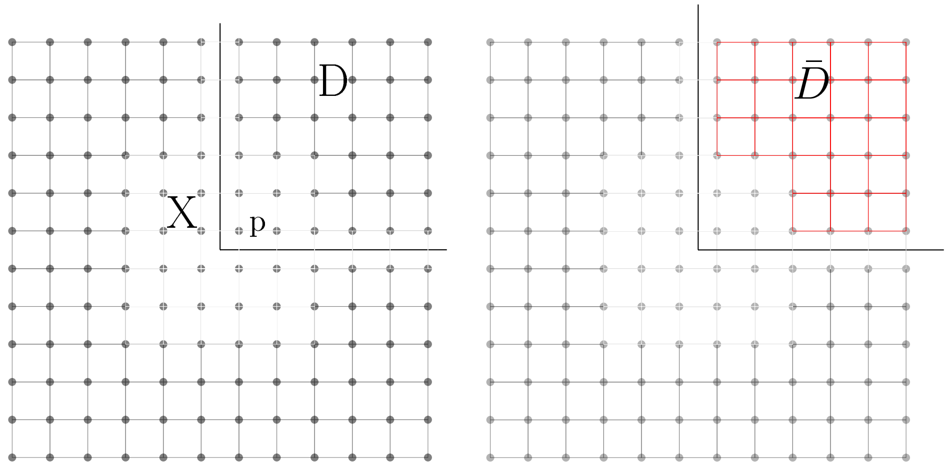


Figure 3.3: Determining the region D and the region $\bar{D}$ (for illustration purposes X is down 4×4 instead of 10×10).

where D is the first quadrant region of $A \backslash X$.

Consider the function $f : \bar{D} \to \mathbb{R}_{>0}$ given by

$$f(p') = e^{-t|p'|}.$$

We now define a step function $\hat{f} : \bar{D} \to \mathbb{R}_{>0}$ to be constant at each unit lattice square as

$$\hat{f}(p') = f(\hat{p'}),$$

where $\hat{p'} = (\lceil x \rceil, \lceil y \rceil)$ is the lattice point at the top right of the square containing $p' = (x, y)$. Also, because $f(p')$ is decreasing in $|p'|$ so $\hat{f} \leq f$.

If $\bar{D}$ is a region containing the points in D and the points in D which completes the unit squares in D, as can be seen in Figure 3.3, then by construction, as each square has unit area $\Delta A = 1$, we have

$$\int\limits_{p' \in \bar{D}} \hat{f}(p')\, dp' = \sum_{\hat{p'} \bar{D}} f(\hat{p'}) \Delta A.$$

Assume that $k > 0$ such that $|p'| > k$ for p' in D. Also we know that $\hat{f} \leq f$, then

$$\sum_{\hat{p'} \in \bar{D}} f(\hat{p'}) = \int\limits_{p' \in \bar{D}} \hat{f}(p')\, dp' \leq \int\limits_{p' \in \bar{D}} f(p')\, dp' \leq \int\limits_{|p'| > k} f(p')\, dp' = \frac{1}{4} \int\limits_{|p'| > k} e^{-t|p'|}\, dp'.$$

Since p' is belongs to the first quadrant of the square grid and the four quadrants are symmetric, then we can write

$$4 \sum_{\hat{p'} \in \bar{D}} f(\hat{p'}) \leq \int\limits_{|p'| > k} e^{-t|p'|}\, dp'$$

Let us change the variables of this integral to polar coordinates to obtain

$$\int_{|p'|\geq k} e^{-t|p'|}\,dp' = \int_{0}^{2\pi}\int_{r=k}^{\infty} e^{-tr} r\,dr\,d\theta = 2\pi \int_{r=k}^{\infty} e^{-tr} r\,dr = 2\pi\frac{e^{-kt}}{t^2}(1+kt).$$

The last equality is by Lemma 3.1.2.

Let $Q_1(t) = 2\pi\frac{e^{-kt}}{t^2}(1+kt)$. This implies that

$$|\sum_{p'\in A\setminus X} e^{-td(p,p')}| < Q_1(t).$$

Therefore, Expression (3.2) is

$$\sum_{p'\in A} e^{-td(0,p')} < \sum_{p'\in X} e^{-td(0,p')} + Q_1(t).$$

So, the 0-spread of tA is

$$E_0(tA) \approx \frac{\#A}{\sum\limits_{p'\in X} e^{-td(0,p')} + Q_1(t)}.$$

Now, we can return to the evaluation of the 0-spread dimension of tA which is by Definition 2.4.1 equal to

$$\begin{aligned}
\frac{t}{E_q(tA)}.\frac{d(E_q(tA))}{dt} &\approx \frac{t}{\frac{\#A}{\sum\limits_{p'\in X} e^{-td(0,p')}+Q_1(t)}}\frac{d}{dt}\left(\frac{\#A}{\sum\limits_{p'\in X} e^{-td(0,p')} + Q_1(t)}\right)\\
&= t\left(\sum_{p'\in X} e^{-t|p'|} + Q_1(t)\right)\frac{\left(\sum\limits_{p'\in X} |p'|e^{-t|p'|} - \frac{d}{dt}Q_1(t)\right)}{\left(\sum\limits_{p'\in X} e^{-t|p'|} + Q_1(t)\right)^2}\\
&= \frac{\sum\limits_{p'\in X} t|p'|e^{-t|p'|} - \frac{d}{dt}Q_1(t)}{\sum\limits_{p'\in X} e^{-t|p'|} + Q_1(t)},
\end{aligned}$$

where $\frac{d}{dt}Q_1(t) = -2\pi\frac{e^{-kt}}{t^3}(2+2kt+t^2k^2)$. Consider $Q_2(t) = -2\pi\frac{e^{-kt}}{t^3}(2+2kt+t^2k^2)$. Then $\dim_0(tA)$ is given by

$$\frac{\sum\limits_{p'\in X} td(0,p')e^{-td(0,p')} + Q_2(t)}{\sum\limits_{p'\in X} e^{-td(0,p')} + Q_1(t)}.$$

Whereas the Taylor series can be used to approximate $Q_1(t)$ and $Q_2(t)$ as $t \gg 0$ to be $O(t^{-1})$. Which are very small that can be neglected and we denoted the remain by $\chi(t) = \frac{\sum_{p' \in X} td(0,p')e^{-td(0,p')}}{\sum_{p' \in X} e^{-td(0,p')}}$. Therefore,

$$\frac{\dim_0(tA)}{\chi(t)} \to 1 \qquad \text{as} \qquad t \to \infty. \tag{3.3}$$

□

We are again plotting the 0-spread dimension for different types of square 60×60, 110×110 and 160×160 with the estimated 0-spread dimension $\chi(t)$ evaluated in Theorem 3.1.3. As can be seen in Figure 3.4, the dimension of metric spaces are approximately the same for larger values of the inter-point distance.

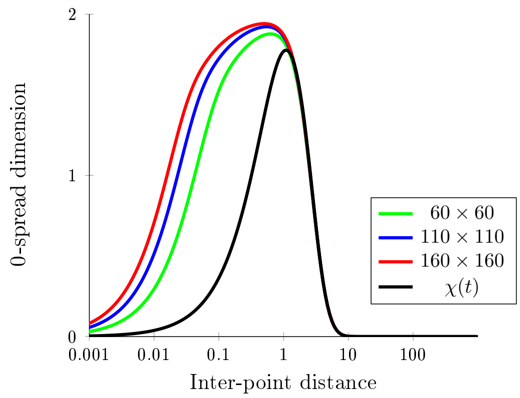


Figure 3.4: The 0-spread dimension of various spaces with the estimation of the 0-spread dimension at different scaling.

In a similar manner to that described in the beginning of Section 3.1, we give the square grid metric space A and a positive scaling factor t. The q-spread of tA for $q = 1, 2$, by Definition 2.4.1, is defined as

$$E_q(tA) = \begin{cases} n^2 . \prod_{p \in A} \left(\frac{1}{\sum_{p' \in A} e^{-td(p,p')}} \right)^{\frac{1}{n^2}} & \text{if} \quad q = 1, \\ \frac{n^4}{\sum_{p \in A} \sum_{p' \in A} e^{-td(p,p')}} & \text{if} \quad q = 2, \end{cases}$$

where the metric d is the usual Euclidean distance formula between two points in A and so is a measure of size. Now we investigate that how the associated size changes under scaling and use this to describe the concept of the q-spread dimension $\dim_q(tA)$ as the growth rate of the q-spread as $q = 1, 2$, which by Definition 3.0.1 is

$$dim(tA) = \frac{d\log(E_q(sA))}{d\log(s)}\Big|_{s=t} = \frac{t}{E_q(sA)}.\frac{d(E_q(sA))}{ds}\Big|_{s=t}.$$

We use numerical evaluation in Maple (see Appendix A.1.1), to determine the q-spread dimensions of different grid squares with 60×60, 110×110 and 160×160 points.

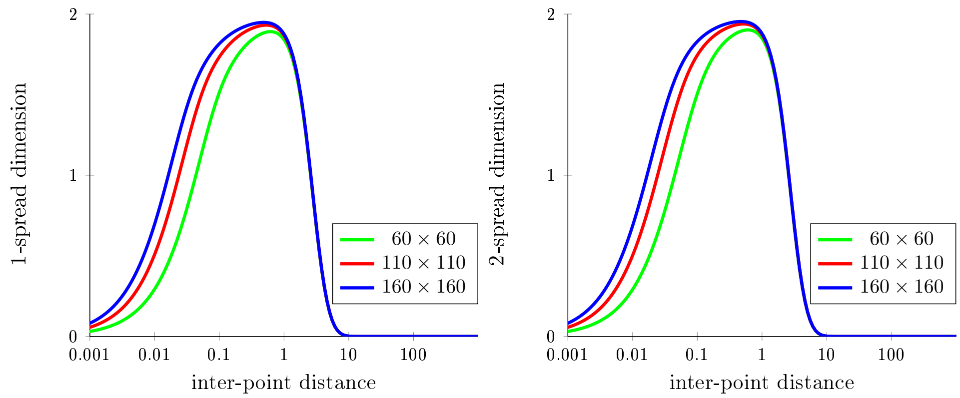


Figure 3.5: A q-spread dimension for grid squares of different sizes at various scaling.

Observe in Figure 3.5 that the q-spread dimension of these grid squares are roughly the same when the inter-point distances are greater than one.

We clarify that by considering a square subset tX of tA with at least 10×10 points that contain the points of a middle square of side length t of the square grid tA, then dividing the q-spread of the metric space tA by their number of points.

$$\frac{E_q(tA)}{n^2} = \begin{cases} \prod\limits_{p\in A}\Big(\frac{1}{\sum\limits_{p'\in A} e^{-td(p,p')}}\Big)^{\frac{1}{n^2}} & \text{if} \quad q = 1, \\ \\ \frac{n^2}{\sum\limits_{p\in A}\sum\limits_{p'\in A} e^{-td(p,p')}} & \text{if} \quad q = 2, \end{cases}$$

these are respectively the geometric average and the harmonic average over the point p of the expression

$$\frac{1}{\sum\limits_{p'\in A} e^{-td(p,p')}}.$$

It follows from the proof of Theorem 3.1.3, this expression equal to:

$$\frac{1}{\sum_{p' \in X} e^{-td(p,p')} + O(t^{-1})}.$$

Also, from the proof of Theorem 3.1.3

$$\chi(t) \approx \frac{\sum_{p' \in X} td(p,p')e^{-td(p,p')}}{\sum_{p' \in X} e^{-td(p,p')}}.$$

Now, as seen in Figure 3.6, the q-spread dimension and the above estimated q-spread dimension are equivalent when inter-point distance becoming larger.

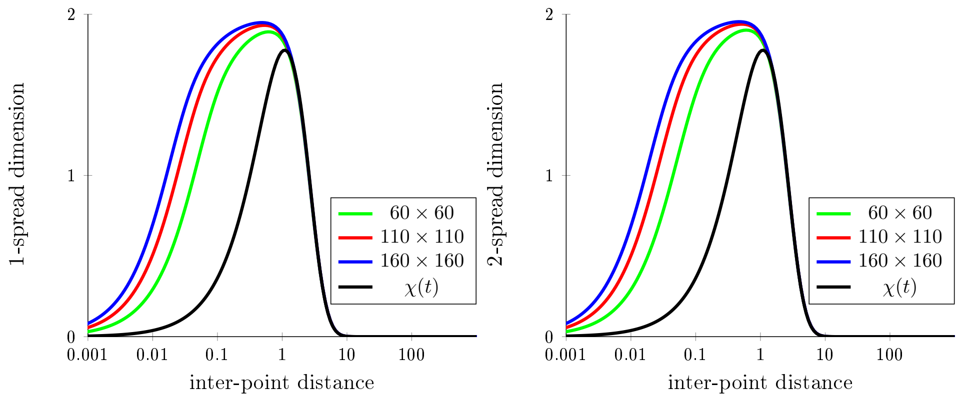


Figure 3.6: A q-spread dimension of grid squares of different sizes compared with the estimated q-spread dimension $\chi(t)$.

As we can see from the graph in Figure 3.7, when the inter-point distance of the 160×160 square grid is very small, the q-spread dimension (for $q = 0, 1, 2$) is approximately the same. we shall describe the details in the following subsection.

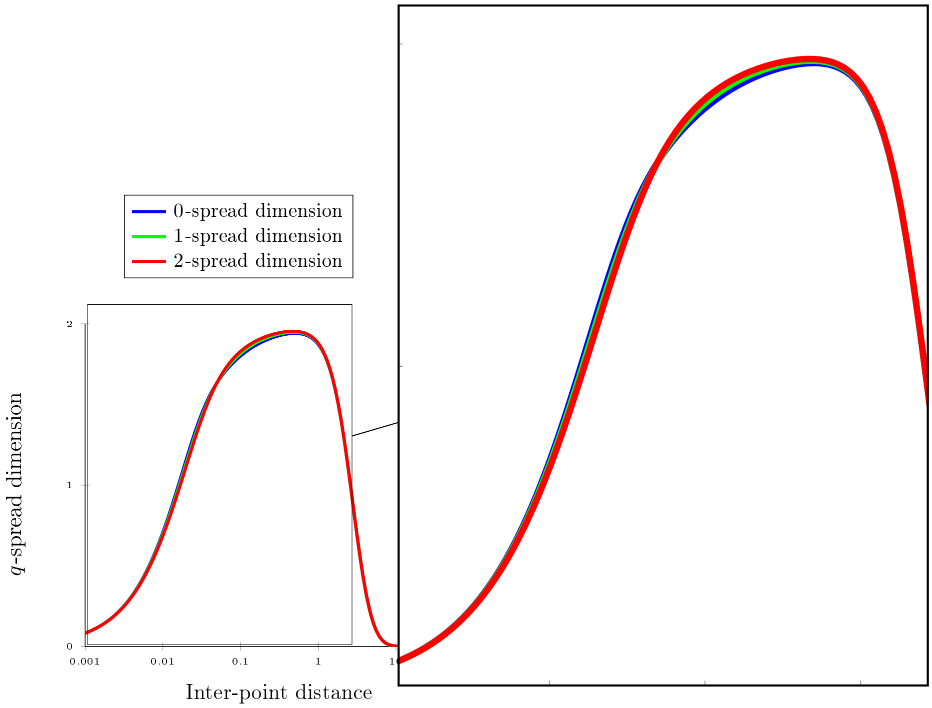


Figure 3.7: The q-spread dimension of the 160×160 square grid at different scales.

§ 3.2 Heuristic for the q-spread dimension of a grid square

In this section, we present a heuristic that approximates the q-spread dimension of a grid square using a solid square. We see from numerical computations that the q-spread dimension is often close to some quadratic formula of a positive τ, independent of $q = 0, 1, 2$.

Let τQ be a $\tau \times \tau$ square subset of $\mathbb{R}^2$. For every $\tau > 0$, this is a solid square, not a grid of points, so τQ is different to tA. Here we are looking first at the 0-spread as a function of side length not distance between points. The square τQ can be approximated by an $n \times n$ square grid of points $\tau \ddot{Q}_n$ with a distance between adjacent points of $\frac{\tau}{n-1}$. This means that $\ddot{Q}_n = \frac{1}{n-1} A$.

Using computer algebra such as Maple (see Appendix A.2), the 0-spread dimensions for $n \times n$ square $\tau \ddot{Q}_n$ for various values of n such as 60, 110 and 160 can be numerically calculated. Then we plot the results, where $\tau > 0$ is the side length of the square.

We can see from Figure 3.8 that the 0-spread dimension of the $\tau \ddot{Q}_n$ for three differently values of n are nearly the same and independent of the number of points, at some smaller scales τ.

Next, we present a heuristic estimate for the contribution to the 0-spread from the bulk of points in a solid square. We see from numerical computa-

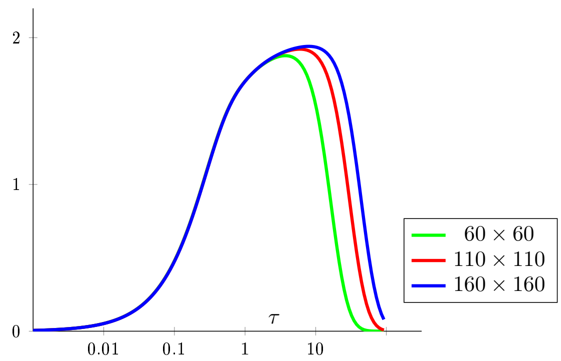


Figure 3.8: The 0-spread dimensions of various square grids $\ddot{Q}_n$ of points at different scales.

tions that for small positive τ the 0-spread is close to the quadratic formula

$$a\tau^2 + b\tau + c,$$

for some positive values of a, b and c. Also, if the distance between adjacent points in the $n \times n$ square grid is very small for large n, then the square grid is approximately the solid square in $\mathbb{R}^2$, which is essentially independent of n. So, the 0-spread of the solid square is supposed to give an approximation to the 0-spread of the $n \times n$ square grid.

Theorem 3.2.1. *If $Q \in \mathbb{R}^2$ is a 1×1 square that is approximated by an $n \times n$ grid square $\ddot{Q}_n$ of lattice points, then we have*

$$E_0(\ddot{Q}_n) \;\rightarrow\; E_0(Q) \qquad \textit{as} \qquad n \;\rightarrow\; \infty.$$

Proof. Since the points of $\ddot{Q}_n$ will be very close to each other for a large number of points, then the square grid $\ddot{Q}_n$ can be approximated to a solid square Q with length sides 1. Take $f : Q \to \mathbb{R}$ be a function on a square region $Q = [0, 1] \times [0, 1] = \{(a, b)| \quad 0 \le a, b \le 1\}$. We can partition Q into n^2 sub-squares Q_{ij} of width $\Delta a = \frac{1}{n}$ and length $\Delta b = \frac{1}{n}$. This partitions the region Q into n^2 sub-squares Q_{ij}, each of which has an area $\Delta A_{ij} = \frac{1}{n^2}$ for each $1 \le i, j \le n$. We can choose a middle point (a_i, b_j) from every sub-square Q_{ij} and consider the expression

$$\sum_i \sum_j f(a_i, b_j)\Delta A_{ij},$$

as $\max \Delta A_{ij} \to 0$, we get

$$\sum_i \sum_j f(a_i, b_j)\Delta A_{ij} \to \int_Q f(a, b)\, dA.$$

By Definition 2.4.1, the 0-spread of $\ddot{Q}_n$ with length sides $\frac{n-1}{n}$ is

$$E_0(\ddot{Q}_n) = \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{1}{\sum\limits_{l=1}^{n}\sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}}$$
$$= \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{1}{\sum\limits_{l=1}^{n}\sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}\Delta A}\Delta A.$$

When $n \to \infty$, the length sides of the grid square $\frac{n-1}{n}$ approaches 1, and ΔA approaches 0, then we have

$$E_0(\ddot{Q}_n) \to \int_Q \frac{1}{\int_Q e^{-\sqrt{(a-a')^2+(b-b')^2}}\, dA}\, dA$$
$$= \int_{a=0}^{1}\int_{b=0}^{1} \frac{1}{\int\limits_{a'=0}^{1}\int\limits_{b'=0}^{1} e^{-\sqrt{(a-a')^2+(b-b')^2}}\, da'\, db'}\, da\, db,$$

which is the 0-spread of Q. □

By the above theorem, the 0-spread of the solid square gives an approximation to the 0-spread of the $n \times n$ square grid. Now if we scale the finite square grid $\ddot{Q}_n$ by a factor for various values of τ, we will show that the 0-spread of the large square grid $\tau\ddot{Q}_n$ is approximately equal to a quadratic function of τ.

Remark 3.2.2. If a large finite grid square metric space $\ddot{Q}_n$ is scaled by a very small factor τ, then there is a function f of τ such that

$$E_0(\tau\ddot{Q}_n) \;\to\; f(\tau) \quad \text{as} \quad n \to \infty.$$

Similarly to the proof of Theorem 3.2.1,

$$E_0(\tau\ddot{Q}_n) \to \int_{a=0}^{\tau}\int_{b=0}^{\tau} \frac{1}{\int\limits_{a'=0}^{\tau}\int\limits_{b'=0}^{\tau} e^{-\sqrt{(a-a')^2+(b-b')^2}}\, da'\, db'}\, da\, db,$$

where $n \to \infty$. We use MATLAB to calculate this integral for various values of τ ranging from 0.0001 to 5 (see Appendix A.2.1). We have used polynomial curve fitting in PYTHON, which involves finding the best polynomials to fit the data to obtain the quadratic formula $0.157\tau^2 + 0.48\tau + 1.01$ which is approximately close to $\frac{\tau^2}{2\pi} + \frac{1}{2}\tau + 1$.

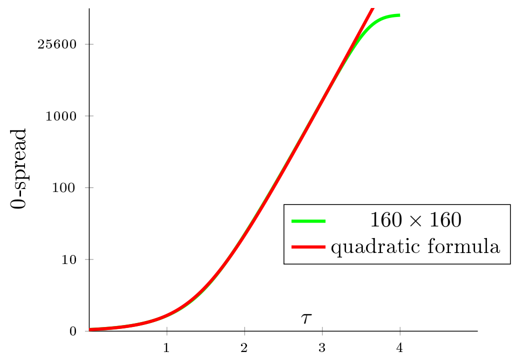


Figure 3.9: Comparison of the 0-spread of square grid $\ddot{Q}_{160}$ with the quadratic formula $\frac{\tau^2}{2\pi} + \frac{\tau}{2} + 1$.

We plot that quadratic expression with the 0-spread of the $\ddot{Q}_{160}$ which gives us a best fit as seen in Figure 5.3.

This means that for small value of τ, the 0-spread of the square grid $\tau\ddot{Q}_n$ for large n is independent to n, so its dimension approximately will not dependent to n, for large n.

The square subset τQ of $\mathbb{R}^2$ and the grid square $\tau\ddot{Q}$ are defined in the same manner as at the beginning of Subsection 3.2. Now, we will look at the 1-spread and 2-spread as a function of side length not distance between points. The square τQ can be approximated by an $n \times n$ square grid of points $\tau\ddot{Q}_n$. We used Maple to compare q-spread dimensions for the 60×60, 110×110 and 160×160 grids square, where $q = 1, 2$, as represented in Figure 3.10.

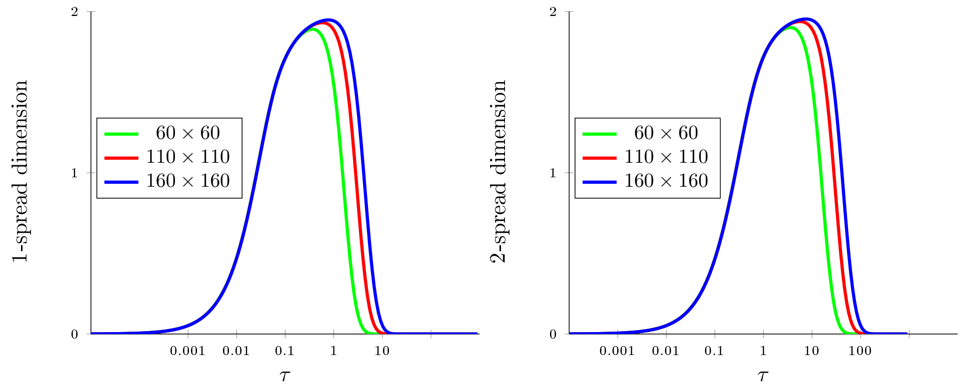


Figure 3.10: A q-spread dimension of the grid square $\ddot{Q}_n$ for different n at various sizes.

In fact, the three expressions that we plotted are similar when τ is very small.

As we mentioned before, the distance between any two adjoining points

$\frac{\tau}{n-1}$ in the $n \times n$ grid square is quite small for large n and small τ. Hence, the grid square is approximately a solid square. The next theorem shows that the 1-spread of the solid square is roughly equal to the 1-spread of the grid square.

Theorem 3.2.3. *If we approximate a 1×1 square subset Q of $\mathbb{R}^2$ by an $n \times n$ grid square $\ddot{Q}_n$ of lattice points, then the following is true*

$$E_1(\ddot{Q}_n) \;\to\; E_1(Q) \qquad as \qquad n \;\to\; \infty.$$

Proof. For larger n, the points of $\ddot{Q}_n$ are very near to each other, that looks like a solid square with sides of length 1. We can take a function $f : Q \to \mathbb{R}$ in a region $Q = [0,\, 1] \times [0,\, 1] = \{(a,\, b)| \quad 0 \le a,\, b \le 1\}$. The region Q can divided into n sub-squares Q_{ij} of equal width $\Delta a = \frac{1}{n}$ and length $\Delta b = \frac{1}{n}$, each having an area $\Delta A = \frac{1}{n^2}$. We can choose a middle point $(a_i,\, b_j)$ in each sub-square and consider the expression

$$\prod_i \big(\prod_j \left(f(a_i, b_j)\right)^{\Delta a}\big)^{\Delta b}.$$

Take the logarithm of above expression

$$\ln\big(\prod_{i,j} \left(f(a_i,\, b_j)\right)^{\Delta A}\big) = \Delta A \sum_{i,j} \ln\left(f(a_i,\, b_j)\right),$$

so

$$\prod_{i,j} \left(f(a_i,\, b_j)\right)^{\Delta A} = e^{\sum_{i,j} \ln (f(a_i, b_j))\Delta A}$$

As $\max \Delta A \to 0$ we have

$$\prod_{i,j} \left(f(a_i, b_j)\right)^{\Delta A} = e^{\int_Q \ln f(a,b)\, dA}.$$

The 1-spread of $\ddot{Q}_n$ by Definition in 2.4.1 as $q = 1$ is

$$\begin{aligned}
E_1(\ddot{Q}_n) &= n^2 \prod_{i=1}^{n} \prod_{j=1}^{n} \Big(\frac{1}{\sum\limits_{l=1}^{n} \sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}}\Big)^{\frac{1}{n^2}} \\
&= \prod_{i=1}^{n} \prod_{j=1}^{n} (n^2)^{n^2} \Big(\frac{1}{\sum\limits_{l=1}^{n} \sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}}\Big)^{\frac{1}{n^2}} \\
&= \prod_{i=1}^{n} \prod_{j=1}^{n} \Big(\frac{n^2}{\sum\limits_{l=1}^{n} \sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}}\Big)^{\frac{1}{n^2}}
\end{aligned}$$

then we can take the logarithm of both sides

$$\begin{aligned}\ln E_1(\ddot{Q}_n) &= \frac{1}{n^2}\ln\Big(\prod_{i,j=1}^{n}\frac{1}{\frac{1}{n^2}}\Big(\frac{1}{\sum\limits_{l,k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}}\Big)\Big)\\ &= \sum_{i,j=1}^{n}\ln\Big(\frac{1}{\sum\limits_{l,k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}\frac{1}{n^2}}\Big)\frac{1}{n^2},\end{aligned}$$

so

$$E_1(\ddot{Q}_n) = e^{\sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n}\ln\Big(\frac{1}{\sum\limits_{l=1}^{n}\sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}\Delta A}\Big)\Delta A}.$$

As $n \to \infty$ the $\max \Delta A \to 0$, then we obtain

$$\begin{aligned}E_1(\ddot{Q}_n) &\to e^{\int_Q \ln\Big(\frac{1}{\int_Q e^{-\sqrt{(a-a')^2+(b-b')^2}}\,dA}\Big)\,dA}\\ &= e^{\int_{a=0}^{1}\int_{b=0}^{1}\ln\Big(\frac{1}{\int_{a'=0}^{1}\int_{b'=0}^{1} e^{-\sqrt{(a-a')^2+(b-b')^2}}\,da'\,db'}\Big)\,da\,db}.\end{aligned}$$

This gives the 1-spread of Q. □

Again, we can scale the $\ddot{Q}_n$ square grid by different positive values of τ and we show that the 1-spread of that square is approximately equal to some quadratic equation of τ.

Remark 3.2.4. Consider a grid square $\ddot{Q}_n$ for large n and a positive value τ. Then there is a function of τ such that

$$E_1(\tau\ddot{Q}_n) \;\to\; f(\tau) \qquad \text{as} \qquad n \to \infty.$$

In the statement of Theorem 3.2.3, the 1-spread of $\ddot{Q}$ approaches to

$$e^{\int_{a=0}^{1}\int_{b=0}^{1}\ln\Big(\frac{1}{\int_{a'=0}^{1}\int_{b'=0}^{1} e^{-\tau\sqrt{(a-a')^2+(b-b')^2}}\,da'\,db'}\Big)\,da\,db}.$$

We apply MATLAB (see Appendix A.2.2) to evaluate the above integral for different values of τ ranging from 0.001 to 5, and use polynomial curve fitting to find the quadratic function $0.157\tau^2 + 0.47\tau + 1.02$ which is also closer to the formula $\frac{\tau^2}{2\pi} + \frac{\tau}{2} + 1$.

In the next theorem, we show that the 2-spread of the solid square is approximately equal to the 2-spread of the grid square $\ddot{Q}_n$.

Theorem 3.2.5. *If we approximate the grid square $\ddot{Q}_n$ by a 1×1 subset Q of $\mathbb{R}^2$, then*

$$E_2(\ddot{Q}_n) \;\to\; E_2(Q) \qquad \textit{as} \qquad n \;\to\; \infty.$$

Proof. For a big value of n, all the points of $\ddot{Q}_n$ are very close to each other, and $\ddot{Q}_n$ is approximately a solid square Q with sides of length 1. We take the function $f : Q \to \mathbb{R}$ on a region $Q = [0,\, 1] \times [0,\, 1] = \{(a,\, b)|0 \leq a,\, b \leq 1\}$; we divide Q into n^2 sub-squares Q_{ij} of equal width and length $\Delta a,\, \Delta b = \frac{1}{n}$. This partitions the region Q into n^2 sub-squares Q_{ij}, each of which has an area $\Delta A_{ij} = \frac{1}{n^2}$. For each sub-square Q_{ij}, we choose a middle point (a_i, b_j) and thus we consider the expression

$$\sum_i \sum_j f(a_i,\, b_j)\Delta A_{ij},$$

as $\max A_{ij} \to 0$, we get

$$\sum_i \sum_j f(a_i,\, b_j)\Delta A_{ij} \to \int_Q f(a,\, b)\, dA.$$

Now, by Definition 2.4.1 for $q = 2$, the 2-spread of $\ddot{Q}_n$ is

$$\begin{aligned} E_2(\ddot{Q}_n) &= \frac{n^4}{\sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n}\sum\limits_{l=1}^{n}\sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}} \\ &= \frac{1}{\sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n}\sum\limits_{l=1}^{n}\sum\limits_{k=1}^{n} e^{-\sqrt{(a_i-a_l)^2+(b_j-b_k)^2}}\frac{1}{n^2}\frac{1}{n^2}}. \end{aligned}$$

As $n \to \infty$, the value $\frac{1}{n^2}$ approaches 0, so

$$\begin{aligned} E_2(\ddot{Q}_n) &\to \frac{1}{\int\limits_Q\int\limits_Q e^{-\sqrt{(a-a')^2+(b-b')^2}}\, dA\, dA} \\ &= \frac{1}{\int\limits_{a=0}^{1}\int\limits_{b=0}^{1}\int\limits_{a'=0}^{1}\int\limits_{b'=0}^{1} e^{-\sqrt{(a-a')^2+(b-b')^2}}\, da'\, db'\, da\, db} \end{aligned}$$

which is the 2-spread of Q. ∎

Here we scale the square grid $\ddot{Q}_n$ by different values of τ and prove that the 2-spread of that square is approximately equal to the quadratic formula $a\tau^2 + b\tau + c$, for some positive values a, b, c provided that n is large.

Remark 3.2.6. Given a grid square $\ddot{Q}_n$ for big n and a positive value τ. Then there is a function of τ such as

$$E_2(\tau\ddot{Q}) \to f(\tau) \quad \text{as} \quad n \to \infty.$$

The 2-spread of $\tau\ddot{Q}_n$ by the statements of Theorem 3.2.5 approaches to

$$\frac{1}{\int\limits_{a'=0}^{1}\int\limits_{b'=0}^{1}\int\limits_{a=0}^{1}\int\limits_{b=0}^{1} e^{-\tau\sqrt{(a-a')^2+(b-b')^2}}\, da'\, db'\, da\, db}$$

the above integral is determined for various values of τ using MATLAB (see Appendix A.2.3) and the curve fitting allows us to calculate the quadratic formula $0.1575\tau^2+0.485\tau+1.02$ that very closer to the expression $\frac{\tau^2}{2\pi}+\frac{\tau}{2}+1$.

Therefore, the 0-spread, 1-spread and 2-spread of the square grid $\tau\ddot{Q}_n$ for large n appear to converge to the quadratic function $\frac{\tau}{2\pi}+\frac{\tau}{2}+1$.

Willerton [55] approximate a 1×1 square Q by the square grid $\ddot{Q}$ of 150×150 points, then the magnitude of $t\ddot{Q}$ is numerical determined for several values of t. Also define the penguin valuation of a square Q scaled by a factor $t>0$, to be

$$P(tQ)=\frac{t^2}{2\pi}+\frac{t}{2}+1.$$

Plotting them together on a graph, (see Figure 4 in [55]), there is a markedly good fit.

Chapter 4

The magnitude and the maximum diversity of the square grid metric spaces

Leinster in [32] established magnitude to be a numerical isometric invariant of metric spaces. Magnitude is defined for a finite metric space A with a metric d by starting from a square matrix $Z = \big(Z_{ab}\big)$ whose columns and rows are indexed by the points of A, with entries

$$Z_{ab} = e^{-d(a,\, b)}. \tag{4.1}$$

Given this, the **weighting** for A is a column vector w such that

$$Zw = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

When the weighting is defined, the **magnitude** $|A|$ is the sum of the entries in the vector w. Here there are two basic principles: the weights are not always positive, and when we have more than one weighting the magnitude is independent of the choice of weighting. If the distance between any pair of points in the metric space A is very small they will appear to be a single point and its magnitude by [Theorem 2.6, [39]] is lower semi-continuous, so

$$\liminf_{t \to 0} |tA| \geq |\cdot| = 1;$$

conversely, if the distances between the points are very large, then the metric space will appear to be a collection of separate points and its magnitude by [Proposition 2.8, [37]] is

$$\lim_{t \to \infty} |tA| = \#A.$$

This means that the magnitude is viewed as the effective number of points, as was first described in the biodiversity literature [52] and which is referred to therein as the effective number of species.

Diversity indices are mathematical measures of species diversity in a given community. Some such measures are the Shannon diversity index, Simpson's diversity index and the Berger Parker diversity index as defined in Section 2.3. Let us consider a community containing S species with relative frequencies of $p_1, \ldots, p_S$. The diversity indices mentioned above have the feature that for a fixed number of species S they are maximized by the uniform relative abundance in which $p_i = \frac{1}{S}$, for $i = 1, 2, \ldots, S$ and take the value S there, so can be thought as effective numbers of species. However, there has been a growing realization that this simple model of biological community is not particularly representative of reality, and does not fully consider the similarities between species. This realization led to a new diversity measure that takes inter-species similarity into account.

Leinster and Cobbold in [35] introduced a new family of diversity measures which takes into account both similarity between the species and their relative abundance. Such a measure is referred to the diversity of order q on relative abundance $p = \{p_1, \ldots, p_S\}$ and similarity matrix Z.

Now consider a list of S species with a known similarity matrix Z; one can ask, what is the maximum diversity of order q, and which probability maximizes it? Leinster [31] provided the answers to these questions, namely that if the similarity matrix of A admits non-negative weighting, then the maximum diversity is simply the magnitude of A. However, if there are any negative weightings, then the maximum is over all $B \subset \{1, \ldots, n\}$ such that Z_B admits a non-negative weighting, so the maximum diversity is the magnitude of that subset, which is independent of q.

This chapter consists of four sections. The first section determines the largest magnitude with a non-negative weighting for all subsets of an 3×3 square grid metric space at various scales to achieve maximum diversity. In the second section, we are interested in the symmetry points of the square grid, and consider only symmetric orbits that are equivalent under the group of symmetries of a square, then for $3 \times 3, \ldots, 10 \times 10$, we determine the maximum magnitude with non-negative weightings of these orbits and unions of these orbits at different scales to ensure maximum diversity. The third section describes how the magnitude of the orbit that contains the four corner points of an $n \times n$ square grid is greater than a magnitude of any other orbits, for sufficiently small scale factor t. Also, when we added any other orbit to the four corner orbit, then the new subset have negative weights on the small-scale. The fourth section studies the weighting of the points in the middle row of the 201×201 grid metric space at different scaling using conjugate gradient method.

§ 4.1 The magnitude and the maximum diversity of a 3×3 square grid

In this section, we determine the maximum diversity of square grid metric space with 3×3 points at various scaling.

Let tA be a 3×3 square grid metric space on the unit grid scaled by a factor $t > 0$ and labeled by $\{[i, j] : 1 \leq i, j \leq 3\}$ which is a subset of $\mathbb{R}^{\nvDash}$, with metric t times the usual Euclidean metric. Its exponential matrix Z with entries $Z_{ij} = e^{-td(i,j)}$ is

$$\begin{bmatrix}
1 & e^{-t} & e^{-2t} & e^{-t} & e^{-t\sqrt{2}} & e^{-t\sqrt{5}} & e^{-2t} & e^{-t\sqrt{5}} & e^{-2t\sqrt{2}} \\
e^{-t} & 1 & e^{-t} & e^{-t\sqrt{2}} & e^{-t} & e^{-t\sqrt{2}} & e^{-t\sqrt{5}} & e^{-2t} & e^{-t\sqrt{5}} \\
e^{-2t} & e^{-t} & 1 & e^{-t\sqrt{5}} & e^{-t\sqrt{2}} & e^{-t} & e^{-2t\sqrt{2}} & e^{-t\sqrt{5}} & e^{-2t} \\
e^{-t} & e^{-t\sqrt{2}} & e^{-t\sqrt{5}} & 1 & e^{-t} & e^{-2t} & e^{-t} & e^{-t\sqrt{2}} & e^{-t\sqrt{5}} \\
e^{-t\sqrt{2}} & e^{-t} & e^{-t\sqrt{2}} & e^{-t} & 1 & e^{-t} & e^{-t\sqrt{2}} & e^{-t} & e^{-t\sqrt{2}} \\
e^{-t\sqrt{5}} & e^{-t\sqrt{2}} & e^{-t} & e^{-2t} & e^{-t} & 1 & e^{-t\sqrt{5}} & e^{-t\sqrt{2}} & e^{-t} \\
e^{-2t} & e^{-t\sqrt{5}} & e^{-2t\sqrt{2}} & e^{-t} & e^{-t\sqrt{2}} & e^{-t\sqrt{5}} & 1 & e^{-t} & e^{-2t} \\
e^{-t\sqrt{5}} & e^{-2t} & e^{-t\sqrt{5}} & e^{-t\sqrt{2}} & e^{-t} & e^{-t\sqrt{2}} & e^{-t} & 1 & e^{-t} \\
e^{-2t\sqrt{2}} & e^{-t\sqrt{5}} & e^{-2t} & e^{-t\sqrt{5}} & e^{-t\sqrt{2}} & e^{-t} & e^{-2t} & e^{-t} & 1
\end{bmatrix}$$

A weighting on A is a column vector w such that

$$Zw = u,$$

where u is a unit column vector. We use Maple (see Appendix B.1) to determine these weightings for different values of t. For example, when $t = 0.001$, we can determine the weighting as follows

$$w = \begin{bmatrix} 0.3203514298 \\ -0.002318084306 \\ 0.3203514298 \\ -0.002318084306 \\ -0.2542313684 \\ -0.002318084306 \\ 0.3203514298 \\ -0.002318084306 \\ 0.3203514298 \end{bmatrix} \tag{4.2}$$

We see from Equation (4.2) that there are some negative weighting, so we need to find the maximum magnitude of the subsets of A that admit a non-negative weighting at various scales, and this maximum is the maximum diversity.

We claim that the subsets which have 0, 1, 2 and 3 points have a non-negative weighting. The empty subsets have a weighting 0 and one-point subsets have a weighting 1. Also, the weighting of a subset consisting of two points is positive, as can be seen from the following example.

Example 4.1.1. Take the subset consisting of two points a distance d apart. The weighting of this subset can be found by solving the following equations

$$\begin{cases} e^{-d}w_a + w_b = 1, \\ w_a + e^{-d}w_b = 1. \end{cases}$$

The solution is

$$w = \begin{bmatrix} \frac{1}{1+e^{-d}} \\ \frac{1}{1+e^{-d}} \end{bmatrix}.$$

Furthermore, any 3 point subset of the square grid has non-negative weighting, as follows from [Proposition 2.4.15, [32]]. Whether or not a subset of tA containing more than three points has a non-negative weighting depends on the value of t. We use Maple code (see Appendix B.1) to evaluate the magnitude of all subsets of the square grid with non-negative weightings, and the maximum magnitude is the maximum diversity.

Now, we find the maximum magnitude of the subsets of tA for different values of $t > 0$, as follows

- If the scale factor of A is $t = 0.1$, then we obtain the subset of four corner points
$$B = \{[1,1],\ [1,3],\ [3,1],\ [3,3]\} \tag{4.3}$$
which has the maximum magnitude with non-negative weighting.

- When the square grid A is scaled by 0.3 we get the subset of the boundary points
$$\{[1,1],\ [1,2],\ [1,3],\ [2,1],\ [2,3],\ [3,1],\ [3,2],\ [3,3]\} \tag{4.4}$$
that has maximum magnitude with non-negative weights.

When the 3×3 square grid is scaled by $t \geq 0.9$, so the distance between each pair of distinct points in the metric space tA is greater than $\log_{10}(\#A - 1)$, then by [Proposition 2.5, [37]], A possesses a positive weighting. Whereas, when the 3×3 square grid is scaled very small, then the four corner points have a larger magnitude with non-negative weights than the magnitude of the subsets consisting of three or fewer points, as the next proposition shows.

Proposition 4.1.2. *Given an 3×3 grid square A scaled by a factor $0 < t \ll 1$, the magnitude of the subset of four corner points B is greater than the magnitude of the subsets of the square grid that contain three-points or fewer.*

Proof. Since the four corner points B of the 3×3 square grid are symmetry, so by Theorem 2.2.13, its magnitude is

$$|tB| = \frac{4}{1 + 2e^{-2t} + e^{-2\sqrt{2}t}},$$

as $t \ll 1$, we approximate the exponential terms in the above expression by the first-order Taylor series expansion, to get

$$\begin{aligned} |tB| = \frac{4}{4 - 2(2+\sqrt{2})t + O(t^2)} &= \frac{1}{1 - \frac{2+\sqrt{2}}{2}t + O(t^2)} \\ &= 1 + \frac{2+\sqrt{2}}{2}t + O(t^2) \\ &\approx 1 + 1.707t + O(t^2). \end{aligned} \tag{4.5}$$

One can see clearly, that the magnitude of tB is greater than the magnitude of 0 and 1 point subsets. So it remains to look at the subsets of the 3×3 square grid that contain 2 or 3 points.

Case 1. From Example 4.1.1, the magnitude of the 2-points subsets tB_1 of the square grid with a distance d apart is

$$\frac{2}{1 + e^{-dt}},$$

when $t \ll 1$, the following an approximate is obtained by applying a first order Taylor series expansion

$$\begin{aligned} |tB_1| &= \frac{2}{2 - dt + O(t^2)} \\ &= \frac{1}{1 - \frac{1}{2}dt + O(t^2)} \\ &\approx 1 + \frac{1}{2}dt + O(t^2), \end{aligned}$$

Since, d is either 1 or $\sqrt{2}$ or $\sqrt{5}$ or $2\sqrt{2}$ or 2, for all cases $2 + \sqrt{2} > d$, so $|tB| > |tB_1|$.

Case 2. Consider the 3-point subset $B_2 = \{a_1, a_2, a_3\}$ of the square grid with distance d_{ij} between a_i and a_j for $i < j$.

Firstly, if $d_{13} = d_{12} + d_{23}$, then by [Theorem 4, [39]], the magnitude of tB_2 is

$$|tB_2| = 1 + \tanh\left(\frac{d_{12}t}{2}\right) + \tanh\left(\frac{d_{23}t}{2}\right).$$

For $t \ll 1$, using Taylor series approximation we obtain

$$|tB_2| \approx 1 + \frac{d_{13}}{2}t + O(t^3).$$

Since, d_{13} is either 2 or $2\sqrt{2}$, for both cases $2+\sqrt{2} > d_{13}$. Therefore, comparing with Equation (4.5) we get $|tB| > |tB_2|$.

Secondly, if $d_{13} \neq d_{12} + d_{23}$, let us first consider the exponential matrix Z_{B_2}

$$\begin{bmatrix} 1 & e^{-d_{12}t} & e^{-d_{13}t} \\ e^{-d_{12}t} & 1 & e^{-d_{23}t} \\ e^{-d_{13}t} & e^{-d_{23}t} & 1 \end{bmatrix}.$$

Then, we can solve the linear equation with respect to w_{B_2},

$$Z_{B_2} w_{B_2} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

where w_{B_2} is the column vector of unknown variables, to get

$$w_{B_2} = \begin{bmatrix} \frac{-e^{-d_{12}t-d_{23}t} - e^{-d_{13}t-d_{23}t} + e^{-2d_{23}t} + e^{-d_{12}t} + e^{-d_{13}t} - 1}{-2e^{-d_{12}t-d_{13}t-d_{23}t} + e^{-2d_{12}t} + e^{-2d_{13}t} + e^{-2d_{23}t} - 1} \\ \\ \frac{-e^{-d_{12}t-d_{13}t} + e^{-2d_{13}t} - e^{-d_{13}t-d_{23}t} + e^{-d_{12}t} + e^{-d_{23}t} - 1}{-2e^{-d_{12}t-d_{13}t-d_{23}t} + e^{-2d_{12}t} + e^{-2d_{13}t} + e^{-2d_{23}t} - 1} \\ \\ \frac{-e^{-d_{12}t-d_{13}t} - e^{-d_{12}t-d_{23}t} + e^{-2d_{12}t} + e^{-d_{23}t} + e^{-d_{13}t} - 1}{-2e^{-d_{12}t-d_{13}t-d_{23}t} + e^{-2d_{12}t} + e^{-2d_{13}t} + e^{-2d_{23}t} - 1} \end{bmatrix}.$$

By the third part of the Theorem 2.2.24, the weighting w_{B_2} is positive. So the magnitude of tB_2 is

$$\begin{aligned} |tB_2| = (&-e^{-2d_{23}t} + 2e^{-d_{23}t-d_{12}t} - e^{-2d_{12}t} + 2e^{-d_{12}t-d_{13}t} - e^{-2d_{13}t} - 2e^{-d_{23}t} \\ &+ 2e^{-d_{23}t-d_{13}t} - 2e^{-d_{12}t} - 2e^{-d_{13}t} + 3)/(2e^{-d_{23}t-d_{12}t-d_{13}t} - e^{-2d_{23}t} \\ &- e^{-2d_{12}t} - e^{-2d_{13}t} + 1). \end{aligned}$$

Since $t \ll 1$, we can approximate the above expression using Taylor series to be

$$1 + 2\frac{d_{12}\,d_{23}\,d_{13}}{-{d_{12}}^2 + 2\,d_{12}\,d_{23} + 2\,d_{12}\,d_{13} - {d_{23}}^2 + 2\,d_{13}\,d_{23} - {d_{13}}^2} t + O\left(t^2\right) \quad (4.6)$$

There are eight possibilities for the distances d_{12}, d_{23}, d_{13}.

1. When d_{12}, d_{23}, d_{13} are 1, 1, $\sqrt{2}$, we have

$$|tB_2| = 1 + 0.773t + O\left(t^2\right),$$

2. When $d_{12} = 1,\ d_{23} = \sqrt{2},\ d_{13} = \sqrt{5}$, we have
$$|tB_2| = 1 + 1.1243t + O\left(t^2\right),$$
3. When $d_{12} = 1,\ d_{23} = 2,\ d_{13} = \sqrt{5}$, we have
$$|tB_2| = 1 + 1.206t + O\left(t^2\right),$$
4. When $d_{12} = 1,\ d_{23} = \sqrt{5}$ and $d_{13} = 2\sqrt{2}$, we have
$$|tB_2| = 1 + 1.4409t + O\left(t^2\right),$$
5. When $d_{12},\ d_{23},\ d_{13}$ are $\sqrt{2},\ \sqrt{2},\ 2$ respectively, we have
$$|tB_2| = 1 + 1.094t + O\left(t^2\right),$$
6. When $d_{12}, d_{23} = 2,\ d_{13} = 2\sqrt{2}$, we have
$$|tB_2| = 1 + 1.547t + O\left(t^2\right),$$
7. When $d_{12}, d_{23} = \sqrt{5}\ \ d_{13} = 2$, we have
$$|tB_2| = 1 + 1.44t + O\left(t^2\right),$$
8. When $d_{12}, d_{23} = \sqrt{5}$ and $d_{13} = \sqrt{2}$, we have
$$|tB_2| = 1 + 1.328t + O\left(t^2\right).$$

From formula (4.5) the magnitude of tB is $1+1.707t+O(t^2)$ which is greater than $|tB_2|$ (for $t \ll 1$) in all eight cases. □

We see above that when t is very small, the maximum diversity is the magnitude of the set of four corner points. While we compute (see Appendix B.1) the magnitude of all set that have more than 3 points at different scaling and we get the following

- When $0 \leq t < 0.23$, the maximum magnitude with non-negative weighting is a magnitude of the four corner points,
- when $0.23 < t \leq 0.87$, the maximum magnitude with non-negative weighting is a magnitude of the boundary points,
- when $t > 0.87$, the maximum magnitude with non-negative weighting is a magnitude of the grid square.

We also, compute the magnitude of all subsets of the 4×4 and 5×5 square grids and we get the magnitude that has non-negative weighting to be the magnitude of orbits and union of orbits. This implies that the maximum diversity occurred for orbits, or unions of such orbits. So we conjectured that maximum diversity always comes from symmetric subsets and concentrated on symmetric subsets. We will explain more details in the next section.

§ 4.2 The maximum diversity of the square grid metric spaces with $3 \times 3, \ldots, 10 \times 10$ points

Speyer [53] showed that all points of a finite metric space have the same weighting if they carry a transitive action of a group of isometries. The symmetry group of the square acts on the $n \times n$ grid square metric space A via isometries but is not transitive, while there are some subsets of the $n \times n$ grid square whose group acts transitively on points. Therefore, we think of the symmetry of the square grid of points only considering symmetric subsets that are invariant under the symmetries of the square. Now, assume a group D_4 of symmetries of the square acts by isometries on the $n \times n$ metric space A. To find the orbit of any $p \in A$, we need to rotate and reflect all points of A around the midpoint to calculate the symmetry functions (see Appendix B.2). Thereafter, we verify the symmetries of all points of A, so for each point in metric space and each of the symmetries, we find the symmetric image of that point; after checking all points of A, this gives a number of equivalence classes which partition A into a union of disjointed subsets which, by Theorem 2.1.7 these equivalent classes are orbits.

The following formulae show that if a group acts isometrically on a metric space and the metric space admits a weighting, then there is an invariant weighting for the metric space.

Proposition 4.2.1. *If the isometry group G acts on the points of a metric space A and w is a weighting for A and the invariant weighting is define, for $p \in A$,*

$$\bar{w}(p) := \frac{1}{\#G} \sum_{g \in G} w(g * p),$$

where $*$ is the group action, then

1 $\bar{w}$ is a weighting of A,

2 $\bar{w}$ is invariant under G, i.e. $\bar{w}(g * p) = \bar{w}(p)$ for all $p \in A$, $g \in G$.

Proof. Part 1. We check that $\bar{w}$ satisfies the weight equations. For $t > 0$ and $p \in A$,

$$\begin{aligned}
\sum_{p' \in A} e^{-td(p,p')} \bar{w}(p') &= \sum_{p' \in A} e^{-td(p,p')} \frac{1}{\#G} \sum_{g \in G} w(g * p') \\
&= \frac{1}{\#G} \sum_{p' \in A} e^{-td(p,p')} \sum_{g \in G} w(g * p') \\
&= \frac{1}{\#G} \sum_{p' \in A} \sum_{g \in G} e^{-td(p,p')} w(g * p')
\end{aligned}$$

Now the set $\{g * p : g \in G\}$ is an orbit that is invariant under G. G acts by isometries, so $d(p, p') = d(g * p, g * p')$ for all $g \in G$ and $p' \in A$. Then we get

$$\sum_{p' \in A} e^{-td(p,p')} \bar{w}(p') = \frac{1}{\#G} \sum_{g \in G} \sum_{p' \in A} e^{-td(g*p, g*p')} w(g * p').$$

But $g * p$ and $g * p'$ are in A, this means that

$$\sum_{p' \in A} e^{-td(g*p, g*p')} w(g * p') = 1.$$

Then,

$$\sum_{p' \in A} e^{-td(p,p')} \bar{w}(p') = \frac{1}{\#G} \sum_{g \in G} 1 = \frac{\#G}{\#G} = 1.$$

This implies that $\bar{w}$ satisfies the weight equation.

Part 2. We need to show that $\bar{w}$ is invariant, for all $p \in A$, $h, g \in G$ we have

$$\begin{aligned} \bar{w}(g * p) &= \frac{1}{\#G} \sum_{h \in G} w(h * (g * p)), \\ &= \frac{1}{\#G} \sum_{hg \in G} w(hg * p)), \\ &= \bar{w}(p). \end{aligned}$$

□

The invariant weighting $\bar{w}$ from Proposition 4.2.1 take the same value at points of an orbit. We partition A into a number of orbits, and now consider **a fundamental domain** to be a subset of A that contains exactly one point from each orbit.

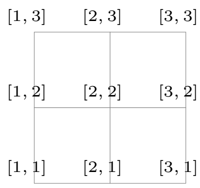
Via some computational code (see Appendix B.2), for each point in the fundamental domain we find its invariant weighting, then the magnitude of A is found as the sum of the individual products of the weighting and the number of points in each orbit. The maximum diversity and the magnitude are the same if there are no negative invariant weights, but when there are some negative invariant weights, linear algebra (see Appendix B.2) can be used to determine the $2^{\#\mathrm{orb}(A)}$ subsets of the fundamental domains. The magnitude of the corresponding orbit and union of orbits can then be evaluated and recorded if the weighting is non-negative. The maximum recorded magnitude is then the maximum diversity of A.

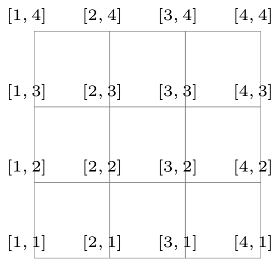
We divided this section into four subsection to determine the maximum diversity of 3×3, 4×4, $\ldots$, 9×9, and 10×10 metric spaces.

4.2.1 The maximum diversity of a square grid with 3×3 and 4×4 points

In this subsection, we compute (see Appendix B.2) the magnitude of orbits and union of orbits of 3×3 and 4×4 square grids that have non-negative weighting at different scaling, then we determine its critical values.

Let A and B be two square grids with $3{\times}3$ and $4{\times}4$ points, respectively.





If the group of symmetries of a square acting on the metric spaces A and B, then these square grids are partitioned into three orbits.

The partitions for A and B are

- $\text{orbit}_1 = \{[1,1],\ [1,3],\ [3,1],\ [3,3]\}$,
- $\text{orbit}_2 = \{[1,2],\ [2,3],\ [3,2],\ [2,1]\}$,
- $\text{orbit}_3 = \{[2,2]\}$,

and

- $\text{orbit}_1 = \{[1,1],\ [1,4],\ [4,4],\ [4,1]\}$,
- $\text{orbit}_2 = \{[1,2],\ [2,1],\ [4,3],\ [3,4],\ [1,3],\ [2,4], [4,2],\ [3,1]\}$,
- $\text{orbit}_3 = \{[2,2],\ [2,3],\ [3,3],\ [3,2]\}$,

respectively. Now consider that fundamental domains of these metric spaces are $\{[3,3],\ [3,2],\ [2,2]\}$ and $\{[4,4],\ [4,3],\ [3,3]\}$, which form triangles of points in Figure 4.1.

Figure 4.1: The fundamental domains of square grids with 3×3 and 4×4 points.

We used certain Maple code (see Appendix B.2) to obtain the invariant weighting equations for each point in the fundamental domain and solved them for various values of t, as shown in Figure 4.2.

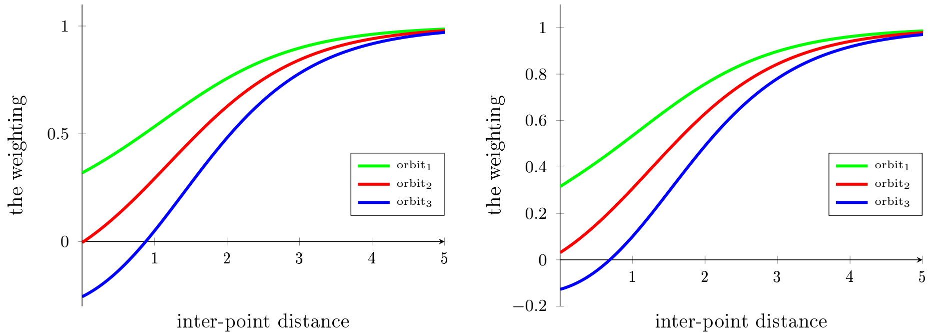


Figure 4.2: The weighting for 3×3 and 4×4 grid squares at various scales.

From Graph 4.2, we note that there are non-positive invariant weights. However, when the 3×3 and the 4×4 are scaled by $t \geq 1$, all the weighting values are non-negative and in this case the maximum diversity is equal to the magnitude of the metric space. But, there are some points in the square grids which have negative weightings when A and B are scaled between 0 and 1. So we have to find subsets of A and B that have maximum magnitude with non-negative weighting as follows

- The first subsets S_1 and S_1' of 3×3 and 4×4 are the orbit$_1$, when the scaled factor t is between 0 and t_0.

  We find the magnitudes of the first subset of A and B to be

  $$|S_1| = 4\left(2\,\mathrm{e}^{-2\,t} + \mathrm{e}^{-2\,t\sqrt{2}} + 1\right)^{-1}$$

  and

  $$|S_1'| = 4\left(2\,\mathrm{e}^{-3\,t} + \mathrm{e}^{-3\,t\sqrt{2}} + 1\right)^{-1}$$

  respectively.

- The second subsets S_2 and S_2' are the union of orbit$_1$ and orbit$_2$, that the scale factor t is $t_0 \leq t < t_1$, where t_0 and t_1 are found at the end of this section.

The magnitudes of the second subset of 3×3 and 4×4 are

$$|S_2| = 4 \left[\frac{4\,e^{-t} + 4\,e^{-t\sqrt{5}} - 2\,e^{-t\sqrt{2}} - 3\,e^{-2\,t} - 2 - e^{-2\,t\sqrt{2}}}{\begin{array}{r} -2\,e^{-4\,t} - e^{-2\,t\left(1+\sqrt{2}\right)} - 4\,e^{-t\left(2+\sqrt{2}\right)} - 2\,e^{-3\,t\sqrt{2}} + e^{-2\,t} \\ + 8\,e^{-t\left(\sqrt{5}+1\right)} + 4\,e^{-2\,t\sqrt{5}} - e^{-2\,t\sqrt{2}} - 2\,e^{-t\sqrt{2}} - 1 \end{array}} \right]$$

and

$$|S_2'| = \frac{N_0(t)}{D_0(t)},$$

respectively, where

$$\begin{aligned} N_0(t) = -4\big(\, & 5\,e^{-3\,t} - 3\,e^{-t} - 4\,e^{-2\,t} - 4\,e^{-t\sqrt{13}} - 3\,e^{-t\sqrt{2}\sqrt{5}} \\ & + 2\,e^{-t\sqrt{5}} + e^{-2\,t\sqrt{2}} + e^{-t\sqrt{2}} + 3 + 2\,e^{-3\,t\sqrt{2}} \,\big), \end{aligned}$$

and

$$\begin{aligned} D_0(t) = & -1 + e^{-3\,t} - e^{-3\,t\sqrt{2}} - 2\,e^{-t\left(\sqrt{2}\sqrt{5}+3\right)} - e^{-t\sqrt{2}\left(\sqrt{5}+3\right)} - 2\,e^{-t\sqrt{5}} \\ & + 4\,e^{-t\left(\sqrt{2}\sqrt{5}+2\right)} + 4\,e^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{13}\right)} - e^{-3\,t\left(1+\sqrt{2}\right)} - 4\,e^{-t\left(\sqrt{5}+3\right)} \\ & - 2\,e^{-t\left(2\sqrt{2}+3\right)} - 2\,e^{-t\left(\sqrt{2}+3\right)} - 2\,e^{-t\left(3\sqrt{2}+\sqrt{5}\right)} + 4\,e^{-t\left(\sqrt{13}+1\right)} \\ & + 4\,e^{-t\left(\sqrt{13}+2\right)} - e^{-4\,t\sqrt{2}} - e^{-5\,t\sqrt{2}} - e^{-t\left(3\sqrt{2}+1\right)} + 4\,e^{-t\left(\sqrt{2}\sqrt{5}+1\right)} \\ & + 2\,e^{-2\,t\sqrt{13}} + 2\,e^{-2\,t\sqrt{2}\sqrt{5}} - 2\,e^{-6\,t} - e^{-t\sqrt{2}\sqrt{5}} - e^{-t\sqrt{2}} - e^{-2\,t\sqrt{2}} \\ & + 2\,e^{-2\,t} - e^{-t}. \end{aligned}$$

- The third subsets S_3 and S_3' are made up from the 3×3 and 4×4 square grids, with scale factor $t \geq t_1$.

  The magnitudes of 3×3 and 4×4 square grids are

$$|S_3| = \frac{N_1(t)}{D_1(t)},$$

and

$$|S_3'| = \frac{N_2(t)}{D_2(t)},$$

respectively, where

$$
\begin{aligned}
D_2(t) = {} & -1 + 9\mathrm{e}^{-3\,t} + \mathrm{e}^{-3\,t\sqrt{2}} + 6\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+3\right)} - 3\,\mathrm{e}^{-t\sqrt{2}\left(\sqrt{5}+3\right)} \\
& + 4\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{13}\right)} + 3\,\mathrm{e}^{-3\,t\left(1+\sqrt{2}\right)} - 20\,\mathrm{e}^{-t\left(\sqrt{5}+3\right)} - 7\,\mathrm{e}^{-t\left(2\,\sqrt{2}+3\right)} \\
& - 9\,\mathrm{e}^{-t\left(\sqrt{2}+3\right)} + 10\,\mathrm{e}^{-t\left(3\,\sqrt{2}+\sqrt{5}\right)} + 4\,\mathrm{e}^{-t\left(\sqrt{13}+1\right)} + 12\,\mathrm{e}^{-t\left(\sqrt{13}+2\right)} \\
& + 3\,\mathrm{e}^{-5\,t\sqrt{2}} - 5\,\mathrm{e}^{-t\left(3\,\sqrt{2}+1\right)} + 2\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+1\right)} - 5\,\mathrm{e}^{-t\left(2\,\sqrt{2}+1\right)} + \mathrm{e}^{-t\left(1+\sqrt{2}\right)} \\
& + 2\,\mathrm{e}^{-t\left(2+\sqrt{2}\right)} + 2\,\mathrm{e}^{-2\,t\sqrt{13}} + 2\,\mathrm{e}^{-2\,t\sqrt{2}\sqrt{5}} + 4\,\mathrm{e}^{-4\,t} + 6\,\mathrm{e}^{-6\,t} + 6\,\mathrm{e}^{-2\,t\sqrt{5}} \\
& - \mathrm{e}^{-t\sqrt{2}\sqrt{5}} - 2\,\mathrm{e}^{-t\sqrt{2}} + \mathrm{e}^{-2\,t\sqrt{2}} - 2\,\mathrm{e}^{-t\sqrt{5}} + 2\,\mathrm{e}^{-2\,t} - 3\,\mathrm{e}^{-t} + 4\,\mathrm{e}^{-5\,t} \\
& - 2\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+3\,\sqrt{2}+1\right)} + 8\,\mathrm{e}^{-3\,t\sqrt{5}} - 8\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{5}+1\right)} - 8\,\mathrm{e}^{-2\,t\left(\sqrt{5}+1\right)} \\
& - 4\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+4\right)} + 8\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{13}+1\right)} + 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}\sqrt{5}+1\right)} + 2\,\mathrm{e}^{-t\sqrt{2}\left(2\,\sqrt{5}+1\right)} \\
& - 4\,\mathrm{e}^{-t\sqrt{5}\left(2+\sqrt{2}\right)} + 8\,\mathrm{e}^{-t\left(\sqrt{13}+3\right)} - 3\,\mathrm{e}^{-t\sqrt{2}\left(\sqrt{5}+2\right)} - 8\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{5}+2\right)} \\
& - 8\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{2}+\sqrt{5}\right)} + 4\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{2}+\sqrt{13}\right)} - 8\,\mathrm{e}^{-2\,t\left(1+\sqrt{2}\right)} \\
& - 4\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+2\,\sqrt{2}+2\right)} - 2\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{2}+3\right)} - 8\,\mathrm{e}^{-t\left(\sqrt{2}+\sqrt{5}+1\right)} \\
& + 8\,\mathrm{e}^{-t\left(\sqrt{2}+5\right)} - 12\,\mathrm{e}^{-t\left(\sqrt{2}+\sqrt{13}+\sqrt{5}\right)} - 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{13}\right)} - 4\,\mathrm{e}^{-t\left(3\,\sqrt{2}+\sqrt{13}\right)} \\
& - 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{5}+2\right)} - 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{13}+\sqrt{5}\right)} - 8\,\mathrm{e}^{-t\left(\sqrt{13}+\sqrt{5}+1\right)} \\
& - 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{13}+1\right)} - 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{13}+2\right)} + 8\,\mathrm{e}^{-t\left(\sqrt{2}+\sqrt{5}+3\right)} \\
& + 8\,\mathrm{e}^{-t\left(5+\sqrt{5}\right)} - 8\,\mathrm{e}^{-2\,t\left(2+\sqrt{2}\right)} + 8\,\mathrm{e}^{-t\left(4\,\sqrt{2}+\sqrt{5}\right)} + 2\,\mathrm{e}^{-t\left(4\,\sqrt{2}+1\right)} \\
& + 4\,\mathrm{e}^{-t\left(3\,\sqrt{2}+\sqrt{5}+2\right)} - 2\,\mathrm{e}^{-t\left(\sqrt{2}+6\right)} + 8\,\mathrm{e}^{-t\left(2\,\sqrt{5}+3\right)} + 2\,\mathrm{e}^{-t\left(3\,\sqrt{2}+2\,\sqrt{5}\right)} \\
& + 12\,\mathrm{e}^{-t\left(\sqrt{2}+2\,\sqrt{5}\right)} + 6\,\mathrm{e}^{-t\left(\sqrt{2}+\sqrt{5}\right)} + 2\,\mathrm{e}^{-t\left(\sqrt{2}+2\,\sqrt{13}\right)} - \mathrm{e}^{-t\sqrt{2}\left(\sqrt{5}+1\right)} \\
& + 10\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{5}\right)} + 12\,\mathrm{e}^{-2\,t\left(\sqrt{2}+\sqrt{5}\right)} - 4\,\mathrm{e}^{-t\left(2\,\sqrt{5}+1\right)} - 4\,\mathrm{e}^{-t\left(\sqrt{5}+2\right)} \\
& - 8\,\mathrm{e}^{-t\left(\sqrt{13}+2\,\sqrt{5}\right)} + 4\,\mathrm{e}^{-t\left(2\,\sqrt{13}+1\right)} + 12\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+2\right)} + 2\,\mathrm{e}^{-4\,t\sqrt{2}} \\
& - 8\,\mathrm{e}^{-t\left(\sqrt{5}+4\right)} - 4\,\mathrm{e}^{-t\left(3\,\sqrt{2}+2\right)} + 4\,\mathrm{e}^{-2\,t\left(2\,\sqrt{2}+1\right)} - 4\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+2\,\sqrt{2}+1\right)} \\
& + 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{5}+3\right)} - 8\,\mathrm{e}^{-t\left(\sqrt{13}+\sqrt{5}+2\right)} - 12\,\mathrm{e}^{-t\left(\sqrt{2}+\sqrt{5}+2\right)} - 2\,\mathrm{e}^{-t\left(5\,\sqrt{2}+1\right)},
\end{aligned}
$$

$$
\begin{aligned}
N_1(t) = {} & -[-9 + 24\,\mathrm{e}^{-t} + 16\,\mathrm{e}^{-t\sqrt{5}} - 2\,\mathrm{e}^{-t\sqrt{2}} - 11\,\mathrm{e}^{-2\,t} + 27\,\mathrm{e}^{-2\,t\sqrt{2}} \\
& + 16\,\mathrm{e}^{-3\,t} - \mathrm{e}^{-2\,t\left(1+\sqrt{2}\right)} - 48\,\mathrm{e}^{-t\left(1+\sqrt{2}\right)} + 8\,\mathrm{e}^{-t\left(2\,\sqrt{2}+1\right)} \\
& + 4\,\mathrm{e}^{-2\,t\sqrt{5}} - 16\,\mathrm{e}^{-t\left(\sqrt{5}+\sqrt{2}\right)} + 4\,\mathrm{e}^{-t\left(2+\sqrt{2}\right)} - 8\,\mathrm{e}^{-t\left(\sqrt{5}+1\right)} \\
& - 2\,\mathrm{e}^{-4\,t} - 2\,\mathrm{e}^{-3\,t\sqrt{2}}],
\end{aligned}
$$

$$
\begin{aligned}
D_1(t) = {} & 20\,\mathrm{e}^{-t\left(2+\sqrt{2}\right)} - 6\,\mathrm{e}^{-4\,t} - 7\,\mathrm{e}^{-2\,t\left(1+\sqrt{2}\right)} + 16\,\mathrm{e}^{-t\left(\sqrt{5}+\sqrt{2}+1\right)} \\
& - 6\,\mathrm{e}^{-3\,t\sqrt{2}} - 5\,\mathrm{e}^{-2\,t} - 8\,\mathrm{e}^{-t\left(\sqrt{5}+1\right)} - 4\,\mathrm{e}^{-2\,t\sqrt{5}} - 3\,\mathrm{e}^{-2\,t\sqrt{2}} \\
& + 2\,\mathrm{e}^{-t\sqrt{2}} + 1,
\end{aligned}
$$

and

$$
\begin{aligned}
N_2(t) = 4\,[&-4 - 2\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+3\right)} - \mathrm{e}^{-t\sqrt{2}\left(\sqrt{5}+3\right)} + 4\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+\sqrt{13}\right)} \\
&- \mathrm{e}^{-3\,t\left(1+\sqrt{2}\right)} + 8\,\mathrm{e}^{-t\left(\sqrt{5}+3\right)} + 3\,\mathrm{e}^{-t\left(\sqrt{2}+3\right)} + 2\,\mathrm{e}^{-t\left(3\,\sqrt{2}+\sqrt{5}\right)} \\
&+ 8\,\mathrm{e}^{-t\left(\sqrt{13}+1\right)} + 5\,\mathrm{e}^{-4\,t\sqrt{2}} - \mathrm{e}^{-5\,t\sqrt{2}} - \mathrm{e}^{-t\left(3\,\sqrt{2}+1\right)} + 6\,\mathrm{e}^{-t\left(\sqrt{2}\sqrt{5}+1\right)} \\
&- 16\,\mathrm{e}^{-t\left(\sqrt{5}+1\right)} - 8\,\mathrm{e}^{-t\left(2\,\sqrt{2}+1\right)} - 5\,\mathrm{e}^{-t\left(1+\sqrt{2}\right)} - 4\,\mathrm{e}^{-t\left(2+\sqrt{2}\right)} \\
&+ 10\,\mathrm{e}^{-2\,t\sqrt{5}} + 2\,\mathrm{e}^{-t\sqrt{2}\sqrt{5}} + \mathrm{e}^{-t\sqrt{2}} + \mathrm{e}^{-2\,t\sqrt{2}} + 4\,\mathrm{e}^{-t\sqrt{5}} + 4\,\mathrm{e}^{-t\sqrt{13}} \\
&+ 14\,\mathrm{e}^{-2\,t} + 8\,\mathrm{e}^{-5\,t} + 6\,\mathrm{e}^{-t\left(\sqrt{2}+\sqrt{5}\right)} - 3\,\mathrm{e}^{-t\sqrt{2}\left(\sqrt{5}+1\right)} + 12\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{5}\right)} \\
&- 16\,\mathrm{e}^{-t\left(\sqrt{5}+2\right)} + 4\,\mathrm{e}^{-t\left(3\,\sqrt{2}+2\right)} - 12\,\mathrm{e}^{-t\left(\sqrt{13}+\sqrt{5}\right)} - 4\,\mathrm{e}^{-t\left(2\,\sqrt{2}+\sqrt{13}\right)} \\
&- 8\,\mathrm{e}^{-2\,t\left(1+\sqrt{2}\right)} - 4\,\mathrm{e}^{-t\left(\sqrt{2}+\sqrt{13}\right)} - 8\,\mathrm{e}^{-t\sqrt{5}\left(1+\sqrt{2}\right)} - 2\,\mathrm{e}^{-t\sqrt{2}\left(\sqrt{5}+2\right)} \\
&+ 2\,\mathrm{e}^{-2\,t\sqrt{13}} + 2\,\mathrm{e}^{-2\,t\sqrt{2}\sqrt{5}} - 4\,\mathrm{e}^{-4\,t} - 2\,\mathrm{e}^{-6\,t}],
\end{aligned}
$$

We plotted three above magnitudes together for various values of t to look at where these were crossed as shown in Figure 4.3 and we found that there are the points where the curves intersect.

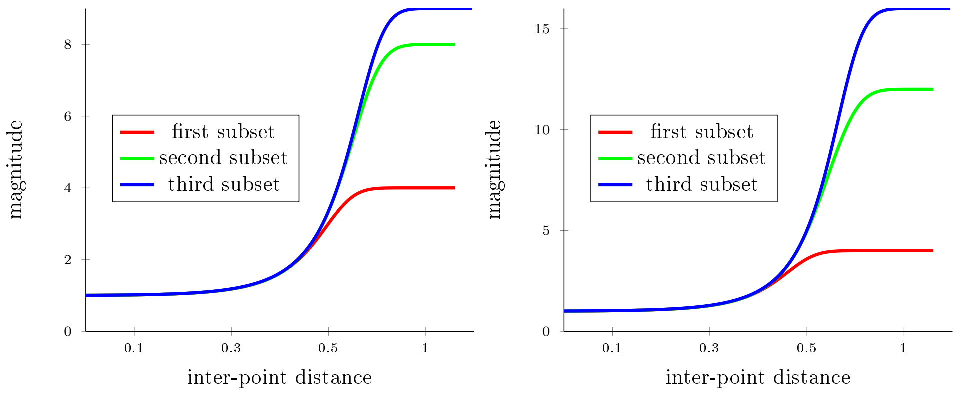


Figure 4.3: The magnitude for the three subsets of 3×3 and 4×4 grid squares at different scales.

From Figure 4.3, we see that the three subsets of 3×3 and 4×4 grid squares have very similar magnitude for low values of t. But there is a small difference, we check it for the value $t = 0.1$ as can be seen as follows

The magnitude of subsets of 3×3 and 4×4 grid squares at $t = 0.1$ are

- the magnitude of first subset is 1.179558317,
- the magnitude of second subset is 1.180421838,
- the magnitude of third subset is 1.184872337

and

- the magnitude of first subset is 1.275555949,
- the magnitude of second subset is 1.276138864,
- the magnitude of third subset is 1.286455041.

respectively.

To calculate graphically the point of intersection curves, we first find the places for the values of t where the curves intersected, then select the regions of the graph around these points. We can apply the same idea algebraically which is called **determining the critical values**, by setting the difference of above formulae of A and B equal to zero such as

$$\begin{aligned} |S_2| - |S_1| = 0 \\ |S_3| - |S_2| = 0 \end{aligned} \tag{4.7}$$

and

$$\begin{aligned} |S_2'| - |S_1'| = 0 \\ |S_3'| - |S_2'| = 0 \end{aligned} \tag{4.8}$$

respectively. The Maple code (see Appendix B.2.1) used to solve the formulea (4.7) and (4.8) to obtain the critical values of t, $t_0 = 0.2323$, $t_1 = 0.877$ for magnitude tA, and $t_0 = 0.1547$, $t_1 = 0.6863$ for magnitude tB, so the maximum magnitudes of square grids with non-negative weighting are gives as

$$|A| = \begin{cases} |S_1|, & 0 \le t \le t_0 \\ |S_2|, & t_0 < t \le t_1, \\ |S_3|, & t > t_1, \end{cases}$$

and

$$|B| = \begin{cases} |S_1'|, & 0 \le t \le t_0 \\ |S_2'|, & t_0 < t \le t_1, \\ |S_3'|, & t > t_1, \end{cases}$$

which is continuous at critical points t_0 and t_1. Now, in both square grids we have when $0 \le t \le t_0$, the points in orbit_1 give the maximum magnitude with non-negative weights, that is, the maximum diversity. And for $t_0 < t \le t_1$, the points in the orbit_1 union orbit_2 have maximum magnitude with non-negative weights, which is maximum diversity and finally, when $t > t_1$ the magnitudes of square grids are maximum diversity.

In this manner, the maximum diversity of A, denoted $D_{max}(A)$ is

$$D_{max}(A) = \begin{cases} |\text{orbit}_1|, & \text{if } 0 \le t \le 0.2323, \\ |\text{orbit}_1 \cup \text{orbit}_2|, & \text{if } 0.2323 < t \le 0.877, \\ |A|, & \text{if } t > 0.877. \end{cases}$$

And the maximum diversity of the 4×4 metric space, denoted $D_{max}(B)$, is equal to

$$D_{max}(B) = \begin{cases} |\mathrm{orbit}_1|, & \text{if } 0 \leq t \leq 0.1547, \\ |\mathrm{orbit}_1 \cup \mathrm{orbit}_2|, & \text{if } 0.1547 < t \leq 0.6863, \\ |B|, & \text{if } t > 0.6863. \end{cases}$$

Furthermore, to examine whether the maximum diversity formulae for A and B are smooth, we use Maple (see Appendix B.2.1) to compute the first derivatives of $|A|$ and $|B|$ with respect to the two critical values of t as

$$\begin{aligned} \frac{d}{dt}|S_1|(t_0) &= 2.066877, \\ \frac{d}{dt}|S_2|(t_0) &= 2.066877, \\ \frac{d}{dt}|S_2|(t_1) &= 2.713363, \\ \frac{d}{dt}|S_3|(t_1) &= 2.713363, \end{aligned}$$

from that, we found

$$\frac{d}{dt}|S_1|(t_0) = \frac{d}{dt}|S_2|(t_0)$$

and

$$\frac{d}{dt}|S_2|(t_1) = \frac{d}{dt}|S_3|(t_1).$$

Similarly for S_i'. This means that the above formulae are smooth, as shown in the following figure.

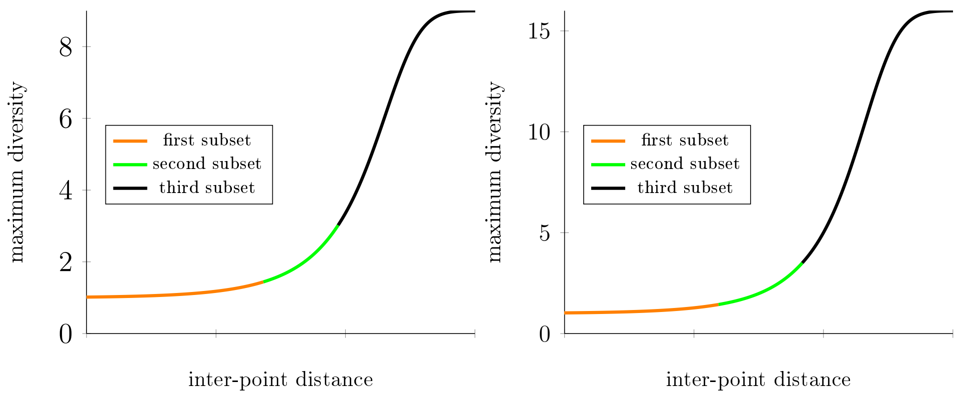
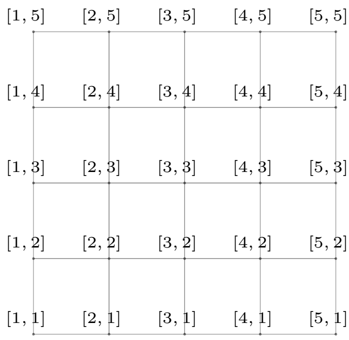


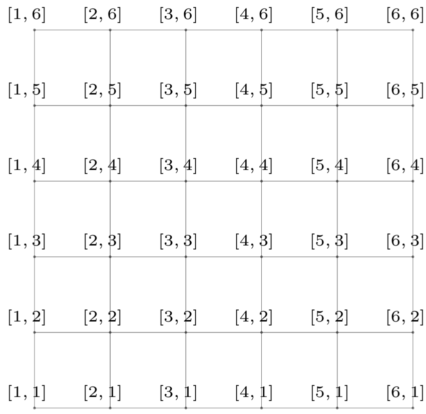
Figure 4.4: The maximum diversity of 3×3 and 4×4 metric spaces at various scales.

4.2.2 The maximum diversity of 5×5 and 6×6 square grid

Here we compute (see Appendix B.2) the magnitude of orbits and union of orbits of 5×5 and 6×6 square grids that have non-negative weighting at various scaling, then we calculate its critical values.

Grid squares with 5×5 and 6×6 points are defined as





To determine the weighting for A and B, we first identify the six orbits that partition the points of the two metric spaces (see Appendix B.2).

The six orbits of the 5×5 are

- $\text{orbit}_1 = \{[1,1],[1,5],[5,5],[5,1]\}$,
- $\text{orbit}_2 = \{[1,2],[2,1],[5,4],[4,5],[1,4],[4,1],[5,2],[2,5]\}$,
- $\text{orbit}_3 = \{[1,3],[3,1],[5,3],[3,5]\}$,
- $\text{orbit}_4 = \{[3,3]\}$,
- $\text{orbit}_5 = \{[2,3],[3,2],[4,3],[3,4]\}$,
- $\text{orbit}_6 = \{[2,2],[4,2],[4,4],[2,4]\}$,

and the orbits of 6×6 are

- $\text{orbit}_1 = \{[1,1],[6,1],[6,6],[1,6]\}$,
- $\text{orbit}_2 = \{[1,2],[2,1],[6,5],[5,6],[1,5],[5,1],[6,2],[2,6]\}$,
- $\text{orbit}_3 = \{[1,3],[1,4],[6,3],[6,4],[3,1],[4,1],[3,6],[4,6]\}$,
- $\text{orbit}_4 = \{[3,3],[4,3],[4,4],[3,4]\}$,
- $\text{orbit}_5 = \{[2,3],[2,4],[5,3],[5,4],[3,2],[4,2],[3,5],[4,5]\}$,
- $\text{orbit}_6 = \{[2,2],[2,5],[5,5],[5,2]\}$.

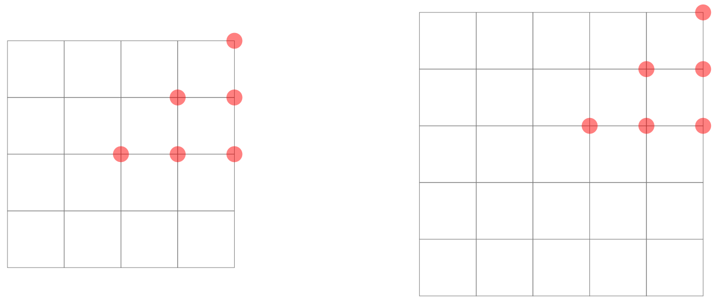


Figure 4.5: The fundamental domains of 5×5 and 6×6 square grids

The triangles shown in Figure 4.5 are the fundamental domains of the 5×5 and 6×6 metric spaces.

These points have distinct invariant weights, and by applying the computational program (see Appendix B.2) the weight equations for points in the fundamental domain can be solved for different values of t from 0.0001 to 30, as represented in Figure 4.6 and by adding individual products of the weighting and the number of points in that orbit; the magnitude can be obtained

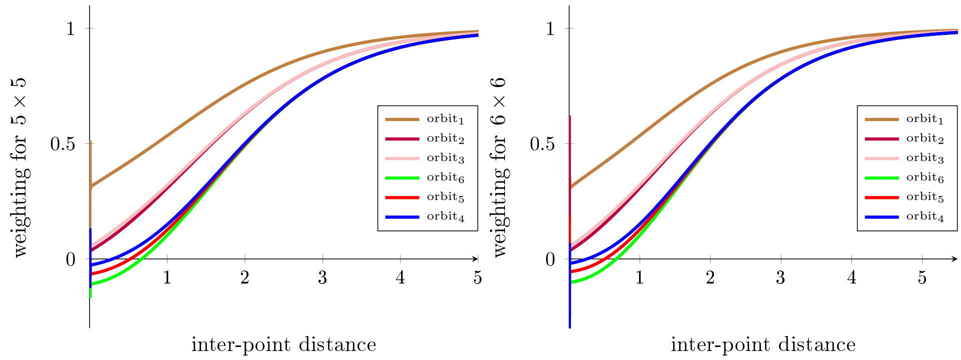


Figure 4.6: The weighting for 5×5 and 6×6 metric spaces at different scales.

We can see from the Figure 4.6, when the inter-points of 5×5 and 6×6 are bigger than 1, all values of weighting are positive, so the maximum diversity is the magnitude of these square grids. Moreover, for some smaller values of inter-points, there are negative weights. We determine the subsets that contains the orbits and the union of orbits of the 5×5 and 6×6 metric spaces that have a maximum magnitude with non-negative weights, and to simplify these subsets we used software such as Maple look at (Appendix B.2).

- The first subset is the orbit_1

- The second subset is the union of orbit_1 and orbit_2

- The third subset is the union of orbit_1, orbit_2 and orbit_3.

- The fourth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_4$.

- The fifth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_5$.

- The last subset is the 5×5 and 6×6 metric spaces.

We have computed the magnitude of the those subsets of 5×5 and 6×6, then plotting them together as shown in the Figure 4.7 and from the figure, we see that the magnitude of the six subsets of 5×5 and 6×6 grid squares are very similar for small values of t. But there is a small difference, we check it for the value $t = 0.1$ as can be seen in the following statements

The magniyude of subsets of 5×5 and 6×6 grid squares at $t = 0.1$ are

- the magnitude of first subset is 1.375226962,
- the magnitude of second subset is 1.375341110,
- the magnitude of third subset is 1.375353511,
- the magnitude of fourth subset is 1.382828470,
- the magnitude of fifth subset is 1.391389478,

- the magnitude of sixth subset is 1.391389477,

and

- the magnitude of first subset is 1.478125582,
- the magnitude of second subset is 1.478169922,
- the magnitude of third subset is 1.478178143,
- the magnitude of fourth subset is 1.490971596,
- the magnitude of fifth subset is 1.496744198,
- the magnitude of sixth subset is 1.499663457,

respectively.

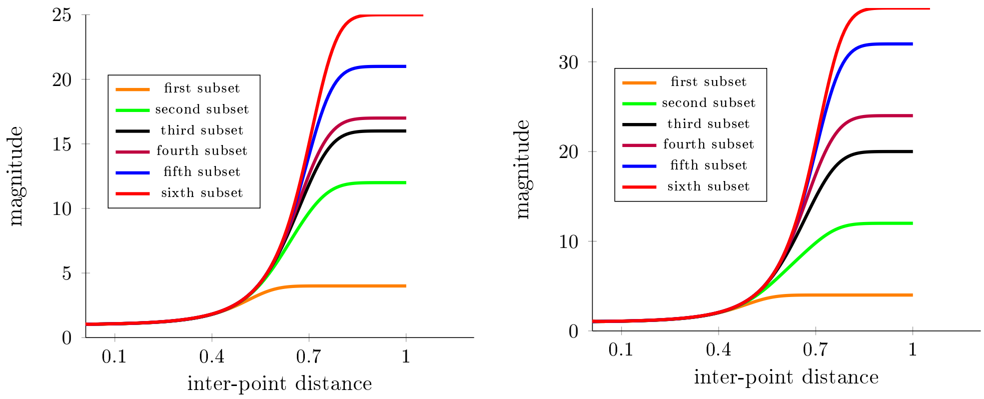


Figure 4.7: The magnitude for the six subsets of 5×5 and 6×6 grid squares at various scales.

We've seen that there are places where the curves intersect and we find the points of the intersection curves in the same way that we found the critical points of the 3×3 and the 4×4 square grids to obtain the critical values of the 5×5 to be

$$\begin{aligned} t_0 &= 0.1159, \\ t_1 &= 0.1167, \\ t_3 &= 0.5195, \\ t_4 &= 0.5757, \\ t_5 &= 0.757, \end{aligned}$$

and the critical values of the 6×6 are

$$\begin{aligned} t_0 &= 0.0927, \\ t_1 &= 0.0933, \\ t_3 &= 0.433, \\ t_4 &= 0.5424, \\ t_5 &= 0.612. \end{aligned}$$

It is clear from the Graph 4.7, for the subsets of each of the square grids that when the scale factor is between 0 and t_0, the maximum diversity is equal to the magnitude of the four corner points. However, as the scale factor is between t_0 and t_1, the maximum diversity is the magnitude of the four corner points with the eight-boundary points that represent the neighboring corners, while in scaling from t_1 to t_2 the maximum diversity is the magnitude of the boundary grid points. For the square grids scaled by factor between t_2 and t_3, the maximum diversity is the magnitude of the boundary grid points with midpoints of the initial square grid. For scale square grids from t_3 to t_4, the maximum diversity is the magnitude of the boundary grid points and midpoints of the initial square grid with midpoints of the first rows of interior points. At a scale factor between t_4 and t_5 , the maximum diversity is the magnitude of the square grid points, though in the latter case with the exception of the four interior points neighboring the corners. As the scale factors greater than t_5, the maximum diversity is the magnitude of the square grids as shown in the Figures 4.8.

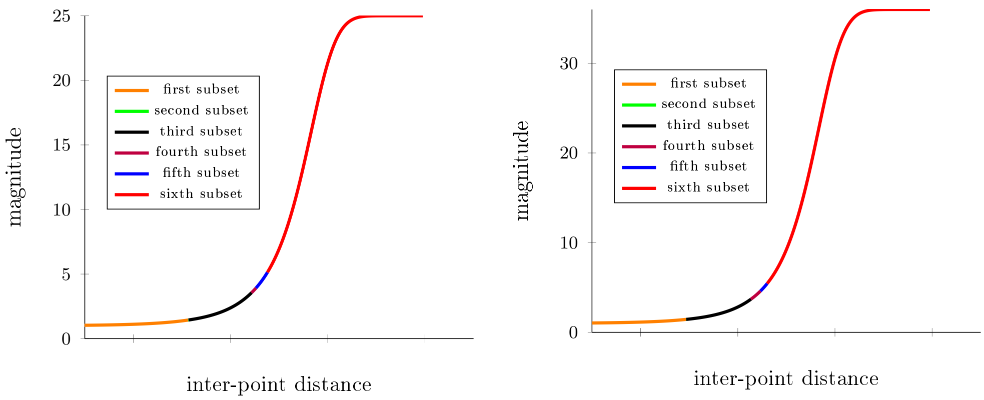
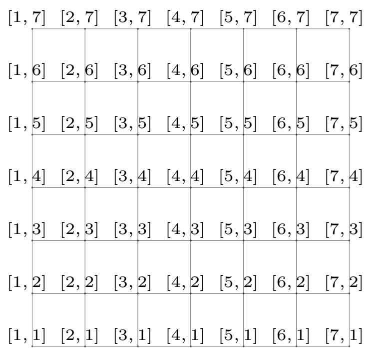


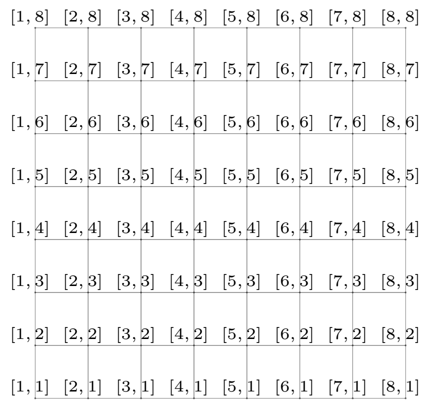
Figure 4.8: The maximum diversity of 5×5 and 6×6 grid squares at different scales.

4.2.3 The maximum diversity of 7×7 and 8×8 square grids

In this subsection, we compute (see Appendix B.2) the magnitude of orbits and union of orbits of 7×7 and 8×8 square grids metric spaces that have non-negative weighting at different scaling.

The points below on the squared grid can be partitioned into ten orbits which are invariant under the symmetries of square.





The ten orbits that partition the 7×7 metric space are

- $\text{orbit}_1 = \{[1,1],[7,1],[7,7],[1,7]\}$,
- $\text{orbit}_2 = \{[1,2],[6,1],[7,6],[2,7],[7,2],[1,6],[6,7],[2,1]\}$,
- $\text{orbit}_3 = \{[1,3],[5,1],[7,5],[3,7],[7,3],[1,5],[5,7],[3,1]\}$,
- $\text{orbit}_4 = \{[1,4],[4,1],[7,4],[4,7]\}$,
- $\text{orbit}_5 = \{[4,4]\}$,
- $\text{orbit}_6 = \{[3,4],[4,3],[5,4],[4,5]\}$,
- $\text{orbit}_7 = \{[3,3],[5,3],[5,5],[3,5]\}$,
- $\text{orbit}_8 = \{[2,4],[4,2],[6,4],[4,6]\}$,
- $\text{orbit}_9 = \{[2,3],[5,2],[6,5],[3,6],[6,3],[2,5],[5,6],[3,2]\}$,
- $\text{orbit}_{10} = \{[2,2],[6,2],[6,6],[2,6]\}$.

The orbits that partition the points of the 8×8 metric space are

- $\text{orbit}_1 = \{[1,1],[8,1],[8,8],[1,8]\}$,
- $\text{orbit}_2 = \{[1,2],[7,1],[8,7],[2,8],[8,2],[1,7],[7,8],[2,1]\}$,
- $\text{orbit}_3 = \{[1,3],[6,1],[8,6],[3,8],[8,3],[1,6],[6,8],[3,1]\}$,
- $\text{orbit}_4 = \{[1,4],[5,1],[8,5],[4,8],[8,4],[1,5],[5,8],[4,1]\}$,
- $\text{orbit}_5 = \{[4,4],[5,4],[5,5],[4,5]]\}$,

- $\text{orbit}_6 = \{[3,4],[5,3],[6,5],[4,6],[6,4],[3,5],[5,6],[4,3]\}$,
- $\text{orbit}_7 = \{[3,3],[6,3],[6,6],[3,6]]\}$,
- $\text{orbit}_8 = \{[2,4],[5,2],[7,5],[4,7],[7,4],[2,5],[5,7],[4,2]\}$,
- $\text{orbit}_9 = \{[2,3],[6,2],[7,6],[3,7],[7,3],[2,6],[6,7],[3,2]\}$,
- $\text{orbit}_{10} = \{[2,2],[7,2],[7,7],[2,7]\}$.

The fundamental domains of the 7×7 and 8×8 metric spaces are the points of the triangles on the square grids in the Figure 4.9.

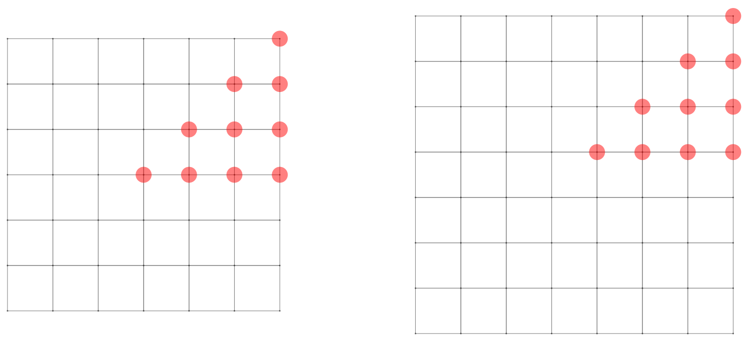


Figure 4.9: The points in the fundamental domains of the 7×7 and 8×8 square grids

We find the weighting for the points in the fundamental domains at various values of t. When we compute these weighting for $t = 0.01$, we obtain some negative weights. The invariant weighting for the points of the 7×7 grid square is

$$w = \begin{bmatrix} 0.3052337457 \\ 0.03734563589 \\ 0.05367790685 \\ 0.05291024745 \\ -0.09616225542 \\ -0.05044423720 \\ -0.04615687010 \\ -0.01591022453 \\ -0.01398006767 \\ -0.01221072246 \end{bmatrix}.$$

The invariant weighting for the points of the 8×8 grid square is

$$w = \begin{bmatrix} 0.3020945816 \\ 0.03753349442 \\ 0.05277179010 \\ 0.05103112775 \\ -0.09286364280 \\ -0.04746400140 \\ -0.04178668675 \\ -0.01408817302 \\ -0.01168125478 \\ -0.009493372626 \end{bmatrix}.$$

Therefore, to evaluate the maximum diversity we need to compute (see Appendix B.2) the subsets of square grids that have the maximum magnitude with non-negative weights at different scaling.

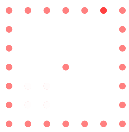
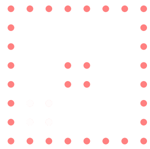
- The first subset is the orbit_1

- The second subset is the union of orbit_1 and orbit_2

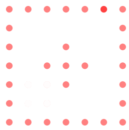
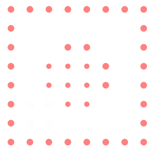
- The third subset is the union of orbit_1, orbit_2 and orbit_3

- The fourth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_4$

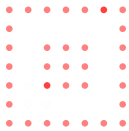
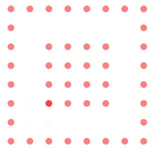
- The fifth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_5$

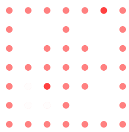
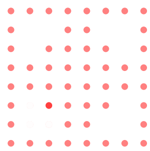
- The sixth subset is the union of $\mathrm{orbit}_1, \ldots, \mathrm{orbit}_6$

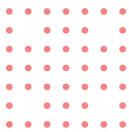
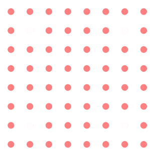
- The seventh subset is the union of $\mathrm{orbit}_1, \ldots, \mathrm{orbit}_7$

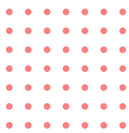
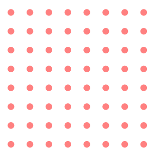
- The eighth subset is the union of $\mathrm{orbit}_1, \ldots, \mathrm{orbit}_8$

- The ninth subset is the union of $\mathrm{orbit}_1, \ldots, \mathrm{orbit}_9$

- The tenth subset is the grid square of points

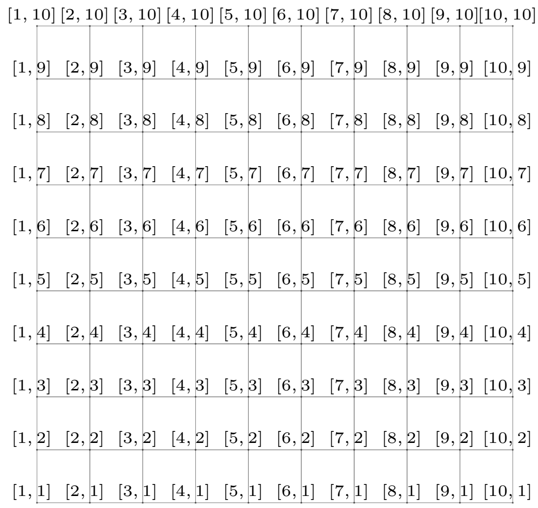
 

From computation evaluation, we see that the scaling factors that transition one subset which has maximum magnitude with non-negative weighting to another subset that has maximum magnitude with non-negative weighting are very close to each other, also the magnitude equations are very big, so it is very difficult to find the critical points for the grid squares greater than 6×6 especially for large subsets.

4.2.4 The maximum diversity of the square grids with 9×9 and 10×10 points

Here, we compute (see Appendix B.2) the magnitude of orbits and union of orbits of 9×9 and 10×10 square grids that have non-negative weighting at different scaling, then we determine the invariant weighting for the points in those orbits at very small scale factor t.

There are fifteen orbits that partition the points of the square grids A and B that have 9×9 and 10×10 points respectively.



The orbits that partition the A and B metric spaces are

- $\text{orbit}_1 = \{[1,1],[9,1],[9,9],[1,9]\}$,
- $\text{orbit}_2 = \{[2,1],[8,1],[9,8],[2,9],[9,2],[1,8],[8,9],[1,2]\}$,
- $\text{orbit}_3 = \{[3,1],[7,1],[9,7],[3,9],[9,3],[1,7],[7,9],[1,3]\}$,
- $\text{orbit}_4 = \{[4,1],[6,1],[9,6],[4,9],[9,4],[1,6],[6,9],[1,4]\}$,
- $\text{orbit}_5 = \{[5,1],[1,5],[9,5],[5,9]\}$,
- $\text{orbit}_6 = \{[5,5]\}$,
- $\text{orbit}_7 = \{[5,4],[4,5],[6,5],[5,6]\}$,
- $\text{orbit}_8 = \{[4,4],[6,4],[6,6],[4,6]\}$,
- $\text{orbit}_9 = \{[5,3],[3,5],[7,5],[5,7]\}$,
- $\text{orbit}_{10} = \{[4,3],[6,3],[7,6],[4,7],[7,4],[3,6],[6,7],[3,4]\}$,
- $\text{orbit}_{11} = \{[3,3],[7,3],[7,7],[3,7]\}$,
- $\text{orbit}_{12} = \{[5,2],[2,5],[8,5],[5,8]\}$,
- $\text{orbit}_{13} = \{[4,2],[6,2],[8,6],[4,8],[8,4],[2,6],[6,8],[2,4]\}$,
- $\text{orbit}_{14} = \{[3,2],[7,2],[8,7],[3,8],[8,3],[2,7],[7,8],[2,3]\}$,

- $\text{orbit}_{15} = \{[2,2],[8,2],[8,8],[2,8]\}$.

and

- $\text{orbit}_{1} = \{[1,1],[10,1],[10,10],[1,10]\}$,
- $\text{orbit}_{2} = \{[1,2],[9,1],[10,9],[2,10],[10,2],[1,9],[9,10],[2,1]\}$,
- $\text{orbit}_{3} = \{[1,3],[8,1],[10,8],[3,10],[10,3],[1,8],[8,10],[3,1]\}$,
- $\text{orbit}_{4} = \{[1,4],[7,1],[10,7],[4,10],[10,4],[1,7],[7,10],[4,1]\}$,
- $\text{orbit}_{5} = \{[1,5],[6,1],[10,6],[5,10],[10,5],[1,6],[6,10],[5,1]\}$,
- $\text{orbit}_{6} = \{[5,5],[6,5],[6,6],[5,6]\}$,
- $\text{orbit}_{7} = \{[4,5],[6,4],[7,6],[5,7],[7,5],[4,6],[6,7],[5,4]\}$,
- $\text{orbit}_{8} = \{[4,4],[7,4],[7,7],[4,7]\}$,
- $\text{orbit}_{9} = \{[3,5],[6,3],[8,6],[5,8],[8,5],[3,6],[6,8],[5,3]\}$,
- $\text{orbit}_{10} = \{[3,4],[7,3],[8,7],[4,8],[8,4],[3,7],[7,8],[4,3]\}$,
- $\text{orbit}_{11} = \{[3,3],[8,3],[8,8],[3,8]\}$,
- $\text{orbit}_{12} = \{[2,5],[6,2],[9,6],[5,9],[9,5],[2,6],[6,9],[5,2]\}$,
- $\text{orbit}_{13} = \{[2,4],[7,2],[9,7],[4,9],[9,4],[2,7],[7,9],[4,2]\}$,
- $\text{orbit}_{14} = \{[2,3],[8,2],[9,8],[3,9],[9,3],[2,8],[8,9],[3,2]\}$,
- $\text{orbit}_{15} = \{[2,2],[9,2],[9,9],[2,9]\}$.

respectively.

By Proposition 4.2.1, all points $[a, b]$ in the same orbit Orb have the invariant weights.

$$w = \frac{1}{\sum\limits_{[c,\,d]\in \text{Orb}} e^{-td([a,\,b],[c,\,d])}}. \tag{4.9}$$

When the scale factor $t > 0$ is very small, we can use a Taylor series approximation to approximate the value of $e^{-td([a,\,b],\,[c,\,d])}$, so

$$\sum_{[c,d]\in\text{Orb}} e^{-td([a,b],[c,d])} = \#\text{Orb} - t \sum_{[c,d]\in\text{Orb}} d([a,b],[c,d]) + O(t^2), \tag{4.10}$$

Consider the points in the fundamental domains of these square grids are

$$\{[9,\,9],\,[9,\,8],\,[9,\,7],\,[9,\,6],\,[9,\,5],\,[8,\,5],\,[7,\,5],\,[6,\,5],\,[5,\,5],\,[6,\,6],\,[7,\,7],\\ [8,\,8],\,[7,\,6],\,[8,\,6],\,[8,\,7]\}$$

and

$$\{[10, 10], [10, 9], [10, 8], [10, 7], [10, 6], [9, 6], [8, 6], [7, 6], [6, 6], [7, 7], [8, 8], [9, 9], [8, 7], [9, 7], [9, 8]\}$$

respectively, which are the points of the triangles on the square grids.

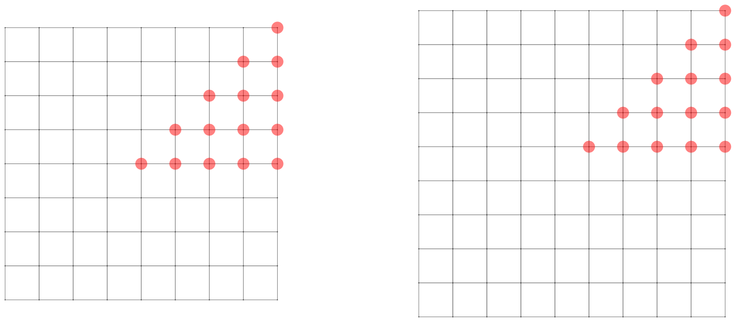
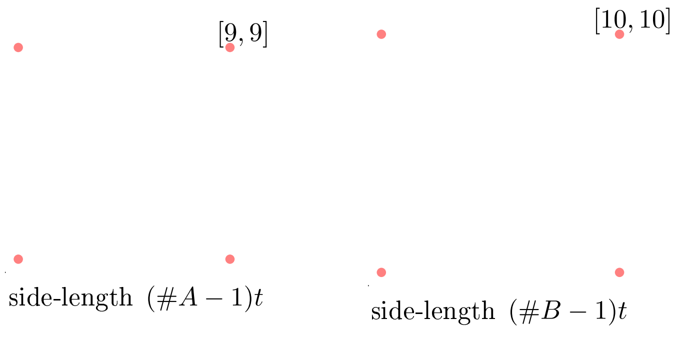


Figure 4.10: The fundamental domains of 9×9 and 10×10 square grids.

We can determine the general formula of the invariant weight of the points in the fundamental domains of 9×9 and 10×10 grid squares (the pattern for order the points of the fundamental domain is the points that complete the biggest square to the points that complete the smallest square in the grid squares) which can be used in the Theorem 4.3.3.

1. The invariant weightings of the first point of these fundamental domains are given by

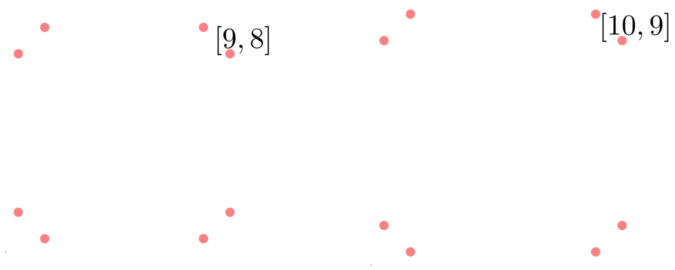


$$\begin{aligned}\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_1} e^{-td([9,9],[c,d])}} &= \frac{1}{1+2e^{-8t}+e^{-\sqrt{2}*8t}} \\ &= \frac{1}{4-(2+\sqrt{2})*8t+O(t^2)},\end{aligned} \tag{4.11}$$

and

$$\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_1} e^{-td([10,10],[c,d])}} = \frac{1}{1+2e^{-9t}+e^{-\sqrt{2}*9t}}$$
$$= \frac{1}{4-(2+\sqrt{2})*9t+O(t^2)}. \tag{4.12}$$

2. The invariant weightings of the second point of these fundamental domains are

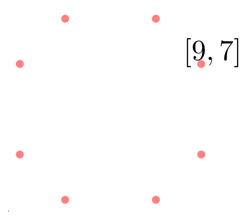


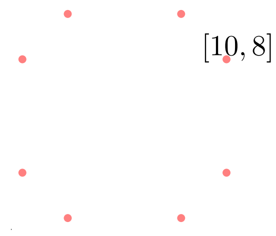
$$\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_2} e^{-td([9,8],[c,d])}}$$
$$= 1/\left(1+e^{-6t}+2e^{-\sqrt{7^2+1^2}t}+e^{-7\sqrt{2}t}+e^{-\sqrt{6^2+8^2}t}+e^{-8t}+e^{-\sqrt{2}t}\right)$$
$$= 1/\left(8-t\left[(2+\sqrt{2})*7+2\sqrt{7^2+1^2}+\sqrt{6^2+8^2}+\sqrt{2}\right]+O(t^2)\right), \tag{4.13}$$

and

$$\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_2} e^{-td([10,9],[c,d])}}$$
$$= 1/\left(1+e^{-7t}+2e^{-\sqrt{8^2+1^2}t}+e^{-8\sqrt{2}t}+e^{-\sqrt{7^2+9^2}t}+e^{-9t}+e^{-\sqrt{2}t}\right)$$
$$= 1/\left(8-t\left[(2+\sqrt{2})*8+2\sqrt{8^2+1^2}+\sqrt{7^2+9^2}+\sqrt{2}\right]+O(t^2)\right). \tag{4.14}$$

3. The invariant weightings of the third point in these fundamental domains of the square grids are



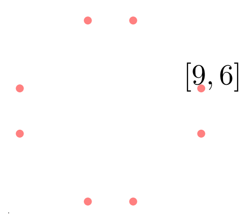


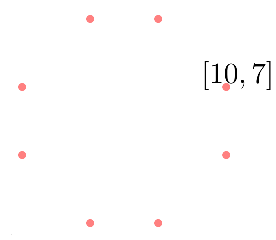
$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_3} e^{-td([9,7],[c,d])}}$$
$$= 1/\left(1 + e^{-4t} + 2e^{-\sqrt{6^2+2^2}t} + e^{-6\sqrt{2}t} + e^{-\sqrt{4^2+8^2}t} + e^{-8t} + e^{-2\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 6 + 2\sqrt{6^2+2^2} + \sqrt{4^2+8^2} + 2\sqrt{2}\right] + O(t^2)\right), \tag{4.15}$$

and

$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_3} e^{-td([10,8],[c,d])}}$$
$$= 1/\left(1 + e^{-5t} + 2e^{-\sqrt{7^2+2^2}t} + e^{-7\sqrt{2}t} + e^{-\sqrt{5^2+9^2}t} + e^{-9t} + e^{-2\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 7 + 2\sqrt{7^2+2^2} + \sqrt{5^2+9^2} + 2\sqrt{2}\right] + O(t^2)\right). \tag{4.16}$$

4. The invariant weightings of the fourth point of theses fundamental domains are given as



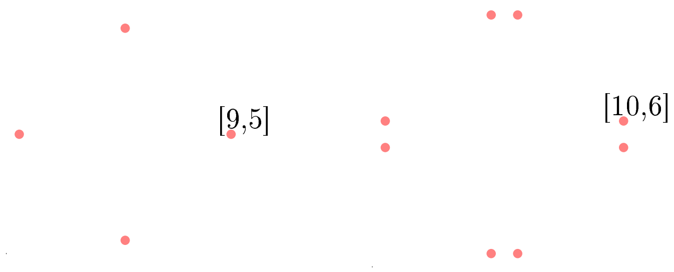


$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_4} e^{-td([9,6],[c,d])}}$$
$$= 1/\left(1 + e^{-2t} + 2e^{-\sqrt{5^2+3^2}t} + e^{-5\sqrt{2}t} + e^{-\sqrt{2^2+8^2}t} + e^{-8t} + e^{-3\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 5 + 2\sqrt{5^2+3^2} + \sqrt{2^2+8^2} + 3\sqrt{2}\right] + O(t^2)\right), \tag{4.17}$$

and

$$
\begin{aligned}
&\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_4} e^{-td([10,7],[c,d])}} \\
&= 1/\left(1+e^{-3t}+2e^{-\sqrt{6^2+3^2}t}+e^{-6\sqrt{2}t}+e^{-\sqrt{3^2+9^2}t}+e^{-9t}+e^{-3\sqrt{2}t}\right) \\
&= 1/\left(8-t\left[(2+\sqrt{2})*6+2\sqrt{6^2+3^2}+\sqrt{3^2+9^2}+3\sqrt{2}\right]+O(t^2)\right).
\end{aligned} \tag{4.18}
$$

5. The invariant weightings of the fifth point of these fundamental domains are

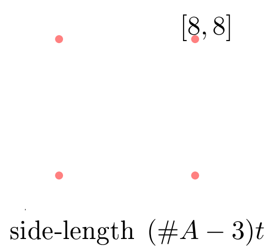


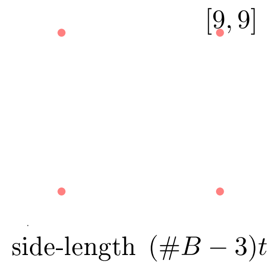
$$
\begin{aligned}
\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_5} e^{-td([9,5],[c,d])}} &= \frac{1}{1+2e^{-4\sqrt{2}}+e^{-8t}} \\
&= \frac{1}{4-(1+\sqrt{2})*8t+O(t^2)},
\end{aligned} \tag{4.19}
$$

and

$$
\begin{aligned}
&1/\sum_{[c,d]\in \text{orbit}_5} e^{-td([10,6],[c,d])} \\
&= 1/\left(1+e^{-t}+2e^{-\sqrt{5^2+4^2}t}+e^{-5\sqrt{2}t}+e^{-\sqrt{1^2+9^2}t}+e^{-9t}+e^{-4\sqrt{2}t}\right) \\
&= 1/\left(8-t\left[(2+\sqrt{2})*5+2\sqrt{5^2+4^2}+\sqrt{1^2+9^2}+4\sqrt{2}\right]+O(t^2)\right).
\end{aligned} \tag{4.20}
$$

6. The invariant weightings of the points $[8,8]$ and $[9,9]$ in the fundamental domains are





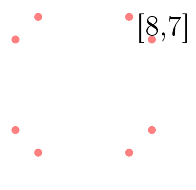
$$\begin{aligned}\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{15}} e^{-td([8,8],[c,d])}} &= \frac{1}{1+2e^{-6t}+e^{-6\sqrt{2}t}} \\ &= \frac{1}{4-(2+\sqrt{2})*6t+O(t^2)},\end{aligned} \tag{4.21}$$

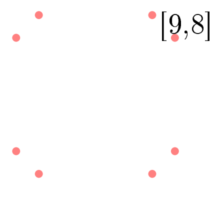
and

$$\begin{aligned}\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{15}} e^{-td([9,9],[c,d])}} &= \frac{1}{1+2e^{-7t}+e^{-7\sqrt{2}t}} \\ &= \frac{1}{4-(2+\sqrt{2})*7t+O(t^2)},\end{aligned} \tag{4.22}$$

respectively.

7. The invariant weightings of $[8,7]$ and $[9,8]$ in the fundamental domains are given by





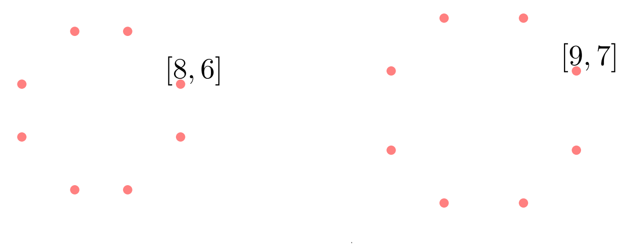
$$\begin{aligned}&\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{14}} e^{-td([9,8],[c,d])}} \\ &= 1/\left(1+e^{-4t}+2e^{-\sqrt{5^2+1^2}t}+e^{-5\sqrt{2}t}+e^{-\sqrt{4^2+6^2}t}+e^{-6t}+e^{-\sqrt{2}t}\right) \\ &= 1/\left(8-t\left[(2+\sqrt{2})*5+2\sqrt{5^2+1^2}+\sqrt{4^2+6^2}+\sqrt{2}\right]+O(t^2)\right),\end{aligned} \tag{4.23}$$

and

$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{14}} e^{-td([9,8],[c,d])}}$$
$$= 1/\left(1 + e^{-5t} + 2e^{-\sqrt{6^2+1^2}t} + e^{-6\sqrt{2}t} + e^{-\sqrt{5^2+7^2}t} + e^{-7t} + e^{-\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 6 + 2\sqrt{6^2+1^2} + \sqrt{5^2+7^2} + \sqrt{2}\right] + O(t^2)\right), \tag{4.24}$$

respectively.

8. The invariant weightings of the $[8,6]$ and $[9,7]$ points in the fundamental domains of the square grids are



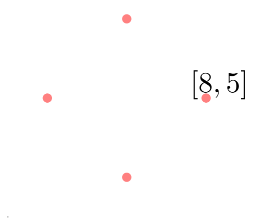
$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{13}} e^{-td([8,6],[c,d])}}$$
$$= 1/\left(1 + e^{-2t} + 2e^{-\sqrt{4^2+2^2}t} + e^{-4\sqrt{2}t} + e^{-\sqrt{2^2+6^2}t} + e^{-6t} + e^{-2\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 4 + 2\sqrt{4^2+2^2} + \sqrt{2^2+6^2} + 2\sqrt{2}\right] + O(t^2)\right), \tag{4.25}$$

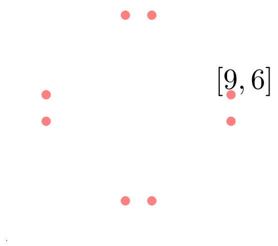
and

$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{13}} e^{-td([9,7],[c,d])}}$$
$$= 1/\left(1 + e^{-3t} + 2e^{-\sqrt{5^2+2^2}t} + e^{-5\sqrt{2}t} + e^{-\sqrt{3^2+7^2}t} + e^{-7t} + e^{-2\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 5 + 2\sqrt{5^2+2^2} + \sqrt{3^2+7^2} + 2\sqrt{2}\right] + O(t^2)\right), \tag{4.26}$$

respectively.

9. The invariant weightings of $[8,5]$ and $[9,6]$ are



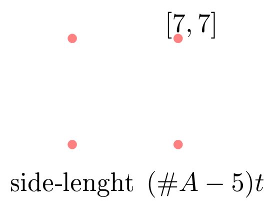


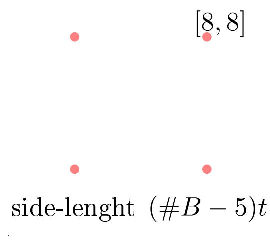
$$\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_{12}} e^{-td([8,5],[c,d])}} = \frac{1}{1+2e^{-t\sqrt{2}*3}+6} = \frac{1}{4-(1+\sqrt{2})*6t+O(t^2)}, \tag{4.27}$$

and

$$\begin{aligned} &\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_{12}} e^{-td([9,6],[c,d])}} \\ &= 1/\left(1+e^{-t}+2e^{-\sqrt{4^2+3^2}t}+e^{-4\sqrt{2}t}+e^{-\sqrt{1^2+7^2}t}+e^{-7t}+e^{-3\sqrt{2}t}\right) \\ &= 1/\left(8-t\left[(2+\sqrt{2})*4+2\sqrt{4^2+3^2}+\sqrt{1^2+7^2}+3\sqrt{2}\right]+O(t^2)\right) \end{aligned} \tag{4.28}$$

10. The invariant weightings of the points [7, 7] and [8, 8] are





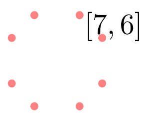
$$\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_{11}} e^{-td([7,7],[c,d])}} = \frac{1}{1+2e^{-4t}+e^{-4\sqrt{2}t}} = \frac{1}{4-(2+\sqrt{2})*4t+O(t^2)}, \tag{4.29}$$

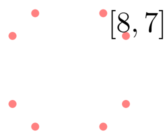
and

$$\frac{1}{\sum\limits_{[c,d]\in \text{orbit}_{11}} e^{-td([8,8],[c,d])}} = \frac{1}{1+2e^{-5t}+e^{-5\sqrt{2}t}} = \frac{1}{4-(2+\sqrt{2})*5t+O(t^2)}, \tag{4.30}$$

respectively.

11. The invariant weightings of $[7,6]$ and $[8,7]$ in the fundamental domains are





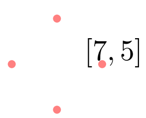
$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{10}} e^{-td([7,6],[c,d])}}$$
$$= 1/\left(1 + e^{-2t} + 2e^{-\sqrt{3^2+1^2}t} + e^{-3\sqrt{2}t} + e^{-\sqrt{2^2+4^2}t} + e^{-4t} + e^{-\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 3 + 2\sqrt{3^2+1^2} + \sqrt{2^2+4^2} + \sqrt{2}\right] + O(t^2)\right), \tag{4.31}$$

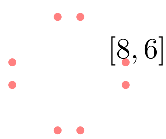
and

$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{10}} e^{-td([8,7],[c,d])}}$$
$$= 1/\left(1 + e^{-3t} + 2e^{-\sqrt{4^2+1^2}t} + e^{-4\sqrt{2}t} + e^{-\sqrt{5^2+3^2}t} + e^{-5t} + e^{-\sqrt{2}t}\right)$$
$$= 1/\left(8 - t\left[(2+\sqrt{2}) * 4 + 2\sqrt{4^2+1^2} + \sqrt{5^2+3^2} + \sqrt{2}\right] + O(t^2)\right), \tag{4.32}$$

respectively.

12. The invariant weightings of $[7, 5]$ and $[8, 6]$ in the fundamental domains are



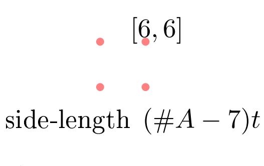


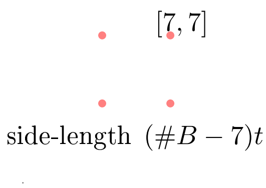
$$\begin{aligned}\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_{9}} e^{-td([7,5],[c,d])}} &= \frac{1}{1 + 2e^{-t\sqrt{2}*2} + 4} \\ &= \frac{1}{4 - (1+\sqrt{2}) * 4t + O(t^2)},\end{aligned} \tag{4.33}$$

and

$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_9} e^{-td([7,6],[c,d])}} = 1/\left(1+e^{-t}+2e^{-\sqrt{3^2+2^2}t}+e^{-3\sqrt{2}t}+e^{-\sqrt{1^2+5^2}t}+e^{-5t}+e^{-2\sqrt{2}t}\right)$$
$$= 1/\left(8-t\left[(2+\sqrt{2})*3+2\sqrt{3^2+2^2}+\sqrt{1^2+5^2}+2\sqrt{2}\right]+O(t^2)\right) \tag{4.34}$$

13. The invariant weightings of [6, 6] and [7, 7] points are



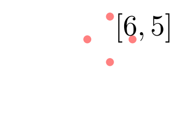


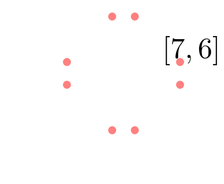
$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_8} e^{-td([6,6],[c,d])}} = \frac{1}{1+2e^{-t\sqrt{2}*2}+e^{-2t}} = \frac{1}{4-(2+\sqrt{2})*2t+O(t^2)}, \tag{4.35}$$

and

$$\frac{1}{\sum\limits_{[c,d]\in \mathrm{orbit}_8} e^{-td([7,7],[c,d])}} = \frac{1}{1+2e^{-t\sqrt{2}*3}+e^{-3t}} = \frac{1}{4-(2+\sqrt{2})*3t+O(t^2)}, \tag{4.36}$$

14. The invariant weightings of [6, 5] and [7, 6] in the fundamental domains are given as





$$\frac{1}{\sum_{[c,d]\in \text{orbit}_7} e^{-td([6,5],[c,d])}} = \frac{1}{1+2e^{-t\sqrt{2}*1}+e^{-2t}} = \frac{1}{4-(1+\sqrt{2})*2t+O(t^2)}, \tag{4.37}$$

and

$$\begin{aligned} &\frac{1}{\sum_{[c,d]\in \text{orbit}_7} e^{-td([7,6],[c,d])}} \\ &= 1/\left(1+e^{-t}+2e^{-\sqrt{2^2+1^2}t}+e^{-2\sqrt{2}t}+e^{-\sqrt{1^2+3^2}t}+e^{-3t}+e^{-\sqrt{2}t}\right) \\ &= 1/\left(8-t\left[(2+\sqrt{2})*2+2\sqrt{2^2+1^2}+\sqrt{1^2+3^2}+\sqrt{2}\right]+O(t^2)\right) \end{aligned} \tag{4.38}$$

15. The invariant weightings of the [5, 5] and [6, 6] are

$$\frac{1}{e^{-td([6,6],[6,6])}} = 1 \tag{4.39}$$

and

$$\frac{1}{\sum_{[c,d]\in \text{orbit}_6} e^{-td([6,6],[c,d])}} = \frac{1}{1+2e^{-t\sqrt{2}*1}+e^{-1t}} = \frac{1}{4-(2+\sqrt{2})*t+O(t^2)}, \tag{4.40}$$

Now the invariant weighting on the grid square A of an 9×9 points can be easily calculated by selecting an arbitrary point $[a,b]$ of the square grid such that $b\le a$ and $1\le a,b\le 5$

1. For $1\le b\le 4$, the invariant weights of the orbits that contain the four points with sides length $(\#A-(2b-1))t$ are equal to

$$\frac{1}{4-(2+\sqrt{2})(\#A-(2b-1))t+O(t^2)}, \tag{4.41}$$

as can be seen from Expressions (4.11), (4.21), (4.29) and (4.35),

2. The invariant weights of the points in the orbit of $[a, b]$, where $b < a$ and $1 < a, b \leq 4$, are equal to

$$1/\big(8 - t\big[(2+\sqrt{2})(\#A - (a+b-1)) + 2\sqrt{(\#A - (a+b-1))^2 + (a-b)^2 +} \\ \sqrt{(\#A - (2a-1))^2 + (\#A - (2b-1))^2} + (a-b)\sqrt{2}\big] + O(t^2)\big), \tag{4.42}$$

as can be observed in Equations (4.13), (4.15), (4.17), (4.23), (4.25) and (4.31),

3. The weighting of each points of the orbits $[a, b]$, where $a = 5$ and $1 \leq b \leq 4$, are equal to

$$\frac{1}{4 - (1+\sqrt{2})(\#A - (2b-1))t + O(t^2)}, \tag{4.43}$$

as can be seen from Equations (4.19), (4.27), (4.33) and (4.37).

Also, the invariant weighting for the grid square B of a 10×10 can be determined by choosing an arbitrary point $[a, b]$ in the square grid such that $b \leq a$ and $1 \leq a, b \leq 5$

1. For $1 \leq b \leq 5$, the invariant weighting of the orbits with sides-length $(\#B - (2b-1))t$ are equal to

$$\frac{1}{4 - (2+\sqrt{2})(\#B - (2b-1))t + O(t^2)}, \tag{4.44}$$

that can be seen from Expressions (4.12), (4.22), (4.30), (4.36) and (4.40),

2. The invariant weighting of the orbits of $[a, b]$, where $b < a$ and $1 \leq a, b \leq 5$, are equal to

$$1/\big(8 - t\big[(2+\sqrt{2})(\#B - (a+b-1)) + 2\sqrt{(\#B - (a+b-1))^2 + (a-b)^2 +} \\ \sqrt{(\#B - (2a-1))^2 + (\#B - (2b-1))^2} + (a-b)\sqrt{2}\big] + O(t^2)\big), \tag{4.45}$$

as seen in the Expressions (4.14), (4.16), (4.18), (4.20), (4.24), (4.26), (4.28), (4.32), (4.34) and (4.38).

We use Maple code (see Appendix B.2), to determine the invariant weighting equations of points in the= fundamental domains of the 9×9 and 10×10

grid squares at $t = 0.01$. The invariant weighting of points for 9×9 square grid is

$$\begin{aligned} w = [&0.2993352826, 0.03759810521, 0.05204502052, 0.04968219598,\\ &0.04873154586, -0.09046078997, -0.04546380615, -0.03907528662,\\ &-0.03761929683, -0.01296539496, -0.01033596374, -0.009799619799,\\ &-0.007988725876, -0.007495290624, -0.007011024439].\end{aligned}$$

The invariant weighting of points for 10×10 square grid is

$$\begin{aligned} w = [&0.2968893377, 0.03759690549, 0.05144925402, 0.04865744587,\\ &0.04710294444, -0.08861467667, -0.04401992904, -0.03724800080,\\ &-0.03501383443, -0.01220637112, -0.009485727106, -0.008669390846,\\ &-0.007094337741, -0.006363739331, -0.005664141309].\end{aligned}$$

From above we can see that there are some negative weights. So, we consider the subsets of the metric spaces which have maximum magnitudes with non-negative weights to represent the maximum diversities at various scaling.

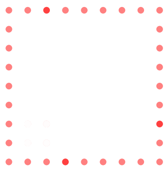
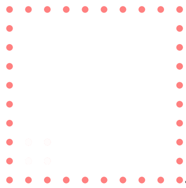
- The first subset is the orbit_1

- the second subset is the union of orbit_1 and orbit_2

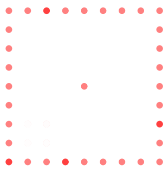
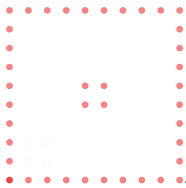
- the third subset is the union of orbit_1, orbit_2 and orbit_3

- the fourth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_4$

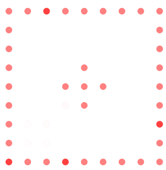
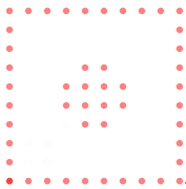
- the fifth subset five is the union of $\text{orbit}_1, \ldots, \text{orbit}_5$

 ,

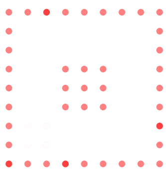
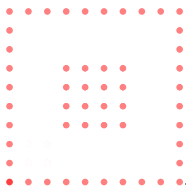
- the sixth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_6$

 ,

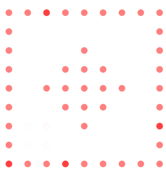
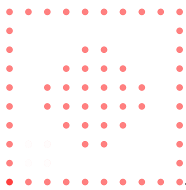
- the seventh subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_7$

 ,

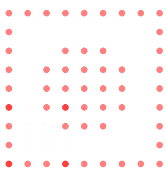
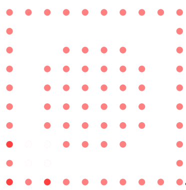
- the eighth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_8$

 ,

- the ninth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_9$

 ,

- the tenth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_{10}$

 ,

- the eleventh subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_{11}$

- the twelfth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_{12}$

- the thirteenth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_{13}$

- the fourteenth subset is the union of $\text{orbit}_1, \ldots, \text{orbit}_{14}$

- the last subset is the 9×9 and 10×10 metric spaces

As can be seen above, if the group of symmetries for the square act by isometries on $n-1 \times n-1$ and $n \times n$ square grids of points, for $n = 4, 6, 8, 10$. This gives some equivalent fundamental domains which partition the metric space into a union of disjointed orbits. When we scale those grid squares by a scale factor t, we can see that as the scale factor increases, the order in which you take the union of orbits, in terms of representative points in a triangular fundamental domain as illustrated (See Figures 4.1, 4.5, 4.9, and 4.10), is as follows. You start in the top right corner. Then you proceed down the right-hand edge until you reach the right angle. Then you jump to the lower-left vertex (at or near the center of the square, according to as n is odd or even, respectively). After that, you move rights through the remaining columns of dots in the triangle, traversing each one from bottom to top.

Also, we calculate the weights of the points on the 9×9 and 10×10 grid squares by finding the invariant weights of the points on these orbits. Furthermore, we observe that when the grid square is scaled by a factor $t > 0$, the invariant weights are not necessarily positive. Therefore, at each scale, there is a subset (as their order described above) of the metric space that has a maximum magnitude with non-negative weighting which is the maximum diversity.

Now, in all cases, when the scale factor is very small, the four corner points have maximum magnitude with non-negative weighting. We shall prove this in the next section.

§ 4.3 The magnitude of the four corner points of an $n \times n$ grid square

In this section, we will find the general formula for the invariant weights of points of the $n \times n$ square grid metric space and we will show that the four corner points of the square grid have a larger magnitude derived from the magnitude of all other orbits for very small scaling factor t. Also, if we consider the set that contains the orbit of four corner points and any other orbit, then that set have negative weights.

The symmetry group of the square acts on the $n \times n$ square grid of points by isometries which partitions the metric space into a union of disjointed orbits.

When n is an odd number and $n > 3$, there are four types of orbit, which are used in the Theorem 4.3.3.

In the first type, the orbit has four points in a square with sides length $\ell = (n - (2b - 1))$, as $1 \leq b \leq \frac{n-1}{2}$. The weighting of this orbit is

$$\frac{1}{1 + 2e^{-\ell t} + e^{-\sqrt{2}\ell t}},$$

as $t \ll 1$, we have

$$\frac{1}{4 - (2 + \sqrt{2})\ell t + O(t^2)}, \tag{4.46}$$

this can be seen from Equation (4.41).

In the second type, the orbit has eight points. The invariant weighting of this orbit is

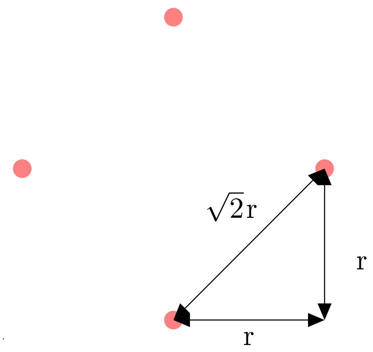
$$1/\big(1 + e^{-(n-(2a-1))t} + 2e^{-\sqrt{(n-(a+b-1))^2+(a-b)^2}t} + e^{-(n-(a+b-1))\sqrt{2}t} + e^{-\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}t} + e^{-(n-(2b-1))t} + e^{-(a-b)\sqrt{2}t}\big)$$

as $t \ll 1$, we get

$$1/\big(8 - t\big[(2+\sqrt{2})(n-(a+b-1)) + 2\sqrt{(n-(a+b-1))^2+(a-b)^2}+ \\ \sqrt{(n-(2a-1))^2+(n-(2b-1))^2} + (a-b)\sqrt{2}\big] + O(t^2)\big), \tag{4.47}$$

where, $1 \leq b < a \leq \frac{n-1}{2}$, as can be viewed from Expression (4.42).

In the third type, the orbit has four points in a diamond shape.



The weighting of this orbit is

$$\frac{1}{1 + 2e^{-\sqrt{2}rt} + e^{-2rt}},$$

when $t \ll 1$, we obtain

$$\frac{1}{4 - (2\sqrt{2}+2)rt + O(t^2)}, \tag{4.48}$$

as can be observed of Equation (4.43).

In the fourth type, we have the single point $\left[\frac{n+1}{2}, \frac{n+1}{2}\right]$. The weighting of this orbit is 1.

Let us begin with the preparatory results, which are important to demonstrate Theorem 4.3.3.

Lemma 4.3.1. *For positive integer numbers n, a, b such that $n > 3$ is an odd number, and $1 \leq b < a \leq \frac{n-1}{2}$ then the following inequality is true*

$$2((n-(2b-1)) + (a-b)) > 2\sqrt{(n-(a+b-1))^2 + (a-b)^2}.$$

Proof. We have $b < a$ and $b \geq 1$, so

$$\begin{gathered} b + b - 1 < a + b - 1 \\ n - (2b-1) > n - (a+b-1). \end{gathered}$$

If we square both sides of the previous inequality, then adding $(a-b)^2$ to both sides gives

$$(n-(2b-1))^2+(a-b)^2 > (n-(a+b-1))^2+(a-b)^2.$$

Taking the square root of both sides of the above expression and multiplying by 2 gives

$$2\sqrt{(n-(2b-1))^2+(a-b)^2} > 2\sqrt{(n-(a+b-1))^2+(a-b)^2}. \quad (4.49)$$

Since $(n-(a+b-1))^2$ and $(a-b)^2$ are positive, we have

$$2\sqrt{(n-(2b-1))^2+2\sqrt{(n-(2b-1))^2(a-b)^2}+(a-b)^2} > \sqrt{(n-(2b-1))^2+(a-b)^2},$$

which implies that

$$\begin{aligned}\sqrt{\left(\sqrt{(n-(2b-1))^2}+\sqrt{(a-b)^2}\right)^2} &> 2\sqrt{(n-(2b-1))^2+(a-b)^2}\\ 2\sqrt{(n-(2b-1))^2}+2\sqrt{(a-b)^2} &> 2\sqrt{(n-(2b-1))^2+(a-b)^2}.\end{aligned}$$

Then the following holds

$$2((n-(2b-1))+(a-b)) > 2\sqrt{(n-(2b-1))^2+(a-b)^2}. \quad (4.50)$$

Therefore, from Inequalities (4.49) and (4.50), the proof is completed. □

Lemma 4.3.2. *Given integer numbers n, a, b. Where n is an odd number, $n>3$ and $1 \leq b < a \leq \frac{n-1}{2}$. Then*

$$(2+\sqrt{2})(n-1) > (2+\sqrt{2})\big[(n-(2b-1))+(a-b)\big]. \quad (4.51)$$

Proof. As $1<b$ and $1<a$, we have

$$\begin{aligned} 3 &< 3b\\ 1 &< 3b-2\\ 1 &< 2b-1-1+b\\ 1 &< 2b-1-a+b\\ n-1 &> n-(2b-1)+(a-b) \end{aligned}.$$

Multiplying each side of the above inequality by $2+\sqrt{2}$, we get Formula (4.51). □

The next theorem shows that, if an $n \times n$ square grid is scaled very small, then the magnitude of the orbit that contains the four corner points is larger than the magnitude of all other orbits of the square grid.

Theorem 4.3.3. *If we consider the orbits under the action of the isometry group of a square $n \times n$ grid tA with $n > 3$, then when $t \ll 1$, the largest magnitude is on the orbit consisting of the four corner points.*

Proof. Suppose we have the square grid A scaled by a factor $t > 0$ and an action of the symmetry group of the square on A, so that the square grid is partitioned by the orbits.

Since from Formula (4.46) when $b = 1$, the magnitude of the four corner points A_0 of a square grid scaled by factor t is equal to

$$\frac{4}{1 + 2e^{-(n-1)t} + e^{-\sqrt{2}(n-1)t}}, \tag{4.52}$$

as $t \ll 1$, the Taylor series approximations gives

$$\begin{aligned} \frac{4}{4 - (2+\sqrt{2})(n-1)t + O(t^2)} &= \frac{1}{1 - \frac{2+\sqrt{2}}{4}(n-1)t + O(t^2)} \\ &= 1 + \frac{2+\sqrt{2}}{4}(n-1)t + O(t^2). \end{aligned} \tag{4.53}$$

We divide the rest of the proof into four parts.

i Let A_1 be any orbit that contain the corners of the square with sides $\ell = (n - (2b - 1))$, such as $1 \leq b \leq \frac{n-1}{2}$. We need to show that $|tA_0| > |tA_1|$,

ii Consider A_2 is any orbit which contains eight points, We shall prove that $|tA_0| > |tA_2|$,

iii Suppose that A_3 is any orbit which consist of points of the square diamond-shape, we will show that $|tA_0| > |tA_3|$,

iv Let A_4 be the orbit $\{[\frac{n+1}{2}, \frac{n+1}{2}]\}$; we want to prove $|tA_0| > |tA_4|$.

Part (i). When $t \ll 1$, the magnitude of the corners of the square with side length $\ell = (n - (2b - 1))$ from Formula (4.46) is equal to

$$\begin{aligned} \frac{4}{4 - (2+\sqrt{2})\ell t + O(t^2)} &= \frac{1}{1 - \frac{2+\sqrt{2}}{4}\ell t + O(t^2)} \\ &= 1 + \frac{2+\sqrt{2}}{4}\ell t + O(t^2), \end{aligned}$$

where $1 \leq b \leq \frac{n-1}{2}$. The last formula is an increasing function of ℓ, so larger squares have bigger magnitudes.

Part (ii). As $t \ll 1$, the magnitude of tA_2 from Formula (4.47) is

$$
\begin{aligned}
&8/\big(8-t\big[(2+\sqrt{2})(n-(a+b-1))+2\sqrt{(n-(a+b-1))^2+(a-b)^2}\\
&\quad+\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}+(a-b)\sqrt{2}\big]+O(t^2)\big)\\
&=1/\big(1-t/8\big[(2+\sqrt{2})(n-(a+b-1))+2\sqrt{(n-(a+b-1))^2+(a-b)^2}\\
&\quad+\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}+(a-b)\sqrt{2}\big]+O(t^2)\big)\\
&=1+t/8\big[(2+\sqrt{2})(n-(a+b-1))+2\sqrt{(n-(a+b-1))^2+(a-b)^2}\\
&\quad+\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}+(a-b)\sqrt{2}\big]+O(t^2),
\end{aligned}
$$

where $1 \leq b < a \leq \frac{n-1}{2}$ and $n > 3$. To show $|tA_0| > |tA_2|$, we need to prove that

$$
\begin{aligned}
(2+\sqrt{2})(n-1) > \frac{1}{2}\big[&(2+\sqrt{2})(n-(a+b-1))+2\sqrt{(n-(a+b-1))^2+(a-b)^2}\\
&+\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}+(a-b)\sqrt{2}\big]. \quad (4.54)
\end{aligned}
$$

We can clearly see that, as $b < a$ $b+b-1 < a+b-1$, so $n-(2b-1) > n-(a+b-1)$.

Multiplying both sides of above inequality by $(2+\sqrt{2})$ gives

$$(2+\sqrt{2})(n-(2b-1)) > (2+\sqrt{2})(n-(a+b-1)). \qquad (4.55)$$

Also, when $a > b \geq 1$ and $n > 3$, we have

$$n-(2b-1) > n-(2a-1) \geq 0,$$

square both sides of above inequality and adding $(n-(2b-1))^2$ to each side, then taking square roots of both sides, we obtain

$$\sqrt{2}(n-(2b-1)) > \sqrt{(n-(2a-1))^2+(n-(2b-1))^2}. \qquad (4.56)$$

Now adding the three formulae, the first one is (4.55), the second formula is from the Lemma 4.3.1, and the third formula is (4.56), we have

$$
\begin{aligned}
&(2+\sqrt{2})(n-(2b-1))+2(n-(2b-1))+2(a-b)+\sqrt{2}(n-(2b-1))\\
&\quad>(2+\sqrt{2})(n-(a+b-1))+2\sqrt{(n-(a+b-1))^2+(a-b)^2}+\\
&\qquad\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}. \quad (4.57)
\end{aligned}
$$

If we add $\sqrt{2}(a-b)$ to each side of Inequality (4.57), then

$$\begin{aligned}(2+\sqrt{2})(n-(2b-1)) &+ \frac{1}{2}(2+\sqrt{2})(a-b)\\ &> \frac{1}{2}\big[(2+\sqrt{2})(n-(a+b-1)) + 2\sqrt{(n-(a+b-1))^2+(a-b)^2}\\ &\qquad + \sqrt{(n-(2a-1))^2+(n-(2b-1))^2} + (a-b)\sqrt{2}\big]. \quad (4.58)\end{aligned}$$

It is obvious that

$$2(2+\sqrt{2})(n-(2b-1))+2(2+\sqrt{2})(a-b) > 2(2+\sqrt{2})(n-(2b-1))+(2+\sqrt{2})(a-b),$$

this implies

$$(2+\sqrt{2})\big[n-(2b-1)+(a-b)\big] > \big[(2+\sqrt{2})(n-(2b-1)+\frac{1}{2}(2+\sqrt{2})(a-b)\big].$$

By Lemma 4.3.2

$$(2+\sqrt{2})(n-1) > (2+\sqrt{2})(n-(2b-1)+\frac{1}{2}(2+\sqrt{2})(a-b). \qquad (4.59)$$

From Formulae (4.58), (4.59), we get the inequality (4.54).

Part (iii). If $t \ll 1$, then the magnitude of tA_3 from Formula (4.48)

$$\begin{aligned}\frac{4}{4-(1+\sqrt{2})\ell t+O(t^2)} &= \frac{1}{1-\frac{1+\sqrt{2}}{4}\ell t+O(t^2)}\\ &= 1+\frac{1+\sqrt{2}}{4}\ell t+O(t^2),\end{aligned} \qquad (4.60)$$

where $\ell = (n-(2b-1))$, as $1 \leq b \leq \frac{n-1}{2}$. Therefore, Expression (4.53) is greater than Expression (4.60).

Part (iv). Since the magnitude of $[\frac{n+1}{2}, \frac{n+1}{2}]$ is equal to one. for nonzero very small scale factor t, the magnitude of tA_0 from Expression (4.53) is greater than one. The proof is completed. □

When an $n \times n$ square grid is scaled very small, then the subsets that contain the union of the four corner points orbit and the points of some other orbits have negative weightings. We shall prove this result in the next theorem.

Theorem 4.3.4. *Given an odd number $n > 3$, and an $n \times n$ square grid tA which is partitioned into the union of disjoint orbits under the action of the isometry group. If we consider a subset B that contains the union of the four corner points orbit with any other orbit, then when $t \ll 1$, B have negative weighting.*

Proof. Suppose that the points of a grid square A are labeled by $\{[i, j] : 1 \leq i, j \leq n\}$ and can be partitioned into the union of disjoint orbits under the symmetry group of the square. We have to find the weighting the disjoint union of two orbits of A. There are four cases as follows

Case 1. The subset B_1 is the union of the four corner points orbit and the middle point orbit,

Case 2. The subset B_2 is the union of the four corner points orbit and a diamond shaped orbit,

Case 3. The subset B_3 is the union of the corner points orbit and a square shaped orbit,

Case 4. The subset B_4 is the union of the four corner points orbit and an eight points orbit.

Case 1. The weighting equations of the first subset B_1 are

$$\begin{aligned} \big(1 + 2e^{-(n-1)t} + e^{-\sqrt{2}(n-1)t}\big)w_{11} + e^{-\frac{\sqrt{2}}{2}(n-1)t}w_{12} &= 1, \\ 4e^{-\frac{\sqrt{2}}{2}(n-1)t}w_{11} + \qquad\qquad w_{12} &= 1, \end{aligned}$$

where w_{11} is an invariant weighting of four corner points and w_{12} is an invariant weighting of the middle point. As $t \ll 1$, the exponential functions of the above expressions can be approximated using the Taylor series of exponential function, to get

$$\begin{aligned} \big(4 - (2+\sqrt{2})(n-1)t + O(t^2)\big)w_{11} + \big(1 - \frac{\sqrt{2}}{2}(n-1)t + O(t^2)\big)w_{12} &= 1, \\ 4\big(1 - \frac{\sqrt{2}}{2}(n-1)t + O(t^2)\big)w_{11} + \qquad\qquad w_{12} &= 1, \end{aligned} \tag{4.61}$$

The values of w_{11} can be obtained, by multiplying the second formula of (4.61) by $1 - \frac{\sqrt{2}}{2}(n-1)t + O(t^2)$, then subtracting the first expression from the second.

$$w_{11} = \frac{1 - 1 + \frac{\sqrt{2}}{2}(n-1)t + O(t^2)}{\big(4 - (2+\sqrt{2})(n-1)t + O(t^2)\big) - 4\big((1 - \frac{\sqrt{2}}{2})(n-1)t + O(t^2)\big)^2}. \tag{4.62}$$

By substituting these formula in the first expression of (4.61) we have

$$w_{12} = \frac{4 - (2+\sqrt{2})(n-1)t + O(t^2) - \big((4 - 2\sqrt{2})(n-1)t + O(t^2)\big)}{4 - (2+\sqrt{2})(n-1)t + O(t^2) - 4\big((1 - \frac{\sqrt{2}}{2})(n-1)t + O(t^2)\big)^2}. \tag{4.63}$$

Simplifying the numerators and the denominators of Formulae (4.62) and (4.63), we get

$$w_{11} = \frac{\frac{\sqrt{2}}{2}(n-1) + O(t)}{(3\sqrt{2}-2)(n-1) + O(t)},$$
$$w_{12} = \frac{-(2-\sqrt{2})(n-1) + O(t)}{(3\sqrt{2}-2)(n-1) + O(t)}.$$

This implies when $n > 1$, the values of w_{11} is positive and w_{12} is negative.

Case 2. Let $[a, b]$ be a point in the diamond shaped orbits such that $1 \leq b < a$ and $a = \frac{n+1}{2}$. So, the weighting equations of subset B_2 are

$$\begin{aligned}\big(1 + 2e^{-(n-1)t} + e^{-\sqrt{2}(n-1)t}\big)w_{21} + \big(2e^{-\frac{1}{2}\sqrt{(n-1)^2+4(b-1)^2}t} \\ + 2e^{-\frac{1}{2}\sqrt{(n-1)^2+4(n-b)^2}t}\big)w_{22} = 1,\end{aligned}$$

and

$$\begin{aligned}\big(2e^{-\frac{1}{2}\sqrt{(n-1)^2+4(b-1)^2}t} + 2e^{-\frac{1}{2}\sqrt{(n-1)^2+4(n-b)^2}t}\big)w_{21} + \big(1 + e^{-(n-(2b-1))t} \\ + 2e^{-\frac{\sqrt{2}}{2}(n-(2b-1))t}\big)w_{22} = 1,\end{aligned}$$

where w_{21} is an invariant weighting of four corner points and w_{22} is an invariant weighting of the diamond shaped orbits. As $t \ll 1$, Using Taylor's approximation formula we have

$$\begin{aligned}\big(4 - (2+\sqrt{2})(n-1)t + O(t^2)\big)w_{21} + \big(4 - (\sqrt{(n-1)^2 + 4(b-1)^2} \\ + \sqrt{(n-1)^2 + 4(n-b)^2})t + O(t^2)\big)w_{22} = 1,\end{aligned}$$

so,

$$\begin{aligned}\big(4 - (2+\sqrt{2})(n-1)t + O(t^2)\big)w_{21} + \big(4 - ((n-1)(\sqrt{1 + (\frac{2(b-1)}{n-1})^2}) \\ + 2(n-b)\sqrt{1 + (\frac{2(n-1)}{n-b})^2})t + O(t^2)\big)w_{22} = 1, \quad (4.64)\end{aligned}$$

and

$$\begin{aligned}\big(4 - (\sqrt{(n-1)^2 + 4(b-1)^2} + \sqrt{(n-1)^2 + 4(n-b)^2})t + O(t^2)\big)w_{21} \\ + \big(4 - (1+\sqrt{2})(n-(2b-1))t + O(t^2)\big)w_{22} = 1,\end{aligned}$$

so,

$$\begin{aligned}\big(4 - ((n-1)(\sqrt{1 + (\frac{2(b-1)}{n-1})^2}) + 2(n-b)\sqrt{1 + (\frac{2(n-1)}{n-b})^2})t + O(t^2)\big)w_{21} \\ + \big(4 - (1+\sqrt{2})(n-(2b-1))t + O(t^2)\big)w_{22} = 1. \quad (4.65)\end{aligned}$$

Since $1 \leq b < \frac{n+1}{2}$, so $(\frac{2(b-1)}{n-1})^2$ and $(\frac{n-1}{2(n-b)})^2$ are less than one. Therefore, Formulae (4.64) and (4.65) can be written as follows

$$\begin{aligned}\big(4-(2+\sqrt{2})(n-1)t+O(t^2)\big)w_{21}+\big(4-\big((n-1)(1+\frac{2(b-1)^2}{(n-1)^2})\\ +2(n-b)(1+\frac{(n-1)^2}{8(n-b)^2})\big)t+O(t^2)\big)w_{22}=1,\end{aligned} \tag{4.66}$$

and

$$\begin{aligned}\big(4-\big((n-1)(1+\frac{2(b-1)^2}{(n-1)^2})+2(n-b)(1+\frac{(n-1)^2}{8(n-b)^2})\big)t+O(t^2)\big)w_{21}\\ +\big(4-(1+\sqrt{2})(n-(2b-1))t+O(t^2)\big)w_{22}=1,\end{aligned} \tag{4.67}$$

where $\epsilon_1 = \frac{2(b-1)^2}{(n-1)^2}$ and $\epsilon_2 = \frac{(n-1)^2}{8(n-b)^2}$. Since $n > 3$ and $b \geq 1$. If we multiply Formula (4.66) by $\big(4-(1+\sqrt{2})(n-(2b-1))t+O(t^2)\big)$ and Formula (4.67) by $\big(4-\big((n-1)(1+\epsilon_1)+2(n-b)(1+\epsilon_2)\big)t+O(t^2)\big)$, then subtract one formula from other to obtain the value of w_{21} and substitute the result into the Expression (4.64) to have w_{22}, then simplifying the resulting expression and neglecting the very small values ϵ_1 and ϵ_2 to obtain

$$w_{21} = \frac{2(n-1)-\sqrt{2}(n-(2b-1))+O(t)}{8(1-\sqrt{2})(n-b)+4(n-1)+O(t)},$$

and

$$w_{22} = \frac{-\sqrt{2}(n-1)+(n-(2b-1))+O(t)}{8(1-\sqrt{2})(n-b)+4(n-1)+O(t)},$$

It is easy to see that w_{21} is positive, and w_{22} is negative.

Case 3. If $[a, b]$ is a point in the square shaped orbits such as $1 < a < \frac{n+1}{2}$ and $a = b$, then the weighting formulae of B_3 are

$$\begin{aligned}\big(1+2e^{-(n-1)t}+e^{-\sqrt{2}(n-1)t}\big)w_{31}+\big(e^{-\sqrt{2}(b-1)t}+2e^{-\sqrt{(n-b)^2+(b-1)^2}t}\\ +e^{-\sqrt{2}(n-b)t}\big)w_{32}=1,\end{aligned}$$

and

$$\begin{aligned}\big(e^{-\sqrt{2}(b-1)t}+2e^{-\sqrt{(n-b)^2+(b-1)^2}t}+e^{-\sqrt{2}(n-b)t}\big)w_{31}+\big(1+2e^{-(n-(2b-1))t}\\ +e^{-\sqrt{2}(n-(2b-1))t}\big)w_{32}=1,\end{aligned}$$

where w_{31} is an invariant weighting of four corner points and w_{32} is an invariant weighting of the square shaped orbits. As $t \ll 1$, we can use the Taylor approximation to get

$$\begin{aligned}\big(4-(2+\sqrt{2})(n-1)t+O(t^2)\big)w_{31}+\big(4-(\sqrt{2}(n-1)+2\sqrt{(n-b)^2+(b-1)^2})t\\ +O(t^2)\big)w_{32}=1,\end{aligned}$$

so,

$$\big(4-(2+\sqrt{2})(n-1)t+O(t^2)\big)w_{31}+\big(4-(\sqrt{2}(n-1)\\ +2(n-b)\sqrt{1+(\frac{b-1}{n-b})^2})t+O(t^2)\big)w_{32}=1,$$

and

$$\big(4-(\sqrt{2}(n-1)+2\sqrt{(n-b)^2+(b-1)^2})t+O(t^2)\big)w_{31}\\ +\big(4-(2+\sqrt{2})(n-(2b-1))t+O(t^2)\big)w_{32}=1.$$

so,

$$\big(4-(\sqrt{2}(n-1)+2(n-b)\sqrt{1+(\frac{b-1}{n-b})^2})t+O(t^2)\big)w_{31}\\ +\big(4-(2+\sqrt{2})(n-(2b-1))t+O(t^2)\big)w_{32}=1.$$

Since $1<b<\frac{n+1}{2}$ and $n\geq 3$, so $\frac{b-1}{n-b})^2<1$. Then the above formulae can be written as

$$\big(4-(2+\sqrt{2})(n-1)t+O(t^2)\big)w_{31}+\big(4-(\sqrt{2}(n-1)\\ +2(n-b)(1+\frac{(b-1)^2}{2(n-b)^2}))t+O(t^2)\big)w_{32}=1, \tag{4.68}$$

and

$$\big(4-(\sqrt{2}(n-1)+2(n-b)(1+\frac{(b-1)^2}{2(n-b)^2}))t+O(t^2)\big)w_{31}\\ +\big(4-(2+\sqrt{2})(n-(2b-1))t+O(t^2)\big)w_{32}=1 \tag{4.69}$$

Multiply Formula (4.68) by $4-(2+\sqrt{2})(n-(2b-1))t+O(t^2)$ and Formula (4.69) by $4-(\sqrt{2}(n-1)+2(n-b)(1+\frac{(b-1)^2}{2(n-b)^2}))t+O(t^2)$, then subtract the one from the other to get w_{31}, after that substitute the value of w_{31} into Expression (4.68) gives w_{32}, then simplifying the resulting expression and neglecting the very small value $\frac{(b-1)^2}{2(n-b)^2}$ to obtain

$$w_{31}=\frac{(2+2\sqrt{2})(b-1)+O(t)}{8\sqrt{2}(n-1)-8\sqrt{2}(n-b)+O(t)}, \tag{4.70}$$

and

$$w_{32}=\frac{-\sqrt{2}(n-1)+(n-(2b-1))+O(t)}{8\sqrt{2}(n-1)-8\sqrt{2}(n-b)+O(t)}. \tag{4.71}$$

Clearly see that the Expression (4.70) is positive and the Expression (4.71) is negative.

Case 4. Consider $[a, b]$ belong to the eight-points orbits such as $1 \leq b < a < \frac{n+1}{2}$. Thus, the weighting equations for the subset B_4 are

$$\begin{aligned}\big(1+2e^{-(n-1)t}+e^{-\sqrt{2}(n-1)t}\big)w_{41}+\big(2e^{-\sqrt{(a-1)^2+(b-1)^2}t}+2e^{-\sqrt{(n-a)^2+(b-1)^2}t}\\ +2e^{-\sqrt{(n-b)^2+(a-1)^2}t}+2e^{-\sqrt{(n-a)^2+(n-b)^2}t}\big)w_{42}=1,\end{aligned}$$

and

$$\begin{aligned}&\big(e^{-\sqrt{(a-1)^2+(b-1)^2}t}+e^{-\sqrt{(n-a)^2+(b-1)^2}t}+e^{-\sqrt{(n-b)^2+(a-1)^2}t}\\ &+e^{-\sqrt{(n-a)^2+(n-b)^2}t}\big)w_{41}+\big(1+e^{-(n-(2a-1))t}+2e^{-\sqrt{(n-(a+b-1))^2+(a-b)^2}t}\\ &\quad+e^{-\sqrt{2}(n-(a+b-1))t}+e^{-(n-(2b-1))t}+e^{-\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}t}\\ &\qquad+e^{-(a-b)\sqrt{2}t}\big)w_{42}=1,\end{aligned}$$

where w_{41} is an invariant weighting of four corner points and w_{42} is an invariant weighting of the eight-points orbits. As $t \ll 1$, we can approximate the above formula by the Taylor expansions

$$\begin{aligned}&\big(4-(2+\sqrt{2})(n-1)t+O(t^2)\big)w_{41}+2\big(4-(\sqrt{(a-1)^2+(b-1)^2}\\ &+\sqrt{(n-a)^2+(b-1)^2}+\sqrt{(n-b)^2+(a-1)^2}+\sqrt{(n-a)^2+(n-b)^2})t\\ &+O(t^2)\big)w_{42}=1,\end{aligned} \tag{4.72}$$

and

$$\begin{aligned}&\big(4-(\sqrt{(a-1)^2+(b-1)^2}+\sqrt{(n-a)^2+(b-1)^2}+\sqrt{(n-b)^2+(a-1)^2}\\ &+\sqrt{(n-a)^2+(n-b)^2})t+O(t^2)\big)w_{41}+2\big(4-(n-(a+b-1))+\frac{\sqrt{2}}{2}(n-(a+b-1))\\ &+\frac{\sqrt{2}}{2}(a-b)+\sqrt{(n-(a+b-1))^2+(a-b)^2}\\ &+\frac{1}{2}\sqrt{(n-(2a-1))^2+(n-(2b-1))^2})t+O(t^2)\big)w_{42}=1.\end{aligned} \tag{4.73}$$

Multiply Formula (4.72) by $\big(4-((n-(a+b-1))+\frac{\sqrt{2}}{2}(n-(a+b-1))+\frac{\sqrt{2}}{2}(a-b)+\sqrt{(n-(a+b-1))^2+(a-b)^2}+\frac{1}{2}\sqrt{(n-(2a-1))^2+(n-(2b-1))^2})t+O(t^2)\big)$ and Formula (4.73) by $\big(4-(\sqrt{(a-1)^2+(b-1)^2}+\sqrt{(n-a)^2+(b-1)^2}+\sqrt{(n-b)^2+(a-1)^2}+\sqrt{(n-a)^2+(n-b)^2})t+O(t^2)\big)$ and subtract one expression from the other, to obtain

$$w_{41}=\frac{C-B+O(t^2)}{AC-B^2+O(t^2)}, \tag{4.74}$$

the values of w_{42} can be find by substitute w_{41} into Formula 4.72

$$w_{42}=\frac{A-B+O(t^2)}{AC-B^2+O(t^2)}, \tag{4.75}$$

where

$$
\begin{aligned}
A &= 4-(2+\sqrt{2})(n-1)t,\\
B &= 4-\big(\sqrt{(a-1)^2+(b-1)^2}+\sqrt{(n-a)^2+(b-1)^2}\\
&\quad+\sqrt{(n-b)^2+(a-1)^2}+\sqrt{(n-a)^2+(n-b)^2}\big)t,\\
C &= 4-\big((n-(a+b-1))+\frac{\sqrt{2}}{2}(n-(a+b-1))\\
&\quad+\frac{\sqrt{2}}{2}(a-b)+\sqrt{(n-(a+b-1))^2+(a-b)^2}\\
&\quad+\frac{1}{2}\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}\big)t.
\end{aligned}
$$

The denominators of Expressions (4.74) and (4.75) are equal to

$$
\begin{aligned}
&16-\big(4(n-(a+b-1))+2\sqrt{2}(n-(a+b-1))+2\sqrt{2}(a-b)\\
&\quad+4\sqrt{(n-(a+b-1))^2+(a-b)^2}+2\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}\\
&\quad+8(n-1)+4\sqrt{2}(n-1)\big)t+O(t^2)-16+\big(8\sqrt{(a-1)^2+(b-1)^2}\\
&\quad+8\sqrt{(n-a)^2+(b-1)^2}\\
&\quad+8\sqrt{(n-b)^2+(a-1)^2}+8\sqrt{(n-a)^2+(n-b)^2}\big)t+O(t^2),
\end{aligned}
\tag{4.76}
$$

by simplifying the above expression we get,

$$
\begin{aligned}
&-8(n-a)-8(n-b)-2\sqrt{2}(n-a)-6\sqrt{2}(n-b)+8(n-a)+8(n-b)\\
&\qquad\qquad+4\sqrt{2}(n-a)+4\sqrt{2}(n-b)+8(a-1).
\end{aligned}
$$

When $1 \le b < a$ and $n > 3$, $8(a-1) > 2\sqrt{2}(a-b)$, so the Expression (4.76) is greater than zero.

Also, the numerator of Formula (4.74) is

$$
\begin{aligned}
&4-\big((n-(a+b-1))+\sqrt{(n-(a+b-1))^2+(a-b)^2}+\frac{\sqrt{2}}{2}(n-(a+b-1))\\
&\quad+\frac{1}{2}\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}+\frac{\sqrt{2}}{2}(a-b)\big)-4\\
&\quad+\big(\sqrt{(a-1)^2+(b-1)^2}+\sqrt{(n-a)^2+(b-1)^2}+\sqrt{(n-b)^2+(a-1)^2}\\
&\quad+\sqrt{(n-a)^2+(n-b)^2}\big),
\end{aligned}
\tag{4.77}
$$

simplifying Formula (4.77) we have,

$$
\begin{aligned}
&-\big((n-(a+b-1))+\sqrt{(n-(a+b-1))^2+(a-b)^2}+\frac{\sqrt{2}}{2}(n-(2b-1))\\
&+\frac{1}{2}\sqrt{(n-(2a-1))^2+(n-(2b-1))^2}\big)+\big((n-1)+\sqrt{(n-b)^2+(a-1)^2}\\
&+\frac{1}{2}\sqrt{(n-a)^2+(n-b)^2}+\frac{\sqrt{2}}{2}(n-\frac{1}{2}(a+b))\big).
\end{aligned}
$$

Since $1 \leq b < a < \frac{n+1}{2}$ and $n > 3$, then the next statements are true

$$
\begin{aligned}
\frac{1}{2}\sqrt{(n-a)^2+(n-b)^2} &> \frac{1}{2}\sqrt{(n-(2a-1))^2+(n-(2b-1))^2},\\
\sqrt{(n-b)^2+(a-1)^2} &> \sqrt{(n-(a+b-1))^2+(a-b)^2},\\
\frac{\sqrt{2}}{2}(n-1) &> \frac{\sqrt{2}}{2}(n-(2b-1)),\\
\frac{2-\sqrt{2}}{2}(n-1)+\frac{\sqrt{2}}{2}(n-\frac{1}{2}(a+b)) &> (n-(a+b-1)),
\end{aligned}
$$

so, Expression (4.77) is bigger than zero. However, the numerator of Formula (4.75) is

$$
\begin{aligned}
&4-(2+\sqrt{2})(n-1)-4+\big(\sqrt{(a-1)^2+(b-1)^2}+\sqrt{(n-a)^2+(b-1)^2}\\
&+\sqrt{(n-b)^2+(a-1)^2}+\sqrt{(n-a)^2+(n-b)^2}\big),
\end{aligned}
\tag{4.78}
$$

simplifying Expression (4.78) we obtain,

$$
-(1+\sqrt{2})(n-1)+2(n-b)
$$

Again, as $b \geq 1$ and $n > 3$, we have $-(1+\sqrt{2})(n-1) > 2(n-b)$. This means Formula (4.78) is less than zero. Which implies that the value w_{41} is non-negative and the value w_{42} is negative. The proof is completed. □

Furthermore, for an even number $n > 2$, there are two cases for the orbits that partition the points of the $n \times n$ square grid.

The first case is the orbit that contains the four points with side length $\ell = n-(2b-1)$, as $1 \leq b \leq \frac{n}{2}$. If $\ell \ll 1$, then the weightings of these orbits is

$$
\frac{1}{4-(2+\sqrt{2})\ell t+O(t^2)}, \tag{4.79}
$$

which can be seen from Formula (4.44).

The second case is the orbit with eight points. When $t \ll 1$, the invariant weightings of these orbits is

$$1/\big(8 - t\big[(2+\sqrt{2})(n-(a+b-1)) + 2\sqrt{(n-(a+b-1))^2+(a-b)^2}+ \\ \sqrt{(n-(2a-1))^2+(n-(2b-1))^2}+(a-b)\sqrt{2}\big] + O(t^2)\big), \tag{4.80}$$

where $1 \leq b < a \leq \frac{n}{2}$, as can be seen from Expression (4.45).

The next statement shows that when the square grid is scaled very small. So the four corner points have a greater magnitude than the magnitude of all other orbits of the square grid and the subsets of the grid square that contains the four corner orbit with any other orbit have a negative weighting.

Corollary 4.3.5. *Suppose that a scale factor t of a square grid tA of an even number $n > 2$ of points is very small. the magnitude of the four corner orbit is bigger than the magnitude of all other orbits as well as if we added any orbit to the four corner points, then the new subset has a negative weighting.*

Proof. Since $n > 2$ is an even, there are two types of the orbits that partition the points of a square grid $n \times n$.

The first type is the orbits that consist of the square-shaped point of the square grid. As $t \ll 1$, by the first part of Theorem 4.3.3, the largest square has a larger magnitude.

The second type is the orbit that consists of the eight points of the $n \times n$ metric space. When $t \ll 1$, form the second part of Theorem 4.3.3, the magnitude of the four corner points of the metric space should be greater than the magnitude of these orbits.

To prove that a new subset that contains the union of the four corner points orbit and any other orbit must have negative weightings. There are two cases to show that.

The first case, a subset of the square grid that contains the union of the four corner point and the square shaped points. From Case 3 of the proof of Theorem 4.3.4, it has negative weighting.

The second case, a subset of the metric space which contain the union of the four corner points and the eight points. From Case 4 of the proof of Theorem 4.3.4, it has negative weighting. The proof is completed. □

From Theorem 4.3.3 and Theorem 4.3.4 and Corollary 4.3.5, we observe that the magnitude of the boundary point at the corner of side length $n-1$ is larger than the magnitude of all other orbits. However, the union of the orbit of side length $n-1$ and each other orbit have a negative weight. Moreover, for $n = 3, 4, \ldots, 9, 10$ when we compute the subsets of the $n \times n$ grid square at a very small scale, we see that.

- The union of any two orbits, must one of them have negative weight,

- The union of more than two orbits, at least one of them have negative weights.

Also, we think that at each scale, one of the types that presented in the figures in the last three pages of Subsection 4.2.4 will have maximum magnitude with non-negative weighting, but had no way to prove this. However, the last case, when the grid square has a maximum magnitude that admits a non-negative weighting was proved by Leinster [Proposition 2.1.3, [32]].

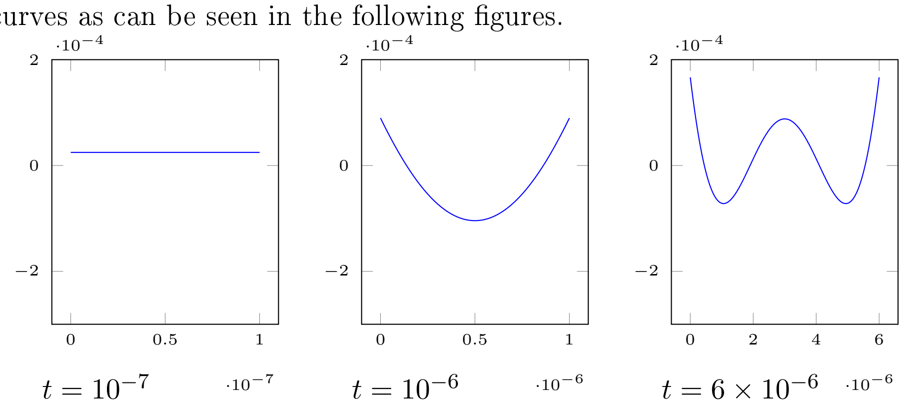
§ 4.4 Finding the weighting of the points in the middle row of the square grid metric space using Krylov subspace method

The programming language Python was used to calculate the weights of the points in the middle row of the 201×201 metric space using the Krylov method as follows.

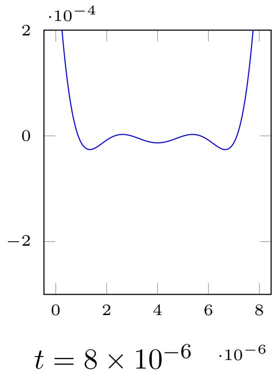
We determine the weighting of the points on the middle row of the 201×201 grid square at various scaling from 0.000001 to 0.6. For each scale, we first obtain the distance matrix for the 201×201 points. After that, we use the conjugate gradient method described in Subsection 2.7 to calculate the weighting of that points. Then, we create a vector of the weighting of the middle row points, and finally we create a text file for that vector with the associated scale factor (see Appendix B.3).

In this section, we will look a little closer at the weights behavior of the points in the middle row of 201×201 grid square at different scaling and trying to see how there can be a smooth transition form the weighting of middle row of the square grid at small scale to the weighting of middle row of the square grid at large scale.

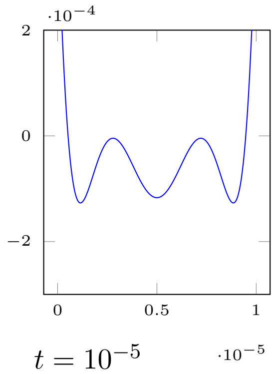
It is not clear what is happening when the grid square is scaled very small. The points of the middle row of the 201×201 grid square have constant positive weighing, when the square grid is scaled by a factor $t = 10^{-7}$. After that those weighting of points have different values when the square grid is scaled between $t = 10^{-6}$ and $t = 62 \times 10^{-5}$ and we get the various positions of curves as can be seen in the following figures.



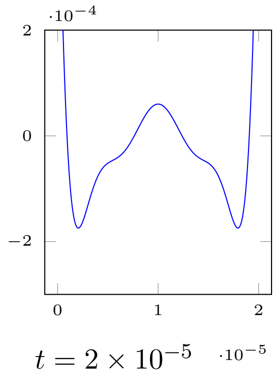
$t = 10^{-7}$ $\quad$ $t = 10^{-6}$ $\quad$ $t = 6 \times 10^{-6}$



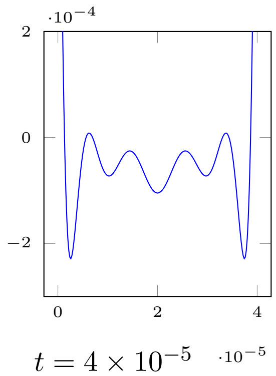
$t = 8 \times 10^{-6}$



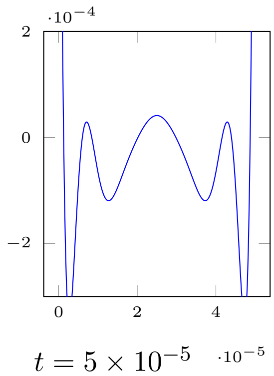
$t = 10^{-5}$



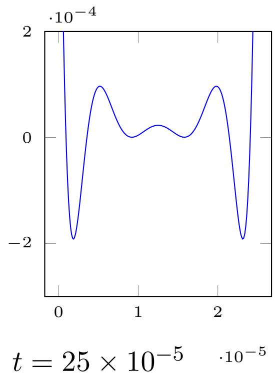
$t = 2 \times 10^{-5}$



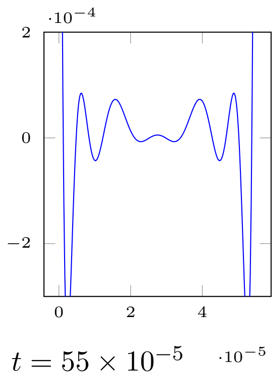
$t = 4 \times 10^{-5}$



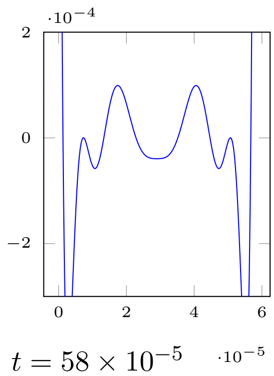
$t = 5 \times 10^{-5}$



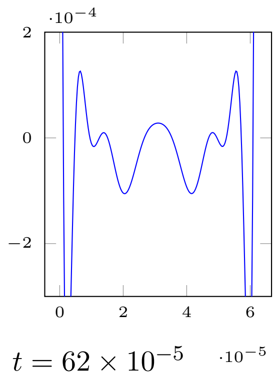
$t = 25 \times 10^{-5}$



$t = 55 \times 10^{-5}$

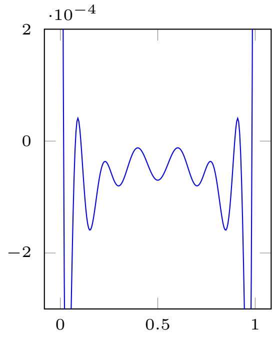


$t = 58 \times 10^{-5}$

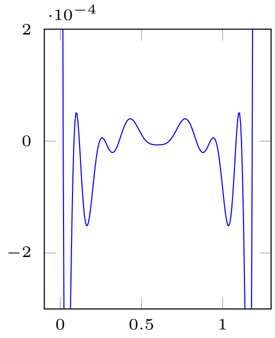


$t = 62 \times 10^{-5}$

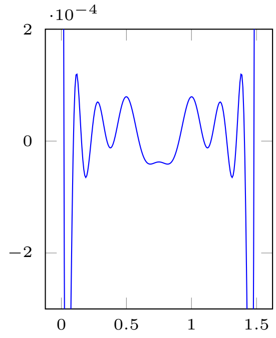
If the square grid with 201×201 points is scaled by the factors between 10^{-4} and 0.6, we have short oscillations happening in the centre comparing to the long oscillations occurring on the bounders. Both short and long oscillations increase in number as scale factor getting bigger. Moreover, the long oscillations decrease in number and tend to one, while the short ones decrease in amplitude and the amplitudes tend to zero, i.e. the oscillations settle at some horizontal level, which are graphically represented in the following figures.



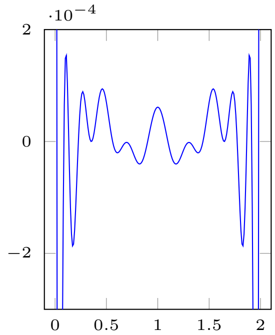
$t = 1 \times 10^{-4}$



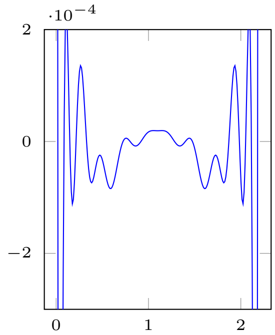
$t = 12 \times 10^{-4}$



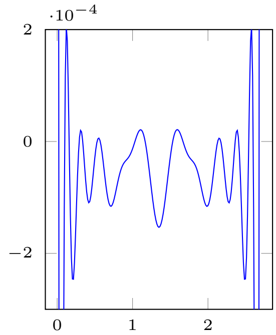
$t = 15 \times 10^{-4}$



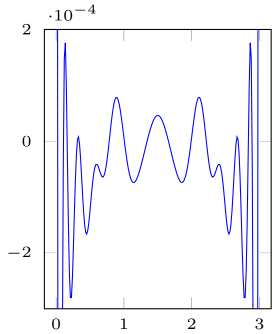
$t = 20 \times 10^{-4}$



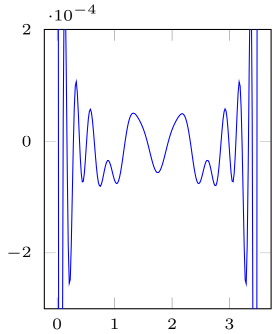
$t = 22 \times 10^{-4}$



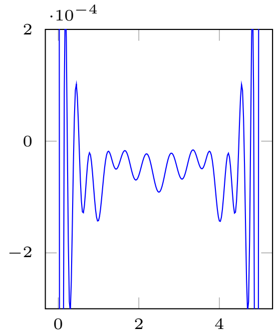
$t = 27 \times 10^{-4}$



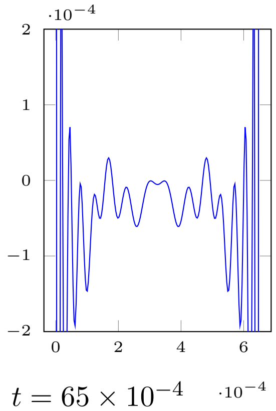
$t = 30 \times 10^{-4}$



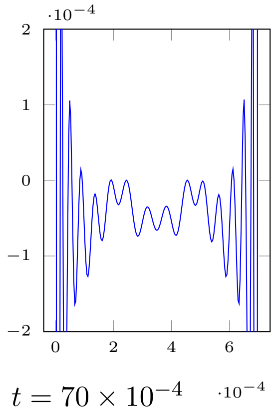
$t = 35 \times 10^{-4}$



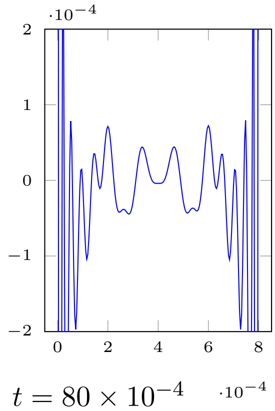
$t = 50 \times 10^{-4}$



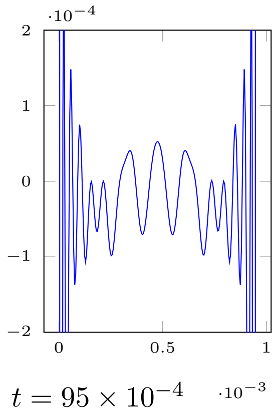
$t = 65 \times 10^{-4}$



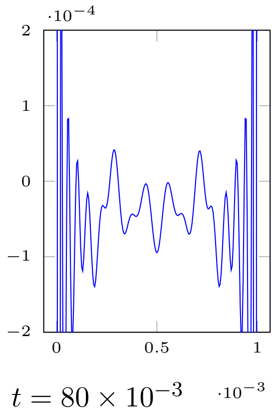
$t = 70 \times 10^{-4}$



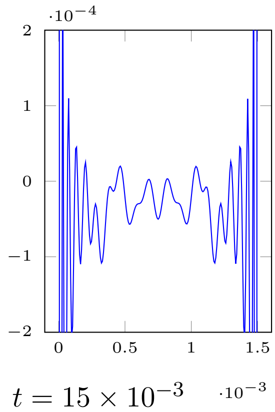
$t = 80 \times 10^{-4}$



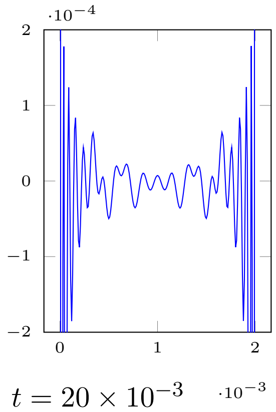
$t = 95 \times 10^{-4}$



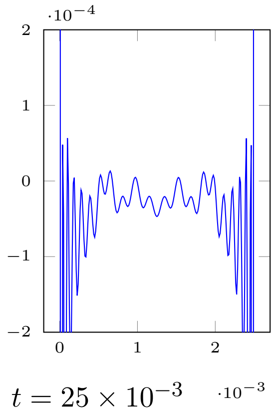
$t = 80 \times 10^{-3}$



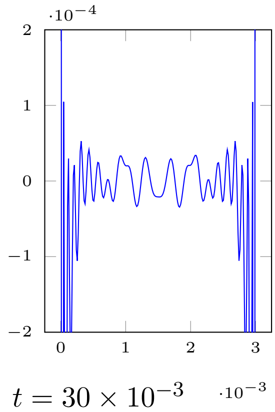
$t = 15 \times 10^{-3}$



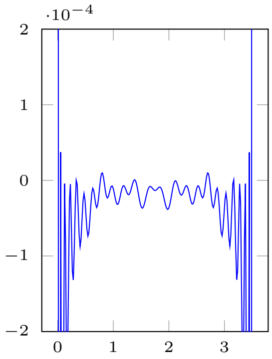
$t = 20 \times 10^{-3}$



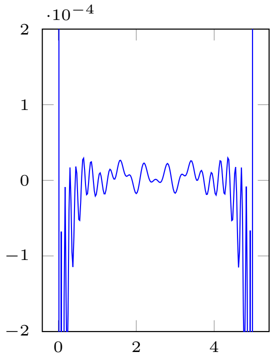
$t = 25 \times 10^{-3}$



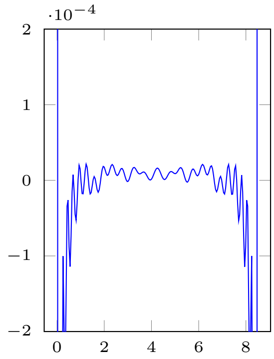
$t = 30 \times 10^{-3}$



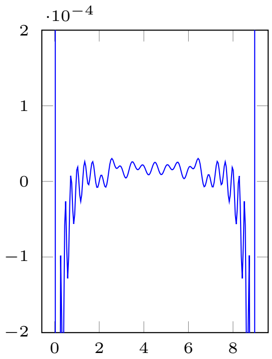
$t = 35 \times 10^{-3}$



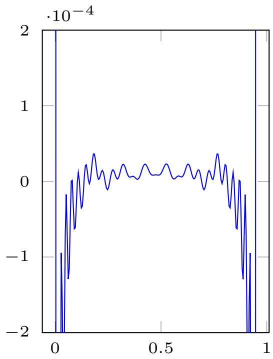
$t = 50 \times 10^{-3}$



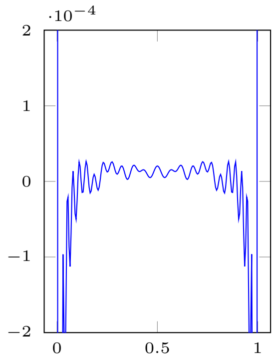
$t = 85 \times 10^{-3}$



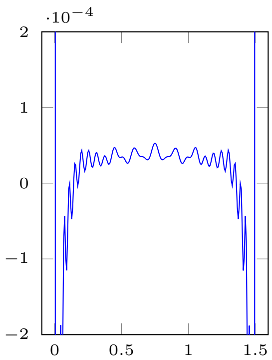
$t = 90 \times 10^{-3}$



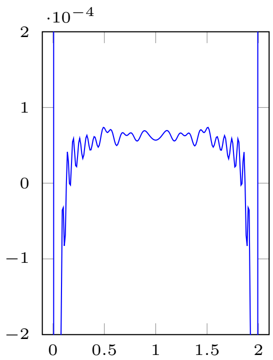
$t = 95 \times 10^{-3}$



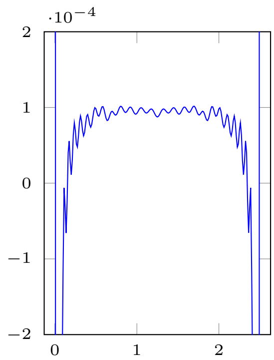
$t = 1 \times 10^{-2}$



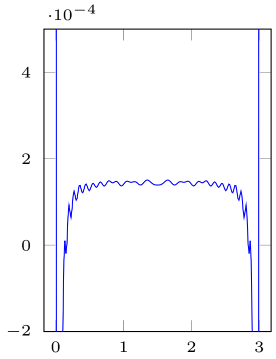
$t = 15 \times 10^{-2}$



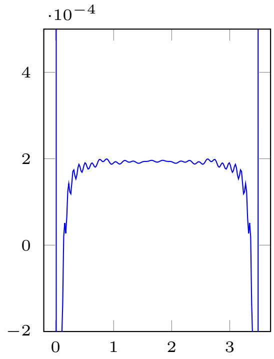
$t = 20 \times 10^{-2}$



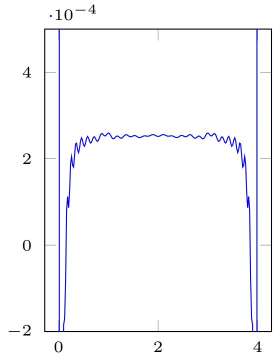
$t = 25 \times 10^{-2}$



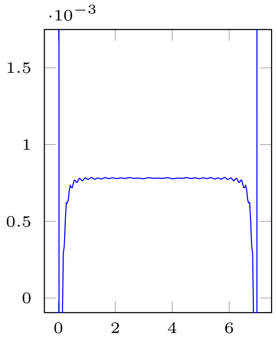
$t = 30 \times 10^{-2}$



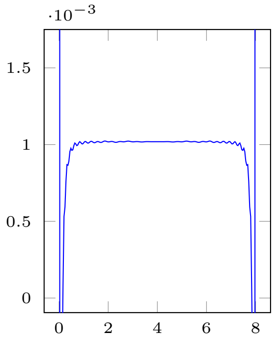
$t = 35 \times 10^{-2}$



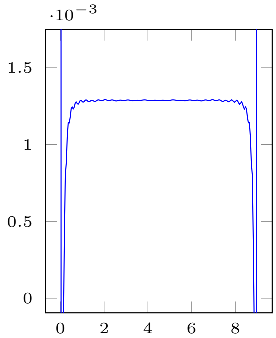
$t = 40 \times 10^{-2}$



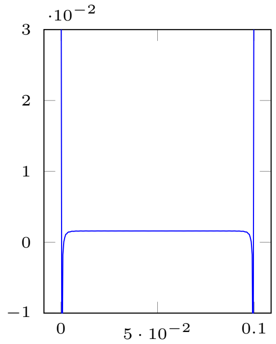
$t = 70 \times 10^{-2}$



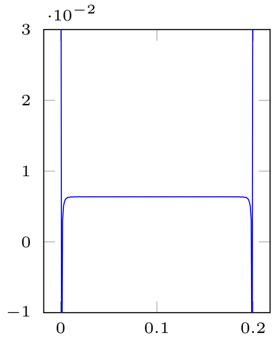
$t = 80 \times 10^{-2}$



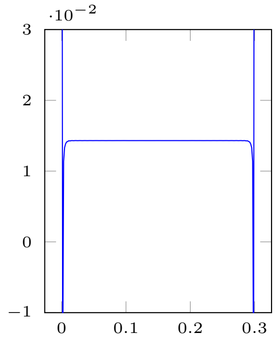
$t = 90 \times 10^{-2}$



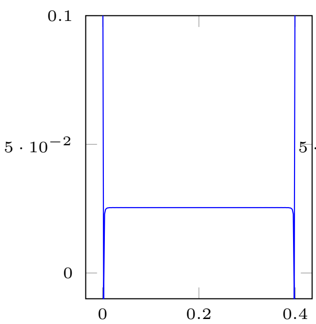
$t = 0.1$



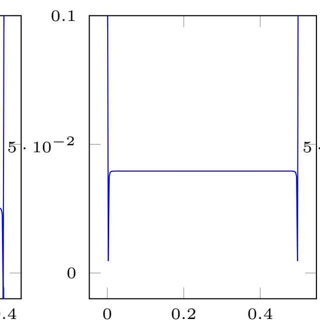
$t = 0.2$



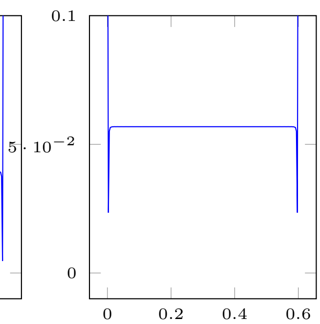
$t = 0.3$



$t = 0.4$



$t = 0.5$



$t = 0.6$

From figures, the following features are apparent.

- The weights of the centre points in the middle row of the grid square are identical and those points increasing as the scale factor gets bigger,
- The weights of the points on the boundary are always positive. As the scale factor gets bigger, the set of points with negative weights shrinks in size, moving close to the boundary, and eventually disappearing, as we see below for $t = 0.6$,
- All points in the middle row having the positive weighting when the metric space is scaled by 0.6.

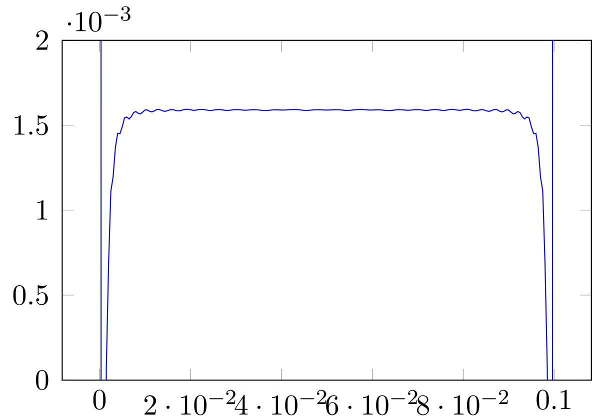


Figure 4.11: The weighting of the points in the middle row of the square grid when the metric space is scaled by 0.1.

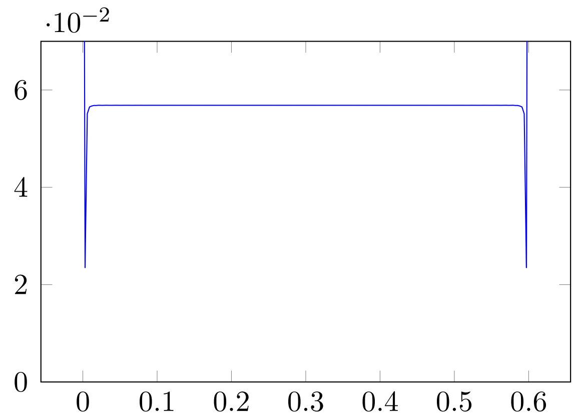


Figure 4.12: The weighting of the points in the middle row of the square grid when the metric space is scaled by 0.6.

Chapter 5

The magnitude dimension and the q-spread of another shapes of metric spaces

This chapter consists of three sections. In the first section, we evaluate a 0-spread of the disk, and similar to the square grid in Section 3.2, we consider D to be a disk of radius R and take $\ddot{D}_n$ to be a large finite grid points metric space and from the numerical calculation, we see that, if the $\ddot{D}_n$ is scaled by a small factor $\tau > 0$, then the squre grid points inside circle is approximately the solid disk in $\mathbb{R}^2$, which is essentially independent of the number of points. So, the 0-spread of the solid disk is supposed to give an approximation to the 0-spread of the large grid points inside circle. Also, the 0-spread of $\tau\ddot{D}_n$ is often close to some quadratic formula of τ for very small τ. In the second and third sections, we numerical evaluate the 0-spread dimension and magnitude dimension of different types of rectangular grid metric spaces respectively.

§ 5.1 0-spread of the solid disk

Here we find the 0-spread of the disk and numerically proved that if a large square grid points inside a circle $\ddot{D}_n$ metric space is scaled by a small factor $\tau > 0$, then 0-spread of $\ddot{D}_n$ is numerical approximations to $0.8\tau^2 + 1.43\tau + 1.02$.

Let us start with the following definition.

Definition 5.1.1. (See [56]) If (A, d) is a metric space equipped with a measure μ such that $\mu(A) < \infty$, then we can define the 0-spread of A by

$$E_0(A) = \int_{a \in A} \frac{d\mu(a)}{\int_{b \in A} e^{-d(a,b)} d\mu(b)}.$$

In the following result, we evaluate the 0-spread of a disc D.

Theorem 5.1.2. *if we consider a disk D of radius R, then a 0-spread of D is equal to*

$$\int_{x=0}^{R} \frac{x\,dx}{\int_{r=0}^{R-x} e^{-r} r\,dr + \frac{1}{\pi}\int_{r=R-x}^{R+x} e^{-r} r \cos^{-1}(\frac{x^2+r^2-R^2}{2rx})\,dr}.$$

Proof. Suppose that $a \in D$, we rotate the disc, so a is in a x-axis. We want to calculate

$$\int_{b\in D} e^{-d(a,b)}\,db. \tag{5.1}$$

Using the cosine rule, we get

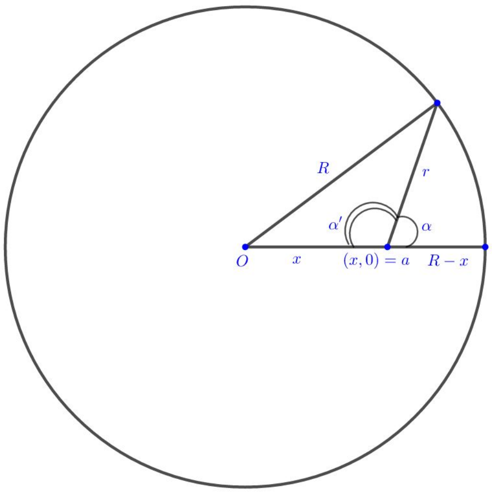


Figure 5.1: The disc D.

$$R^2 = x^2 + r^2 - 2rx\cos(\alpha'),$$

this implies that

$$\alpha' = \cos^{-1}(\frac{x^2+r^2-R^2}{2rx}).$$

We can see from Figure 5.1, that $\alpha = \pi - \alpha'$, so

$$\pi - \alpha = \cos^{-1}(\frac{x^2+r^2-R^2}{2rx}).$$

Also from Figure 5.2 we can find the region.

$$\int_{b\in D} e^{-d(a,b)}\,db = \int_{b\in D'} e^{-d(a,b)}\,db + \int_{b\in D''} e^{-d(a,b)}\,db.$$

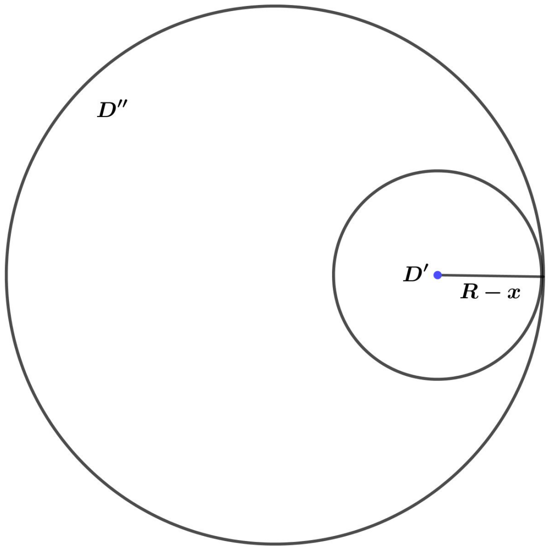


Figure 5.2: The region D' and D''.

Now, we rewrite the above formula in a polar coordinates to obtain

$$\begin{aligned}
\int_{b\in D} e^{-d(a,b)}\, db &= \int_{\Theta=0}^{2\pi}\int_{r=0}^{R-x} e^{-r} r\, dr\, d\Theta + \int_{\Theta=\alpha}^{2\pi-\alpha}\int_{r=R-x}^{R+x} e^{-r} r\, dr\, d\Theta,\\
&= \int_{\Theta=0}^{2\pi} d\Theta \int_{r=0}^{R-x} e^{-r} r\, dr + \int_{r=R-x}^{R+x}\int_{\Theta=\pi-\alpha'}^{\pi+\alpha'} e^{-r} r\, d\Theta\, dr,\\
&= 2\pi \int_{r=0}^{R-x} e^{-r} r\, dr + 2\int_{r=R-x}^{R+x} e^{-r} r\alpha'\, dr,\\
&= 2\pi \int_{r=0}^{R-x} e^{-r} r\, dr + 2\int_{r=R-x}^{R+x} e^{-r} r \cos^{-1}\Big(\frac{x^2+r^2-R^2}{2rx}\Big)\, dr.
\end{aligned}$$

The 0-spread of D is

$$\begin{aligned}
E_0(D) &= \int_{\phi=0}^{2\pi}\int_{x=0}^{R} \frac{x\, dx\, d\phi}{2\pi \int_{r=0}^{R-x} e^{-r} r\, dr + 2\int_{r=R-x}^{R+x} e^{-r} r\cos^{-1}\big(\frac{x^2+r^2-R^2}{2rx}\big)\, dr},\\
&= \int_{\phi=0}^{2\pi} d\phi \int_{x=0}^{R} \frac{x\, dx}{2\pi \int_{r=0}^{R-x} e^{-r} r\, dr + 2\int_{r=R-x}^{R+x} e^{-r} r\cos^{-1}\big(\frac{x^2+r^2-R^2}{2rx}\big)\, dr},\\
&= \int_{x=0}^{R} \frac{x\, dx}{\int_{r=0}^{R-x} e^{-r} r\, dr + \frac{1}{\pi}\int_{r=R-x}^{R+x} e^{-r} r\cos^{-1}\big(\frac{x^2+r^2-R^2}{2rx}\big)\, dr}.
\end{aligned}$$

□

Now, if we scale a large finite grid points inside a disk $\ddot{D}_n$ by scale factor

$\tau > 0$, then the 0-spread of $\tau\ddot{D}_n$ defined by the Definition 2.4.1 as

$$E_0(\tau\ddot{D}_n) = \sum_{i=1}^{n^2} \frac{1}{\sum\limits_{j=1}^{n^2} e^{-\tau d(p_i,\, p_j)}},$$

where the distance between the points $d(p_i,\, p_j)$ is the usual distance in Euclidean space.

Now, if the scale factor $\tau > 0$ is very small, then the points of $\ddot{D}_n$ will be very close to each other for a large number of points, then the square grid inside the circle $\ddot{D}_n$ can be approximated to a solid disk D with length sides 1. So, the disk D can be approximated by an grid of points inside disk $\tau\ddot{Q}_n$.

Next, we show that the 0-spread of the $\tau\ddot{D}_n$ is numerical approximations to some quadratic function of τ.

Remark 5.1.3. If a large finite grid points inside disk metric space $\ddot{D}_n$ is scaled by a very small factor τ, then there is a function f of τ such that

$$E_0(\tau\ddot{D}_n) \;\to\; f(\tau) \qquad \text{as} \qquad n \to \infty.$$

Since the points of $\ddot{D}_n$ will be very close to each other for the large number of points and small scale factor, then the grid points inside $\ddot{D}_n$ can be approximated to the disc D. So, by the proof of Theorem 5.1.2,

$$E_0(\tau\ddot{D}_n) \to \int_{x=0}^{R} \frac{x\,dx}{\int_{r=0}^{R-x} e^{-r} r\,dr + \frac{1}{\pi}\int_{r=R-x}^{R+x} e^{-r} r \cos^{-1}(\frac{x^2+r^2-R^2}{2rx})\,dr}.$$

We use Matlab (see Appendix C.1) to calculate this integral for various values of τ ranging from 0.0001 to 5. We have used polynomial curve fitting in Python, which involves finding the best polynomials to fit the data to obtain the quadratic formula

$$0.8\tau^2 + 1.43\tau + 1.02. \tag{5.2}$$

Willerton (See [55]) approximated a finite grid of points $\ddot{D}$ to a circle D of radius 1, then numerically calculated the magnitude of $\ddot{D}$ scaled by a factor of τ and plotted that magnitude and the penguin valuation (see end of Section 3.2) of τD together (see [Figure 5, [55]]). Now we plotted the Expression 5.2 with the penguin valuation of $\tau D = \frac{\tau^2}{2} + \frac{\pi\tau}{2} + 1$ as seen the Figure 5.3.

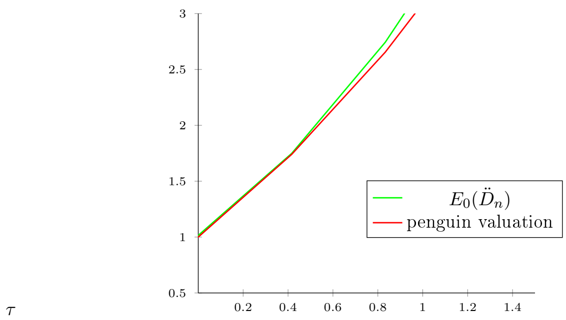


Figure 5.3: Comparison of the 0-spread of the disc with the penguin valuation $\frac{\tau^2}{2} + \frac{\pi}{2}\tau + 1$.

§ 5.2 The 0-spread dimension for various rectangular grid

In Section 3.1, we found the 0-spread dimension of square grids with 60×60, 110×110 and 160×160 points as the growth rate of the 0-spread of the square. In this section, we will present the concept of 0-spread dimension of two types rectangular grid metric spaces which is the instantaneous growth rate of the 0-spread of the metric space. This concept is a scale-dependent dimension, as we will see that the rectangular grids can have 0-spread dimension close to zero, one, or two, depending on the scale.

It is informative to look at the 0-spread dimension as rectangular grids is scaled. We used a number of computer calculations, as performed using Maple (see Appendix C.2). Firstly, starting with the 0-spread dimensions of 1×1600, 1×6400 and 1×14400, we notice that if the points are very close to each other, the 0-spread dimension is close to zero, then the line at that scale is look like a point. However, when the line of points is scaled up, it looks more and more like a line, the 0-spread dimension is close to one. Moreover, when the line of points is scaled up further and further, the 0-spread dimension drops to zero as shown in Figure 5.4.

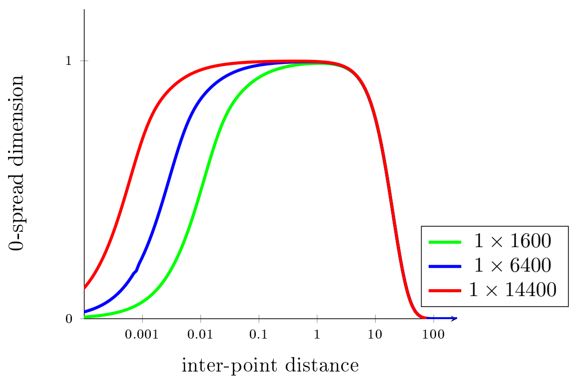


Figure 5.4: The 0-spread dimensions of various lines at different scaling.

Secondly, we will look at the 0-spread dimension of the rectangular grids with 20×80, 20×320 and 20×720 points. Again, at small scales the 0-spread dimension is close to zero while the grid looks like a small point. Then when it is scaled up there is a regime, where the large space 20×720 looks like a line and the 0-spread dimension is approximately one. Whilst, if it is scaled up more, then the width is apparent and the 0-spread dimension heads towards two. Finally, if it is scaled up even more, then the point-like nature becomes apparent and the 0-spread dimension descends to zero as can be represented in Figure 5.5.

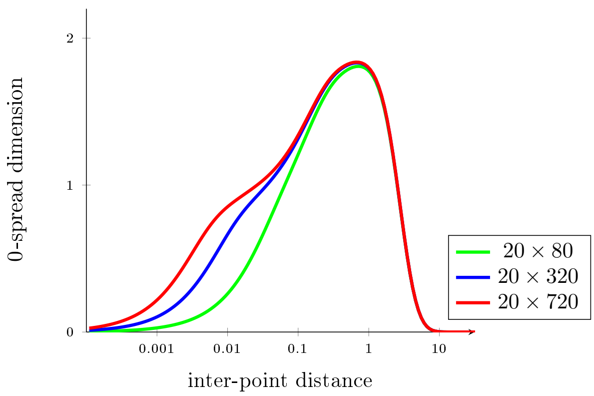


Figure 5.5: The 0-spread dimensions of different rectangle grids at various scaling.

Finally, we can plotted the 0-spread dimension of three cases of rectangular grids with equally spaced points together as shown in Figure 5.10.

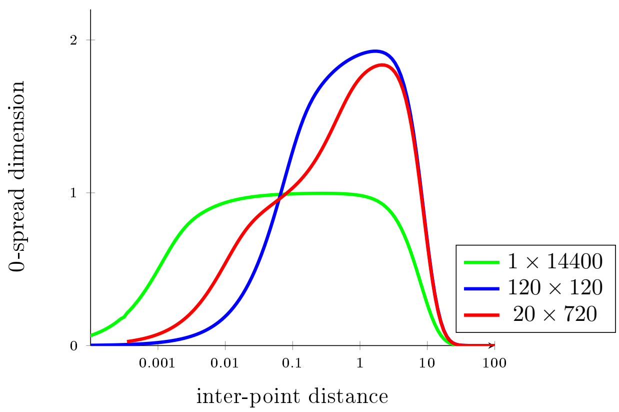


Figure 5.6: The 0-spread dimensions of various rectangle grids with 14400 points.

Furthermore, from figures 5.4 and 5.5, we can see that the 0-spread dimensions of those rectangular grids become closer and closer for sufficiently large τ, also we see from Figure 5.6 that the 0-spread dimensions of 20×720 and 120×120 rectangular grids become closer and closer and approximately independent of the number of points, as the scale factor getting bigger..

§ 5.3 The magnitude dimension for various rectangular grid

In this section, we will present the concept of the magnitude dimension of various rectangular grid metric spaces which is defined as follows

Definition 5.3.1. (see [40]) The magnitude dimension $\dim(|A|)$ of a metric space A is the instantaneous growth of its magnitude function.

$$\dim(|A|) = \lim_{t \to \infty} \frac{\log(|tA|)}{\log(t)}.$$

This concept of dimension is scale-dependent. For example, depending on the scale, the points can have a magnitude dimension close to zero, one, or two. We look at three types of rectangular grids and the magnitude dimension at various lengths can then be computed numerically using Krylov method in Python (See Appendix C.3). Firstly beginning with the magnitude dimensions of various lines with 1×1600, 1×6400 and 1×14400 points, we see that when the points are very close together the magnitude dimension is close to zero, so the line at that scale is point-like. As the line of points is scaled up, it looks more and more like a line, the magnitude dimension is close to one. As the line of points is scaled up further and further, the magnitude dimension drops to zero again as can be represented in Figure 5.7.

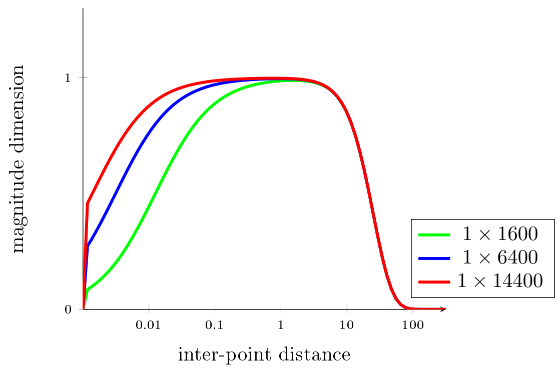


Figure 5.7: The magnitude dimensions of various lines at different scales.

It looks like the computation method breaks down when the scale factor is very small in Figure 5.7. Then, we compute the magnitude dimension of the rectangular grids with 20×80, 20×320 and 20×720 points. Again, at very small scales the magnitude dimension is close to zero whilst the grid looks like a small point. After that as it is scaled up there is a regime, where the large space looks line-like and the dimension is approximately one. when it is scaled up further, the width is apparent and the magnitude dimension heads towards two. Then, as it is scaled up further, the point-like nature becomes apparent and the magnitude dimension descends to zero as can be seen in Figure 5.8.

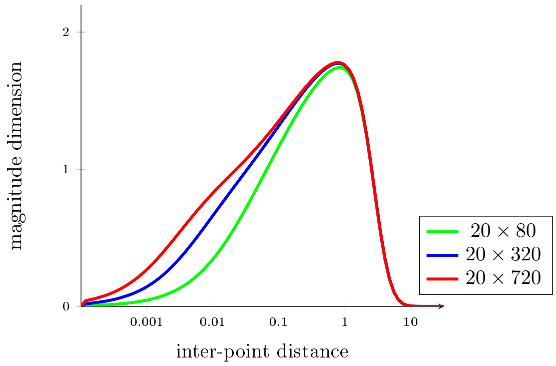


Figure 5.8: The magnitude dimensions of 20×80, 20×320 and 20×720 rectangle grids at various scales.

Finally, we find the magnitude dimension of the square grids with 40×40, 80×80 and 120×120 points, we see that this starts off looking like a point at small scales, with the magnitude dimension being close to zero, after that as the square grid is scaled up, it looks more like a genuine square and has a magnitude dimension of just under two. Thereafter as the square grid is scaled up further, the point-like nature is apparent and the magnitude dimension drops to zero as can be shown in Figure 5.9.

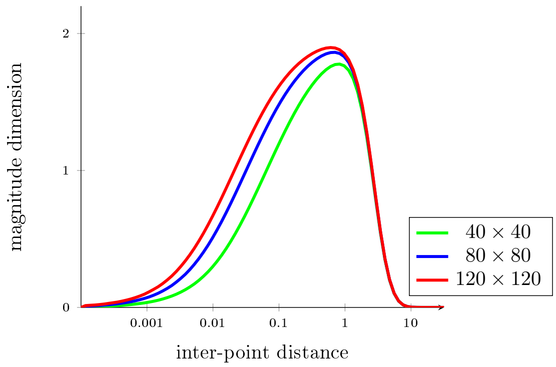


Figure 5.9: The magnitude dimensions of various $n \times n$ square grids at different scales.

Now we can look at the magnitude dimension of three types of rectangular grids with 14400 points as shown in Figure 5.10.

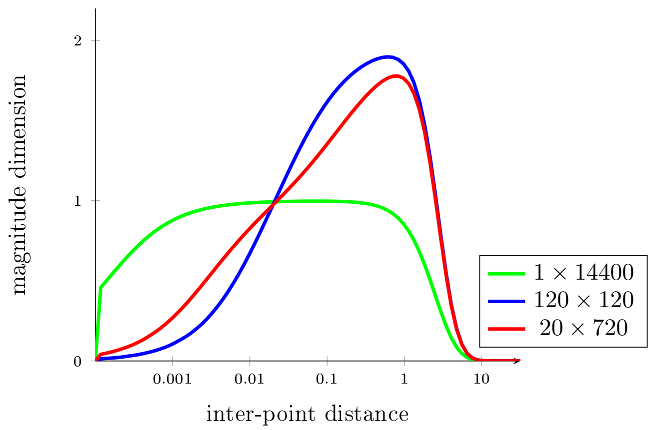


Figure 5.10: The magnitude dimensions of various rectangle grids with 14400 points.

In additional, from Figures 5.7, 5.8 and 5.9, we find out that the magnitude dimensions of those rectangular grids become closer and closer when the scale factor is getting bigger, and we see from Figure 5.10 that the magnitude dimensions of 20×720 and 120×120 rectangular grids get closer and closer which are approximately independent of the number of points, for sufficiently large scale factor τ.

Also, we plotted the 0-spread and the magnitude of the 40×40 grid square metric space at different scaling as shown in the figure 5.11. From

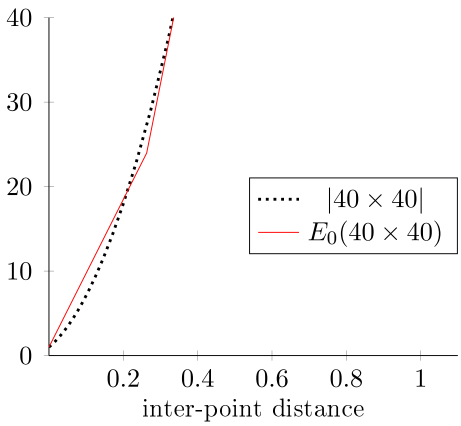


Figure 5.11: The magnitude and the 0-spread of a 40×40 grid square metric space at various scales.

above figure, we see that when the scale factor is bigger than one, then the 0-spread and magnitude of the 40×40 grid square metric space get closer and closer together. So the 0-spread dimension and the magnitude dimension of grid square with 40×40 points are also identical when the scale factor is bigger than one as seen in the figure 5.12.

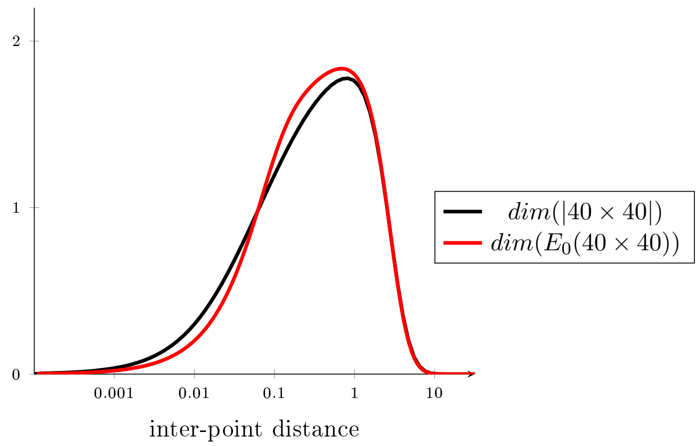


Figure 5.12: The magnitude dimension and the spread dimension of grid square with 1600 points.

This happen because by Proposition 3.1.1, the 40×40 grid square metric space is homogeneous and by Theorem 2.6.3, their magnitude and 0-spread are similar.

§ 5.4 Future works

- In Section 4.2, we compute the subsets of $n \times n$ square grids, for $n = 3, \ldots, 10$ at different scaling that have maximum magnitude with non-negative weighting to be maximum diversity and we see that those subsets are always orbits or union of such orbits. This implies that the maximum diversity occurred for orbits, or unions of such orbits. So we conjectured that maximum diversity of $n \times n$ grid square always comes from symmetric subsets and union of symmetric subsets.

- In Section 4.4, we compute the weights of the points in the middle row of the 201×201 metric space using the Krylov method at different scaling factors t, then we look at their behavior. We will explain why this happens in the future.

- In Sections 3.1 and 5.3, we plotted the 0-spread dimension and magnitude dimension of various rectangular grids (see Figures 5.4, 5.5, 5.7, 5.8, 5.9) at different scaling. We see that when the scale factor is big than 1, then the 0-spread dimension and magnitude dimension of those rectangular grids are identical. We will explain why this happens in the future.

- In Section 5.2, we plotted the 0-spread dimension of 20×720 and 120×120 rectangular grids at various scaling (see Figure 5.6) and we see that the 0-spread dimension of those rectangular grids get closer and closer and approximately independent of the number of points, as the scale factor bigger than one. We will explain why this happens in the future.

- In Section 5.3, we plotted the magnitude dimension of rectangular grids with 14400 points at various scaling (see Figure 5.12) and we see that the magnitude dimension of those rectangular grids become closer and closer and approximately independent of the number of points for sufficiently large scale factor. We will explain why this happens in the future.

Appendix A

Numerical computation of the q-spread dimension of a metric space

The computer codes described in this chapter is used in Chapter 3 to determine the q-spread dimension of the square grid metric space and the heuristic q-spread dimension. This chapter is divided into two sections. The first section computes the q-spread, q-spread dimension and we approximate the q-spread of the large square grid to the q-spread of a small square grid such as 10×10. The second section computes the heuristic 0-spread, the heuristic 1-spread and the heuristic 2-spread, respectively.

§ A.1 Finding the q-spread of the square grid

The computer code was used to identify the q-spread for a finite metric space which has an $n \times n$ square grid of points such that the distance between any two points is the usual distance in Euclidean space.

Now, if n is an even number, then the points of the grid square can be partitioned into four equivalent parts under the action of a subgroup of order four of the symmetry group of the square containing the rotation of the points by $0°$ and $180°$ and reflection of the points about the y-axis, and the x-axis about the midpoint. After that, we create a procedure to compute these symmetries of the square and return the image of a point under them.

We create a new subset and calculate these symmetric images for each point in the set of square grid points and for each of the above four symmetries of the square. This image is added to the new subset and removed from that set of points and the above process repeated until the set of square grid points becomes empty. Thus by a process of exhaustion, we partition the grid points into orbits for the action of the subgroup.

If we choose a representative from each orbit for the action of the subgroup, then we will get one of the four equivalent pieces. For instance, if a 4×4 square grid is $\{[i\,,\,j]:\ 1 \leq i, j\ \leq\ 4\}$. The orbits are

$$\{[1,1],[4,4],[4,1],[1,4]\},\{[1,2],[4,3],[4,2],[1,3]\},$$
$$\{[2,1],[3,4],[3,1],[2,4]\},\{[2,2],[3,3],[3,2],[2,3]\}.$$

Now, we select one point from each of the above orbits in order to get the four parts that partition A, which are

$$\{[1,1],[1,2],[2,1],[2,2]\},\{[4,4],[4,3],[3,4],[3,3]\},$$
$$\{[4,1],[4,2],[3,1],[3,2]\},\{[1,4],[1,3],[2,4],[2,3]\}.$$

Then the q-spread (see Definition 2.4.1) of one of these parts of A for $q = 0, 1, 2$ can be found for different scales of t and the result multiplied by four to get the q-spread of A. After that, convert these results to the data and put them to the text file.

A simple piece of the Maple code is given below:

```
# load  packages,
with(LinearAlgebra):
with(plots):

# Define $n^2$ points and put them in a   matrix A.

A[i, j] := [i,  j]:

# Define four symmetries of the square

# The identity rotation,

R[0] := proc(p) return[p[1], p[2]]; end proc:

# The 180 degree rotation,

R[1] := proc(p)return[(n+1)-p[1], (n+1)-p[2]]; end proc:

# Reflection through the $y$-axis,

R[2] := proc(p) return[(n+1)-p[1], p[2]];  end proc:

# Reflection through the $x$-axis,

R[3] := proc(p) return[p[1], (n+1)-p[2]]; end proc:

# Convert the matrix of points $A$ to a set,
```

```
original_list_of_points := convert(A, set):

# First, we consider an empty subset and
# consider p is the first point in the set A,
# then add the image of symmetry of square of a
# point p  in a subset, and removed from A,
# and repeated the process again until the set A
# is empty.

k := 1:
while original_list_of_points <> {} do
subset[k] := []:
p := original_list_of_points[1];
for i from 0 to 3 do
subset[k] := [op(subset[k]), R[i](p)];
end do;
original_list_of_points := original_list_of_points
minus {R[0](p), R[1](p), R[2](p), R[3](p)}:
newsubset[k] := subset[k];
k := k + 1:
end do:

# k-1 is the number of subsets that we obtained
# from  the partition A,

# calculate q-spread Eq for q = 0, 1, 2,

E_0 := 4*add(1/add(add(exp(-t*Distance(
       newsubset[i][1], A[j][c])), c = 1..n),
       j = 1..n ), i = 1..k-1):

E_1 := n^2*mul(1/add(add(exp(-t*Distance(
       newsubset[i][1], A[j][c])), c = 1..n),
       j = 1..n)^(4/n^2), i = 1..k-1):

E_2 := n^4/(4*(add(add(add(exp(-t*Distance(
       newsubset[i][1], A[j][c])), c = 1..n),
       j = 1..n), i = 1..k-1))):

# The text file for the E0 loglog data and
# the other q-spread are the same.
# l is the number of points of the square grid
```

```
stem := "/home/smp13sam/maple11/":
data_E0 := sprintf("0_spread_of_grid_%g.txt", l);
fopen(cat(stem, data_E0), WRITE):
pdata[l] := loglogplot(E0[l], t = 0.0001 .. 1000);
writedata(data_E0, convert(op(1, op(1, pdata[l])),
matrix), [float, float]);
```

The q-spread of different n is converted to the data in the text file. We use these to evaluate the q-spread dimension.

A.1.1 Approximating the q- spread dimension of a square grid

The Maple code was used to determine the q-spread dimension for $n \times n$ square grid A in Section ??. We have some expression for $E_q(tA)$ from Section A.

There are two approaches to calculate the q-spread dimension (see Definition 3.0.1).

- Get Maple to compute the logarithmic derivative of the q-spread of the square grid A as $t > 0$

$$dim_q(tA) = \frac{d(\log(E_q(tA)))}{d(\log(t))}.$$

- We read the q-spread text file from Section A and use these data to approximate derivative to be

$$dim_q(t_iA) = \frac{E_q(t_{i-1}A) - E_q(t_{i+1}A)}{t_{i-1} - t_{i+1}},$$

  where $i = 2, \ldots, 199$ are the numbers of the data in the text file.

  After that, we put the dimension data with the data representing t in a text file and get latex to plot it.

The code below is for a 0-spread. Furthermore, other q-spread code are identified in the same manner.

```
# Read the text file that contains the $q$-spread data
# with $t$ data,

data_E0 := sprintf("0_spread_of_grid_%g.txt");
data:=readdata(data_E0, 2);

# Evaluate the dimension $q$ spread,
# where i is the number of data in the text file,

for i from 2 to 199 do
```

```
dim[i] := (data[i-1][2] - data[i+1][2])/
(data[i-1][1] - data[i+1][1]):
end do:
dim_data := {seq([data][i][1], dim[i]], i = 2..199)};

# Open a text file and write the data to it

data_dim_E0 :=  sprintf("dimension_0_spread.txt");
fopen(cat(stem, data_dim_E0), WRITE):
writedata(file, convert(dim_data, listlist),
[float, float]);
end do:
```

A.1.2 Estimate q-spread of a square grid

The below Maple code is described in Section 3 to compare the q-spread of an $n \times n$ grid square A divided by the number of points n^2 with the estimated q-spread B for a 10×10 grid square such that contains the square with a length-side of one, as seen in Formula 3.1.

$$E_q(tB) = \frac{1}{\sum_{i=1}^{10} \sum_{j=1}^{10} e^{-td((a,b),(c_i,d_j))}},$$

where (a, b) is the point nearest to the middle of the square grid, say $(\frac{n}{2} + 1, \frac{n}{2} + 1)$ and (c_i, d_j) are finite points of A around (a, b). Also, we compute the estimated q-spread dimension for a 10×10 grid square B using the logarithmic derivative of the estimated q-spread. Then, each of the above calculations is converted to data and saved into a text file. Get Latex to plot these data.

The program code below is for a 0-spread, and the other q-spread code are the same. Also the code to find the four subsets are same as the code in Section A

```
E0/n^2 :=
(4*add(1/add(add(exp(-t*Distance(Subset[i][1], A[j][c])),
c = 1..n), j = 1..n), i = 1..k-1))/n^2:
# stem is the location where the text file can be saved.
stem := "/home/smp13sam/maple14/":
f_0 := sprintf("0spread_dividedofnumberofpoint.txt");
fopen(cat(stem, f_0), WRITE):
data := loglogplot(E0, t = 0.0001..1000);
writedata(f_0, convert(op(1, op(1, data)),
matrix), [float, float]):
```

```
estimate_E0 :=
1/add(add(exp(-t*Distance([n/2, n/2],  B[j][c])),
c = 1..10), j = 1..10);
approximate_spread:=
          loglogplot(estimate_E0, t = 0.001..1000):
f_1:=sprintf("estimate_E0.txt");
fopen(cat(stem, f_1), WRITE):
writedata(f_1, convert(op(1, op(1, approximate_spread)),
                               matrix), [float, float]):

estimate_dimension_E0 :=
t*(add(add(exp(-t*Distance([n/2, n/2], B[j][c]))*
Distance([n/2, n/2], B[j][c]), c = 1..10), j = 1..10))/
add(add(exp(-t*Distance([n/2, n/2], B[j][c])),
c = 1..10), j = 1..10):
approximate_dimension :=
loglogplot(estimate_dimension_E0, t = 0.001..1000):
f_2:=sprintf("approximate_dimension.txt");
fopen(cat(stem, f_2), WRITE):
writedata(f_2,
         convert(op(1, op(1, approximate_dimension)),
                            matrix), [float, float]):
```

To achieve a better approximation, we need to take a sufficiently large number of points. The main constraints on how large a number of points one can reasonably consider are the computational time and the memory available. I have used the Iceberg at the University of Sheffield to run my programs, choosing the number of points 60×60, 110×110 and 160×160. This program used about 9GB to 90GB of RAM and could take between 9 to 64 hours to evaluate a q-spread at different scales.

§ A.2 Calculation of a heuristic q-spread dimension

The code in this section is used in Section 3.2 to calculate the heuristic q-spread. All the code used are the same as those in Appendix A, but rather than scale A by a factor t, it is instead scaled by a factor τ, where $\tau = \frac{t}{n-1}$, to calculate the q-spread and the q-spread dimension, for $q = 0, 1, 2$.

A.2.1 Heuristic 0-spread

The 0-spread of the square grid by the proof of Theorem 3.2.1 is

$$\int_{a=0}^{1}\int_{b=0}^{1} \frac{1}{\int\limits_{a'=0}^{1}\int\limits_{b'=0}^{1} e^{-\tau\sqrt{(a-a')^2+(b-b')^2}}\,da'\,db'}\,da\,db.$$

The MATLAB code used to calculate the above integral for different values of τ are:

```
# Let i be an initial point,
# We will running the same  block of code
# several times, each time with a different value used
# to perform a loop.
i = 1
for tau = 0.0001: 0.001 : 5
result_integral(i) =
integral2(@(a, a')arrayfun(@(a, b)1./integral2(
@(a', b')exp(-tau.*sqrt((a - a').^2 + (b - b').^2)),
0 , 1, 0, 1), a, a'), 0, 1, 0, 1);
i = i + 1;
end
```

Further, the above integration is computed through the width of the square scaled by τ.

```
i = 1;
for tau = 0.0001: 0.01 : 5
result_integral(i) =
integral2(@(a, b)arrayfun(@(a, a')1./integral2(
@(a', b')exp(-sqrt((a - a').^2 + (b - b').^2)),
0 , tau, 0, tau), a, a'), 0, tau, 0, tau);
i = i + 1;
end
```

In both cases we obtain the same result.

A.2.2 Heuristic 1-spread

The 1-spread, by the proof of Theorem 3.2.3, is:

$$e^{\int\limits_{a=0}^{1}\int\limits_{b=0}^{1} \ln\left(\frac{1}{\int\limits_{a'=0}^{1}\int\limits_{b'=0}^{1} e^{-\tau\sqrt{(a-a')^2+(b-b')^2}}\,da'\,db'}\right)da\,db}.$$

The MATLAB code used to evaluate this integral is given by:

```
function result = shint4(a, b)
k = 0;
L = length(a : 0.01 : b);
result = zeros(1, L);
for tau = a : 0.01 : b
k = k + 1;
result(k) = exp(integral2(@(x1, x2)arrayfun(@(x1, x2)
            log(1./integral2(@(y1, y2)exp(-tau.*
            sqrt((x1 - y1).^2 + (x2 - y2).^2)),
            0, 1, 0, 1)), x1, x2), 0, 1, 0, 1));
end
end
```

A.2.3 Heuristic 2-spread

By proof of Theorem 3.2.5, the 2-spread is:

$$\frac{1}{\int\limits_{a=0}^{1}\int\limits_{b=0}^{1}\int\limits_{a=0}^{1}\int\limits_{b'=0}^{1} e^{-\tau\sqrt{(a-a')^2+(b-b')^2}}\,da'\,db'\,da\,db}$$

The MATLAB code used to find this integral is given by:

```
function result = shint3(a, b, h)
i = 0;
tau = length(a : h : b);
result = zeros(1, L);
for tau = a : h : b
i = i + 1;
rr = (integral2(@(x1, x2)arrayfun(@(x1,  x2)(integral2(
     @(y1,y2)exp(-tau.*sqrt((x1-y1).^2+(x2 -y2).^2))
     , 0, 1, 0, 1)), x1, x2), 0, 1, 0, 1));
result(i) = 1/rr;
end
end
```

Appendix B

Computation to find the maximum diversity for a grid square metric space

In this chapter, we consider some of the forms of code that can be used in Chapter 4. We have divided this chapter into three sections. The first section focuses on the code used to find the magnitude of all subsets of a square grid with non-negative weighting, then recorded all of those magnitudes that admits non-negative weightings to have a maximum magnitude which is equal to a maximum diversity. In the second section, we find the symmetric subsets under the group of action, then find the magnitude of each of these orbits for a square grid, which we then plotted together to obtain the critical values for these orbits, and we also compare the magnitude of all of these orbits and their union to obtain the largest magnitudes at different scaling. The last section evaluates the weighting of the points in the middle row of the 201×201 grid square at various scales.

§ B.1 Determining the subsets of the $n \times n$ square grid that have a maximum magnitude with non-negative weightings

We have programming code to find a maximum diversity for $n \times n$ grid square such that the distance between its points is the usual distance in Euclidean space.

Assume that A is a metric space with $n \times n$ matrix of points called $p_1, \ldots, p_{n^2}$ where p_i is a pair of numbers $[x, y]$ for $i = 1. \cdots n^2$ and x, y are points in x-axis and y-axis respectively such that $p_1 = [1, 1]$ and $p_{n^2} = [n, n]$ and let tA be the metric space A with the metric d scaled up by a factor of t, for $t > 0$.

Define Z to be $n^2 \times n^2$ matrix whose rows and columns are indexed by the points of A and (p_i, p_j)-entry of Z is $Z_{p_i p_j} = e^{-td(p_i, p_j)}$ where $td(p_i, p_j)$

is a distance between the point p_i and the point p_j in A scaled by a factor t, where **Distance** is a distance function in Maple which tends (p_i, p_j) to

$$\sqrt{(p_i[1] - p_j[1])^2 + (p_i[2] - p_j[2])^2}.$$

Also define the column vector weights $w = (w_{p_1}, \ldots, w_{p_{n^2}})$ that satisfy the weighting equation $Zw = (1, \ldots, 1)^T$ where $(1, \ldots, 1)^T$ is a transpose of $(1, \ldots, 1)$ which are n^2 equations with n^2 unknowns variables. and add up the entries of w together to obtain the magnitude of A.

Now to evaluate the maximum diversity of A we will check all entries of w. If all entries of w are non-negative, then the maximum diversity of A is equal to the its magnitude. However if there are some non-positive entries, then we will check all subsets of A. For each of those subsets we define the exponential distance matrix Z_B and find the weight equation of it, then using some linear algebra to decide whether Z_B has non-negative weighting and if it does, then record its magnitude and the maximum of all the recorded magnitude of B is equal to the maximum diversity of A.

Here is some useful Maple code:

```
# load  packages,

with(LinearAlgebra):
with(combinat);

# Define the exponential matrix Z

A := Matrix(n, n, 0):
for i from 1 to n do
for j from 1 to n do
A[i, j] := [i, j];
end do;
end do;
listofpoints := convert(A, list):
M := Matrix(nops(listofpoints), nops(listofpoints),
                                shape = symmetric):
for i from 1 to nops(listofpoints) do
for j from 1 to i do
M[i, j] := Distance(A(i), A(j));
end do;
end do;
Z := map(x->exp(-t*x), M):
# Finding the weightings and the magnitude
W:=LinearSolve(Z, Vector(nops(listofpoints), 1)):
Magnitude:= add(W[i],  i = 1..nops(listofpoints)):
```

```
B := 0:
a := 0:
Listofsubsets := subsets(listofpoints);
weight_is_negative := false:
max_magnitude_B := 0:
while`not`(Listofsubsets[finished])do
d := Listofsubsets[nextvalue]():
M_B:=Matrix(nops(d),nops(d)):
for i from 1 to nops(d) do
for j from 1 to nops(d) do
M_B[i, j] := Distance(d[i], d[j]):
end do:
end do:
Z_B := map(x -> exp(-t*x), M_B):
W_B :=
 LinearSolve(subs(t=0.9, Z_B), Vector(nops(d), 1)):
for i in W_B do
if i < 0 then
weight_is_negative := true:
end if:
od:
if weight_is_negative = false then
magnitude_B := simplify(add(W_B[i], i = 1..nops(d))):
if magnitude_B > max_magnitude_B then
max_magnitude_B := magnitude_B:
B := d:
end if:
end if:
weight_is_negative := false:
a := a + 1:
end do:
```

We calculate the maximum diversity of the 3×3 and 4×4 metric spaces at different scales. However, we have used Iceberg, to run these code for 5×5, 6×6, $\ldots$ square grids at various scaling. Whereas, the program used about 65GB of RAM and take about 85 hours to determine the maximum diversity of the all subsets of those square grids at the selected small scale factor t, but we did not get the result. Therefore, we are thinking of the symmetric subsets of the square grid which have a maximum magnitude as explained in the next section.

§ B.2 Determining the orbits of the square grid which have a maximum magnitude with non-negative weights

The programming code involved in identifying the maximum diversity for a metric space with an $n \times n$ square grid of points with the usual Euclidean distance between any two points. Consider a metric space A with points $p_{11}, p_{21}, \ldots, p_{nn}$ scaled by a factor $t > 0$, where

$$p_{ij} = [i, j]$$

for $i, j = 1, 2, \ldots, n$.

To evaluate a weighting for these points, we need to partition the points of square grid into a number of parts under the eight-fold symmetry group of the square: an identity rotation, a $90°$ rotation, a rotation of $180°$, a rotation by $270°$, a flip about horizontal axis, a flip about the vertical axis, a flip about the main diagonal and a flip about the other diagonals.

Let $[a, b]$ be any point of A and let $[\frac{n+1}{2}, \frac{n+1}{2}]$ be the midpoint of A. Now, rotations and reflections of $[a, b]$ about a midpoint that is not at the origin are:

1. The identity rotation of $[a, b]$ about the midpoint is $[a, b]$,
2. If $[a, b]$ is rotated $90°$ anticlockwise about the midpoint, its image is
$$[\frac{n+1}{2}, \frac{n+1}{2}] + R_{90}\Big[[a, b] - [\frac{n+1}{2}, \frac{n+1}{2}]\Big] = [(n+1) - b, a],$$
3. If $[a, b]$ is rotated clockwise through $180°$ about the midpoint, its image is
$$[\frac{n+1}{2}, \frac{n+1}{2}] + R_{180}\Big[[a, b] - [\frac{n+1}{2}, \frac{n+1}{2}]\Big] = [(n+1) - a, (n+1) - b],$$
4. The image of $[a, b]$ after a $270°$ clockwise rotation about the midpoint is
$$[\frac{n+1}{2}, \frac{n+1}{2}] + R_{270}\Big[[a, b] - [\frac{n+1}{2}, \frac{n+1}{2}]\Big] = [b, (n+1) - a],$$
5. If $[a, b]$ is reflected about the x-axis (horizontal) through the midpoint, its image is
$$[\frac{n+1}{2}, \frac{n+1}{2}] + R_{h}\Big[[a, b] - [\frac{n+1}{2}, \frac{n+1}{2}]\Big] = [a, (n+1) - b],$$
6. When $[a, b]$ is reflected through the y-axis (vertical) about the midpoint, its image is
$$[\frac{n+1}{2}, \frac{n+1}{2}] + R_{v}\Big[[a, b] - [\frac{n+1}{2}, \frac{n+1}{2}]\Big] = [(n+1) - a, b],$$

7. If $[a, b]$ is reflected about the main diagonal $y = x$ about the midpoint, then its image is

$$[\frac{n+1}{2}, \frac{n+1}{2}] + R_{d1}\Big[[a, b] - [\frac{n+1}{2}, \frac{n+1}{2}]\Big] = [b, a],$$

8. The image of $[a, b]$ reflected through the diagonal line $y = -x$ about the midpoint is

$$[\frac{n+1}{2}, \frac{n+1}{2}] + R_{d2}\Big[[a, b] - [\frac{n+1}{2}, \frac{n+1}{2}]\Big] = [(n+1) - b, (n+1) - a].$$

We will first describe the procedures to compute these symmetries of the square and return a symmetric point. Secondly, we will create a new set and convert the points of A to a set referred to as the original list of points; for every point in the original list of points and for each of the above eight symmetries of the square, we determine the symmetric image of that point. We then add the image to the new set and delete it from the original list. The new set contains the disjointed orbits of A, then the next step is to find the weight equations for the first point in each orbit, then solve these weight equations for w.

1. If all entries in w are non-negative, then the maximum diversity of A is equal to its magnitude.
2. If there are some negative entries in w, then we check the subsets B of the new set by defining the exponential distance matrix Z_B, and then
   - Use linear algebra to decide whether Z_B has a non-negative weighting.
   - If it does, then record the magnitude of Z_B, which is equal to the sum of the weighting entries.

   Finally, the magnitude of the maximum Z_B recorded that have non-negative weightings is equal to the maximum diversity.

Some useful Maple code is given below:

```
# load  packages,

with(LinearAlgebra):
with(plots):
with(combinat):

# Define an $n \times n$ matrix of points.
# for i, j from 1 to n,
```

```
A[i, j] := [i, j];

# Define procedures that compute the symmetries of the
# square and return the image of the symmetric point,

sy[0] := proc(p) return[p[1], p[2]]; end proc:
sy[1] := proc(p) return[(n+1)-p[2], p[1]]; end proc:
sy[2] :=
   proc(p) return[(n+1)-p[1], (n+1)-p[2]]; end proc:
sy[3] := proc(p) return[p[2], (n+1)-p[1]]; end proc:
sy[4] := proc(p) return[(n+1)-p[1], p[2]]; end proc:
sy[5] := proc(p) return[p[1], (n+1)-p[2]]; end proc:
sy[6] :=
   proc(p) return[(n+1)-p[2], (n+1)-p[1]]; end proc:
sy[7] := proc(p) return[p[2], p[1]] end proc:

# To  identify orbits,  we want  to convert A  to
# the set,

original_list_of_points := convert(A, set):

# Let k be an initial point,
k := 1:
# To create a disjointed orbit
# Let p be the first point of the original set,
# First find the image of p,
# then removed the image of p from original set

while original_list_of_points <> {} do
new_subset[k] := []:
p := original_list_of_points[1];
for i from 0 to 7 do
if member(sy[i](p), s[k]) = false then
s[k] := [op(s[k]), sy[i](p)];
end if;
end do;
original_list_of_points :=
original_list_of_points minus
             {sy[0](p), sy[1](p), sy[2](p), sy[3](p),
             sy[4](p), sy[5](p), sy[6](p), sy[7](p)}:
subset[k] := new_subset[k];
k := k + 1:
end do:
```

```
# To evaluate the weight equations of k-1 new orbits,
# begin by finding the exponential distance between
# the first point of each orbit and other points of A
# and multiply by representative weight vector,
# after that solve these weight equations.

for i from 1 to k-1 do
for j from 1 to k-1 do
distance[j] :=
add(exp(-t*Distance(subset[i][1], subset[j][c]))*w[j],
c = 1..nops(subset[j]));
end do;
equation[i] := add(distance[j], j = 1..k-1) = 1;
end do:
a := 1:
weighting_of_subset := {}:
equation_subset := {}:
while a <> k do
equation_subset := equation_subset union{equation[a]};
weighting_of_subset := weighting_of_subset union {w[a]};
a := a + 1;
end do:
system := convert(equation_subset, list):
variable := convert(weighting_of_subset, list):
B, b := GenerateMatrix(system, variable):
weighting := LinearSolve(B, b):

# Plot the weightings for different values of t
plot([seq(weighting[i], i = 1..k-1)], t = 0..8);

# Multiply the number of points in each orbit by their
# weights, then add together to obtain the magnitude of A.

magnitude := add(nops(subset[i])*weighting[i], i = 1..k-1):
# To evaluate the maximum magnitude with non-negative weightings
# of the subsets of square grid at different values of t.
# Find the weights for each subset d and
# check if there are some negative weights, if yes,
# check another subset, while if not,
# evaluate the magnitude of that subset,
# where this process is repeated until the list of subsets
# become empty,
```

```
# Where max_d is a subset that takes a maximum magnitude,
max_d := []:
subweights := {}:
subequations := {}:
magnitude_of_subset := 0:
weight_is_negative := false:
List_of_subsets := subsets({seq(subset[i], i = 1..k-1)}):
while`not`(List_of_subsets[finished]) do
d := List_of_subsets[nextvalue]();
for i from 1 to nops(d) do
for j from 1 to nops(d) do
distance_of_subset[j] :=
add(exp(-t*Distance(d[i][1], d[j][c]))*w[j],
                                c = 1..nops(d[j])):
end do;
eq_of_subset[i] :=
     add(distance_of_subset[j], j = 1..nops(d)) = 1;
end do:
for e from 1 to nops(d) do
subequations := subequations union {eq_of_subset[e]};
subweights := subweights union {w[e]};
end do:
subsystem := convert(subequations, list):
subvariable := convert(subweights, list):
sB, sb := GenerateMatrix(subsystem, subvariable):
weighting_of_subset :=
          subs(t = 0.02, LinearSolve(sB, sb)):
for h in weighting_of_subset do
if h < 0 then
weight_is_negative := true:
end if:
end do:
print(weight_is_negative):
if weight_is_negative = false then
submagnitude :=
add(nops(d[i])*weighting_of_subset[i], i = 1..nops(d)):
if submagnitude > magnitude_of_subset then
magnitude_of_subset := submagnitude:
max_d := d;
end if;
end if;
weight_is_negative := false:
subequations := {}:
subweights := {}:
```

```
end do;
```

We have used Iceberg, the University of Sheffield's central high-performance computing resource, to run these code for different square grids of points between 3×3 to 10×10. The program used about 2GB to 95GB of RAM and could take between 1 to 100 hours to determine the maximum diversity of the square grid for various scale factors.

B.2.1 Determining the critical values of the magnitude of the symmetric subsets of the square grid

In the previous Appendix B.2, we identified all the symmetric subsets of square grids that have a maximum magnitude with non- negative weighting at different scales. We now evaluate the magnitude of each of these subsets and plot them together. Also, the critical values are calculated and the derivatives of these magnitudes at the (number of subsets -1) critical values are computed. For instance, the 3×3 grid square has three symmetric subsets, the following code is used to determine the magnitude of each subset and plot them together with the critical values and the derivatives of the magnitude formulae at the critical values.

```
# load of packages,
with(LinearAlgebra):
with(plots):

# Define the three subsets of the square grid
d1 := {[[1, 1], [3, 1], [3, 3], [1, 3]]}:
d2 := {[[1, 1], [3, 1], [3, 3], [1, 3]]} union
{[[1, 2], [2, 1], [3, 2], [2, 3]]}:
d3 := {[[2, 2]]} union {[[1, 1], [3, 1], [3, 3], [1, 3]]}
     union {[[1, 2], [2, 1], [3, 2], [2, 3]]}:
# Define the distance between the points in same subset
# and find a weight equation of these subsets
# k = 1, 2, 3

for i from 1 to nops(dk) do
for j from 1 to nops(dk) do
distance_of_subset_k[j] :=
add(exp(-t*Distance(dk[i][1], dk[j][c]))*w[j],
                                 c = 1..nops(dk[j])):
end do;
equation_k[i] :=
add(distance_of_subset_k[j], j = 1..nops(dk)) = 1;
end do:
equation_subset_k := {}:
```

```
weights_k := {}:
for e from 1 to nops(dk) do
equation_subset_k :=
equation_subset_k union {equation_k[e]};
weights_k := weights_k union {w[e]};
end do:
system_subset_k := convert(equation_subset_k, list):
variable_subset_k := convert(weights_k, list):
sBk, sbk :=
GenerateMatrix(system_subset_k, variable_subset_k):
weighting_subset_k:=
simplify(LinearSolve(sBk, sbk));
magnitude_subsetk := simplify(
add(nops(dk[i])*weighting_subset_k[i], i = 1..nops(dk)));

# We identified the magnitude_subset1, magnitude_subset2,
# and magnitude_subset3. Then the critical values are

t0 := fsolve(
magnitude_subset2 - magnitude_subset1 = 0, t = 0..0.3);
# the result is t0 := 0.2321907228

t1 := fsolve(
magnitude_subset3 - magnitude_subset2 = 0, t = 0.1..1);
# the result is t1 := 0.8776945691

# plot the magnitude_subset1, magnitude_subset2, and
# magnitude_subset3 together

a1 : =plots[semilogplot](magnitude_subset1, t = 0..t0):
a2 := plots[semilogplot](magnitude_subset2, t = t0..t1):
a3 := plots[semilogplot](magnitude_subset3, t = t1..30):
display(a1, a2, a3);


#define the equations as functions
f1 := unapply(magnitude_subset1, t):
f2 := unapply(magnitude_subset2, t):
f3 := unapply(magnitude_subset3, t):

# The derivative of the  magnitude_subset1 at t0,
simplify(subs(x = t0, diff(f1(x), x)));
# The result is 2.066877690
```

```
# The derivative of the  magnitude_subset2 at t0,
simplify(subs(x = t0, diff(f2(x), x)));
# The result is 2.066877546

# The derivative of the  magnitude_subset2 at t1,
simplify(subs(x = t1, diff(f2(x), x)));
# The result is 2.713363781

# The derivative of the  magnitude_subset3 at t1,
simplify(subs(x = t1, diff(f3(x), x)));
# The result is 2.713363798
```

Also, we used Iceberg to run the above code for the square grids. The critical values for subsets of 3×3 to 6×6 were obtained which these take between 1 to 40 hours and use about 1GB to 35GB of RAM.

§ B.3 Determining the weighting of the middle row points for the square grid with the odd large number of points

The code in this section is used in Subsection 4.4 to evaluate the weighting of the points of the middle row of an $n \times n$ square grid metric space for large and odd-numbered n at different scaling from 0.000001 to 1. For each scale, we obtain the distance matrix for the points, then use the conjugate gradient method described in Subsection 2.7 to determine the weighting of the points of the metric space. After that, we create a vector of the weighting of the middle row points, then create a text file for that vector with the associated scale factor.

A simple segment of the Python code is given as follows

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.spatial
from krypy.linsys import LinearSystem, Cg
import sys
# l is a change from 1 to 20
l = sys.argv[1]
# Define the range of the scale factor t
t = int(10)**(-int(l)/5)

# The grid will be $n \times n$ points.
n = 201
N = n**2
print("Number of points is", N)
```

```
points = np.array([[i, j] for i in range(n)
          for j in range(n)])

# Obtain the distance matrix of the points.
D = scipy.spatial.distance.pdist(points, metric='euclidean')
D = scipy.spatial.distance.squareform(D)

# Give an initial guess of the weighthing to be fixed in to
# the algorithm.
w = np.ones(N)/N

# Calculate the magnitude for each t, iteratively feeding
# the previous weighting in as a start point.

linear_system = LinearSystem(np.exp(-t*D), np.ones(N),
                 self_adjoint=True, positive_definite = True)
w = Cg(linear_system,  x0 = w).xk

#""" Evalute the weighting of middle row points"""

middle_W = []
for i in range((n**2-(n-1))//2, (n**2-(n-1))//2+(n)):
middle_W.append(w[i])

# Creat a text file that contain the weighting
# of the points in the middle row
f = open("weighting_middle_row_201x201_%g.txt"
                                        % int(l), "w");
for W in middle_W:
f.write("{0}\t{1}\n".format(t, W[0]))
x = 0
for W in middle_W:
f.write("{0}\t{1}\n".format(x, W[0]))
x += t/(n-1)
```

We applied Iceberg, the University of Sheffield's central high-performance computing resource, to run these code for 201×201 square grid metric space. The program used about 37GB RAM and 7 minutes to find the weighting for the points of the middle row of 201×201 square grid at each scale.

Appendix C

Compute the 0-spread of the disk and the magnitude of the rectangular grid metric space

The computer code describes in this chapter is used in Chapter 5 to determine the 0-spread and the magnitude of various metric spaces.

§ C.1 Determining the 0-spread of the disk

The Matlab code in this section is used in Section 5.1 to calculate the 0-spread of the disk.

```
unction result1 = shint121(n, h)
k = 0;
L = length(5 : h : n);
result1 = zeros(1, L);
for R = 6 : h : n
k = k + 1;
f1 = @(x)arrayfun(@(x)(integral(@(r) r .* exp(-r),
                                    0, R - x)), x);
f2 = @(x)arrayfun(@(x)(integral(@(r) r .* exp(-r).*
    acos(( r.^2 + x.^2 - R.^2) / (2 .* x .* r)),
                             R - x, R + x)), x);
f = @(x)(x./(f1(x) + 1 ./ pi .* f2(x)));
result1(k) = integral(@(x)arrayfun(f, x), 0, R);
end
end
```

§ C.2 Determining the 0-spread of the rectangular grid metric space

The computer code was used to calculate the 0-spread (see Definition 2.4.1) for a finite metric space which has an $n \times m$ rectangular grid of points at different scaling.

A simple piece of the Maple code is given as:

```
# load  packages,
with(LinearAlgebra):
with(Student:-Precalculus):
n := 20:
m := 80:
A := Matrix(n, m, 0):
for i from 1 to n do
for j from 1 to m do
A[i, j] := [i, j];
end do;
end do;
E0 := add(1/add(add(exp(-t*Distance(A(i), A[j][c])),
            c = 1..m), j = 1..n), i = 1..n*m):
stem:="/home/smp13sam/maple8/spread_of_rectangle/":
with(plots):
f_1 := sprintf("spread_of_rectangle_1x%g.txt", m);
fopen(cat(stem, f_1), WRITE):
pdata := loglogplot(E0 , t = 0.00001..10000):
writedata(f_1, convert(op(1, op(1, pdata)), matrix),
                                 [float, float]):
```

The 0-spread of different n and m is converted to the data in the text file. We use these to evaluate the 0-spread dimension (see A.1.1).

§ C.3 Determining the magnitude of the rectangular grid metric space

The code in this section is used in Section 5.3 to identify the notion of magnitude dimension of different rectangular grid metric spaces which is the instantaneous growth rate of the magnitude of the spaces.

Firstly, the magnitude of various rectangular grids can be found at different scaling. Then, convert these results to the data and put them to the text file. After that, we used these data to determine the magnitude dimension

A simple segment of the Python code is given by

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.spatial
```

```
from krypy.linsys import LinearSystem, Cg
import sys
l = sys.argv[1]
# Define the range of the scale factor t
log_min = -4
log_max = 1.5
num_points = 81
log_t = np.linspace(log_min, log_max, num_points)
t = int(10)**log_t
# The grid will be $n \times m$ points.
n =l
m = l
N = n*m
print(n,m)
print("Number of points is", N)
points = np.array([[i, j] for i in range(n)
                               for j in range(m)])
# Obtain the distance matrix of the points.
D = scipy.spatial.distance.pdist(points,
                                metric='euclidean')
D = scipy.spatial.distance.squareform(D)
magnitude = np.zeros_like(t)
# Give an initial guess of the weighthing.
w = np.ones(N)/N
# Calculate the magnitude for each t, iteratively
# finding the previous weighting in as a start point.
for i in range(len(t)):
linear_system = LinearSystem(np.exp(-t[i]*D), np.ones(N),
self_adjoint = True, positive_definite = True)
w = Cg(linear_system,  x0 = w).xk
magnitude[i] = sum(w)
# Open a text file that contain the data of
the magnitude scales by a factor t
col_format = "{:<25}"*2 + "\n"# to left-justfied columns
# with 25 character width
f = open("magnitude_of_rectangle_grid_nxm_{0}.txt".
                                      format(N), "w")
for x in zip(t, magnitude):
f.write(col_format.format(*x))
f.close()
```

Now we will read the text file and evaluate the magnitude dimension as can be seen in the following Python code.

```
import numpy as np
```

```
import matplotlib.pyplot as plt
from os import listdir
N = 6400
log_min = -4
log_max = 1.5
num_points = 81
log_t = np.linspace(log_min, log_max, num_points)
t = int(10)**log_t
mag_file = []
f = open("magnitude_of_rectangle_grid_nxm_6400.txt", "r")
for line in f:
values = [float(s) for s in line.split()]
mag_file.append(values[1])
dimension = np.zeros_like(t)
for i in range(1, len(t) - 1):
dimension[i] =
      ((np.log10(mag_file[i+1]) - np.log10(mag_file[i-1])) /
      (log_t[i+1] - log_t[i-1]))
f1 =
open("mag_dimension_of_rectangle_nxm_{0}.txt".format(N), "w")
for i  in range(len(t)):
f1.write("{0}\t{1}\n".format(log_t[i], dimension[i]))
f1.close()
```

We used Iceberg, the University of Sheffield's central high-performance computing resource, to run these code for different rectangular grids. The program used between 3GB and 32GB RAM and between 2 and 8 minutes, to find the magnitude at various scaling.

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