Domestication effects on wheat morphology and production

The University of Sheffield

School of Bioscience

Yixiang Shan

Thesis for the degree of Doctor of Philosophy

September 2023

Student Number: 190182733

Acknowledgements

This work is funded by Sheffield–China Scholarships Council PhD Scholarship Programme.

I could not have completed my PhD without my supervisor, Prof. Colin Osborne. Colin is a mentor that I look up to. He is very knowledgeable in the field of plants. He gave me a lot of valuable scientific advice for my work. At the same time, he gave me a great deal of autonomy and respected my ideas, making me feel human. Thank you, Colin.

I also want to thank my family. My father and mother always support me to study aboard. My wife, Menghan Wang, has given me a lot of understanding and support throughout our time together in Sheffield.

I would also like to thank my friends in the School of Bioscience at the University of Sheffield; Bong and Karn, you were my best lab mates, and I will never forget the time we shared together on my PhD; Kim, Bobby, Mohammod, Sarah, Maggi and Ben, you were my most respected colleagues in the school; Luke, Rob, Gareth and Holly, you are all very popular mentors and thank you for your help on my work.

Outside of Sheffield University, I'd like to mention the following teachers, Prof. Jochem Evers at Wageningen University and Dr. Andrea Harper at the University of York. Thank you for your instructions on computing technologies.

Declaration

I declare that this dissertation is my own PhD work. The research chapters in each of these were designed by me in collaboration with my supervisor Prof. Colin Osborne. Some professors in other fields were consulted and referenced. Prof. Jochem Evers in Wageningen University helps to instruct modelling work in Chapter 3. Dr. Andrea Harper in University of York helps to instruct GWAS analysis in Chapter 4. Prof. Rob Freckleton in the University of Sheffield helps to instruct experiment design in Chapter 5.

The work on the experiments was all done by me personally. I received some help from fellow lab members and university research support staff, including transplanting wheat and harvesting. Much of the work on the experiment, especially the measurements and data collection, was done independently by me.

The writing of this manuscript was done by me in the first draft, with the help of my supervisor, Prof. Colin Osborne, for revisions and suggestions. References in which others are cited have been attributed. This paper has not been submitted to any other previous degree or professional qualification.

Abstract

Wheat is one of the world's most important food crops, and increasing wheat production is an important solution to hunger. From its ancient wheat ancestors to the edible modern varieties available to people today, wheat has undergone a long evolutionary process involving domestication, chromosome doubling, selective breeding, and the Green Revolution. During these historical processes, wheat morphology has changed dramatically. We have also found that wheat crop improvement can be achieved by domesticating the phenotype for the purpose of increasing yield. However, phenotypic improvement in wheat has encountered a number of difficulties. The most important of these is the domestication bottleneck. Namely, the wild traits of wheat have been lost in evolution and its germplasm pool has been shrinking in domestication selection.

Therefore, we conducted the present project focusing first on the wheat morphological traits that have emerged and disappeared during the evolutionary process. Secondly, we took the values of these traits that wheat had possessed and carried out modelling work to predict the ideal high yielding wheat based on existing trait variation. We also conducted experiments to investigate the loss of loci associated with certain yield traits in wheat during the evolution of domestication, as well as changes in individual competitiveness during wheat domestication.

The results showed that there was a loss of morphological traits in wheat during domestication, but natural selection and genetic mutations also created new domains of phenotypic trait values. Morphological traits of wheat showed different characteristics at different historical periods. Some traits have risen or declined in one direction during wheat evolution, others have changed only at certain stages; still others have shown opposite trends before and after the period. For one of the important wild traits, awns, we also found the locus associated with its disappearance during landrace improvement. Using these morphological traits to model and optimise their values, we created virtual ideotypes of wheat. They were taller and had more tilers than the original wheat, which also resulted in yield gains. However, these yield advantages were not apparent under high density planting. Finally, we found that individual competitiveness of wheat increased during domestication. Higher individual competitiveness in domesticated wheat may be detrimental to the efficiency of population yield at high densities.

Our results elucidate the relationship between wheat phenotype, domestication and yield. This helps agronomists to better understand crop domestication, as well as for future breeding efforts.

Keywords: wheat, phenotype, yields, morphology, domestication

Contents

Chapter 1: General Introduction

1.1 Introduction

In order to grow more food to meet global demand in 2050 (Döös, 2002), the challenge is to find ideotypes of crops as breeding targets to make crop growth faster and stronger, thereby boosting yields (Donald, 1968a). Current research in this area uses theory from plant sciences to identify bottlenecks to production and identify new phenotypes that would increase yields. My PhD thesis will focus on studying the relationships of domestication, morphology and yield in wheats. Domestication has led to significant improvements in crop yield (Preece *et al.*, 2015). In a comparison of wild cereals and their domesticated relatives, the latter's yield was more than 50% greater than that of wild populations (Preece *et al.*, 2017). For 10,000 years, people have cultivated crop species, selecting trait values that promoted high yields (Rasmusson, 1987). However, the process of domestication led to an important bottleneck (Flint-Garcia, 2013). When humans selected crops with particular traits, they gave up other traits that they had no interest in. Through the process of selection by farmers, many undesirable alleles from the wild ancestors, along with some potentially beneficial alleles such as those conferring disease resistance (Ma *et al.*, 2019), were not carried through to early domesticates (Gustafson *et al.*, 2009).

At the same time, the process of domestication has led to a change in the environment of the crop from the wild to farmland (Jackson & Buell, 2022). The change in the external environment leads to natural selection in addition to artificial selection. Natural selection drives crops to evolve in response to changes in the environment (Henry & Nevo, 2014). With external security and abundant resources (water or nitrogen), natural selection will tend to evolve traits that are more resource-acquiring on an individual basis, such as bigger seeds, taller shoots and larger leaves (Milla *et al.*, 2015). But do these high-resource-acquisition plants (and often gigantism) have traits we need for modern agriculture? Many agronomists disagree. Most of them believe that too much individual competitiveness may be beneficial to the individual, but detrimental to group production (Denison *et al.*, 2003). Therefore domestication, containing artificial selection and unconscious natural selection, is thought to have been an important factor that has caused evolutionary changes in crop morphology

(Smith, 2007). Morphological trait changes have, in turn, influenced crop biomass allocation to modify growth (Markesteijn & Poorter, 2009).

Almost all breeders want multiple populations of crop species in their germplasm repository to provide a diversity of morphological traits to use as breeding materials. Generating diversity in morphological traits using wild material is particularly important to break through the domestication bottleneck and explore the growth potential of our major crops (Kovach & McCouch, 2008). Although some morphological trait values were lost during domestication, the process also created new trait values. This is because the phenotype is determined by both genotypes and environments, and domesticated crops are grown in environments beyond their natural ranges (Williams *et al.*, 2008), which means that the results of breeding are sometimes unpredictable, despite being under the control of humans (Diamond, 2002). Meanwhile, genetic recombination can also create new trait values in breeding, for example in the case of rice hybridization (Virmani, 1996). These observations lead to the expectation that today's crops have valuable traits that never appeared in their wild progenitors. Meanwhile, unconscious natural selection in specific cultivated fields, as mentioned above, also creates new phenotypic values during domestication and even breaks the original domain of trait values (Zohary, 2004). Based on this understanding, I hypothesise that the diversity of trait values in wild crops and modern ones should be like that presented in Figure 1. Even though the morphospace of wild trait values is larger than that of domesticated ones (Area 1), the wild morphospace does not cover the modern morphospace totally (Area 2) because new trait values have arisen in domesticated populations (Area 3). **My first objective in Chapter 2 is therefore to test these ideas by comparing the morphospaces defined by the wild trait values and domesticated trait values of a crop species.** For this work, I will use wheat, since it is economically important globally and in both the UK and China. The hypothesis (H) are listed below.

H2.1: The morphospace of wheat progenitors should be larger than that of domesticated wheats.

H2.2: The morphospace of domesticated wheats should expand beyond that covered by wild ones.

H2.3: Wheat traits were changed at different timepoints and have different evolutionary strategies during its long history.

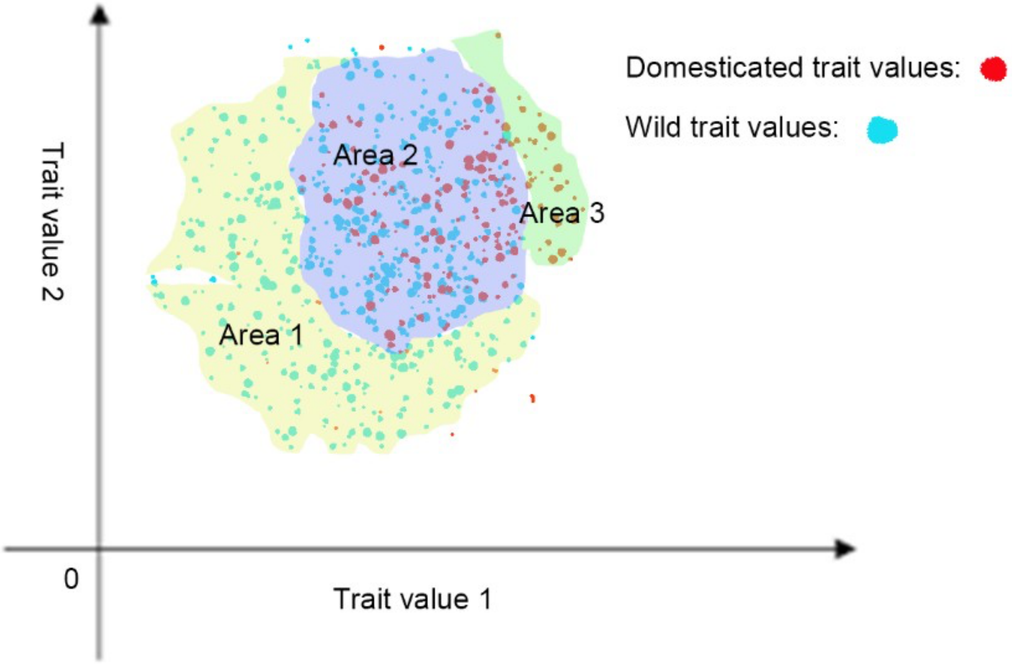


Figure 1 : The hypothesized morphospace of wild and domesticated traits. Each small point represents the range of trait values from a single population, i.e. accession. The points of wild trait values are blue and those of domesticated trait values are red. The overlap of points from wild and domesticated forms can be categorized into three areas, denoted with yellow, purple and green colours respectively. The purple area 2 shows the overlap of wild trait values and domesticated trait values. The yellow area 1 shows trait values that only belong to wild progenitors (i.e. they are absent in domesticated accessions). The green area 3 shows new trait values that were created during domestication (i.e. absent from wild accessions).

The mechanism of how morphology changes carbon allocation is important in crop growth (Mccarthy & Enquist, 2007). The potential sizes and numbers of leaves, branches and fruits are determined by genetics, but their actual values in growth arise from the internal competition for carbohydrates and external limitation by the environment, which influence yield (Burnett *et al.*, 2016). Donald proposed the idea of defining phenotypic traits that benefit yield and combining them to build an ideotype that might achieve the highest yield (Donald, 1968b). In the first objective of my PhD, I will have measured the morphological trait values for multiple wild and domesticated accessions of a crop under a common environment. Variation among accessions in this case arises entirely from genetics. But I cannot screen all of these varieties in the field to fully consider the limitation by environmental factors. I also want to test whether variation beyond the observed range of trait values has the potential to lead to greater yields. To address these two issues, I will apply an advanced computing method to simulate crop morphology and growth *in silico*. In collaboration with Wageningen University, I will use a new FSP (functional-structural plant) model (Vos *et al.*, 2010). Using this platform, plant morphology, physiological metabolism, external environment and dynamic growth process can all be simulated. Importantly, the FSP model is specifically designed to simulate the relationships between crop structure (i.e. morphology) and function (i.e. physiological behaviour, including photosynthesis and growth). Running this model requires me to collect more data from the literature. Previous research about wheat trait values can help me to set default ranges of values for all model parameters. Within this range, I can modify some trait values and see how this variation is relevant to crop yield. This work can be achieved using the FSP model. **My second objective in Chapter 3 is therefore to use this model to test the relationships between the morphological variation observed in the first objective and the growth of the crop under simulated field conditions**. I will also use the model to explore extreme trait values observed within existing wheat diversity, and their effects on plant growth. If these trait values could be generated in breeding populations, how would they influence yield?

H3.1: Combining yield-friendly traits to generate ideotype in the FSP model will lead to yield increases.

H3.2: Maintaining these yielding advantages of the ideotype is more challenging in high density farming.

After identifying which traits were changed by domestication and if they would benefit yield, we are also interested in knowing which genetic changes cause the corresponding trait variation. Especially for landraces, the genetic resources of these wheat accessions are rich, representing potential reservoirs of desirable allelic forms of valuable traits that can be used as breeding material (Adhikari *et al.*, 2022). It has been proved that landraces of *T. aestivum* exhibit more allelic variability in economically important traits than modern varieties (Lopes *et al.*, 2015). The variable yielding traits of wheat landrace are associated with morphology at different locations (Reynolds *et al.*, 1994) (Loss & Siddique, 1994) (Ashfaq *et al.*, 2003). It becomes very interesting to see whether these wheat landraces have similar or different trait profiles and whether the same traits are associated with the same genetic loci on the chromosomes. I therefore wanted to identify genetic markers for important morphological traits using a diversity panel. Our collaborator at University of York has a diversity panel of genotyped wheat landraces that is suitable for this work. Following computing technology improvement, a GWAS (genome-wide association study) will be used to identify gene loci related to targeted traits (Korte & Farlow, 2013). The study analyses the genomes of a large number of individuals to detect correlations between specific genetic markers (such as SNPs) and the presence or absence of a trait (Yang *et al.*, 2012). I apply GAPIT software packages to find loci that cause variation in yield traits (Wang & Zhang, 2021). **Therefore, my third objective in Chapter 4 is to apply GWAS to identify loci that cause variation in yield traits of wheat landrace improvement.**

H4.1: Yield-related traits showing variation among landraces is associated with specific genetic loci.

All these above mainly focus on the relation of morphology and yield of individual wheat plants. However, real-world farming is always a group challenge, such that yield depends on the performance of the crop as a whole rather than individual plants. In addition to the yield brought about by its own phenotype, we therefore need to pay extra attention to the competitiveness of plants (Asif *et al.*, 2014). This determines whether they will be able to grow with their neighbours and have access to sufficient environmental resources (sunlight, water, space and nitrogen) **Adhikari S, Kumari J, Jacob SR, Prasad P, Gangwar OP, Lata C, Thakur R, Singh AK, Bansal R, Kumar S, *et al.* 2022**. Landraces-potential treasure for sustainable wheat improvement. *Genetic Resources and Crop Evolution* **69**: 499–523.

Ashfaq M, KHAN A, Ali Z. **2003**. Association of Morphological Traits with Grain Yield in Wheat (Triticum aestivum L.).

Asif M, Iqbal M, Randhawa H, Spaner D. **2014**. *Managing and breeding wheat for organic systems: enhancing competitiveness against weeds*. Springer Science & Business Media.

Burnett AC, Rogers A, Rees M, Osborne CP. **2016**. Carbon source–sink limitations differ between two species with contrasting growth strategies. *Plant, cell & environment* **39**: 2460–2472.

Denison RF, Kiers ET, West SA. **2003**. Darwinian Agriculture: When Can Humans Find Solutions Beyond the Reach of Natural Selection? *The Quarterly Review of Biology* **78**: 145–168.

Diamond J. **2002**. Evolution, consequences and future of plant and animal domestication. *Nature* **418**: 700–707.

Donald CM. **1968a**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Donald CM. **1968b**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Döös BR. **2002**. Population growth and loss of arable land. *Global Environmental Change* **12**: 303–311.

Flint-Garcia SA. **2013**. Genetics and Consequences of Crop Domestication. *Journal of Agricultural and Food Chemistry* **61**: 8267–8276.

Gustafson P, Raskina O, Ma X, Nevo E. **2009**. Wheat evolution, domestication, and improvement. *Wheat: science and trade. Wiley, Danvers*: 5–30.

Henry RJ, Nevo E. **2014**. Exploring natural selection to guide breeding for agriculture. *Plant Biotechnology Journal* **12**: 655–662.

Jackson D, Buell CR. **2022**. Crop Domestication: Past, Present and Future. *Plant and Cell Physiology* **63**: 1527–1528.

Korte A, Farlow A. **2013**. The advantages and limitations of trait analysis with GWAS: a review. *Plant methods* **9**: 1–9.

Kovach M, McCouch S. **2008**. Leveraging natural diversity: back through the bottleneck. *Current Opinion in Plant Biology* **11**: 193–200.

Lopes MS, El-Basyoni I, Baenziger PS, Singh S, Royo C, Ozbek K, Aktas H, Ozer E, Ozdemir F, Manickavelu A. **2015**. Exploiting genetic diversity from landraces in wheat breeding for adaptation to climate change. *Journal of experimental botany* **66**: 3477–3486.

Loss SP, Siddique KHM. **1994**. Morphological and physiological traits associated with wheat yield increases in Mediterranean environments. *Advances in agronomy* **52**: 229–276.

Ma Y, Liu M, Stiller J, Liu C. **2019**. A pan-transcriptome analysis shows that disease resistance genes have undergone more selection pressure during barley domestication. *BMC Genomics* **20**: 12.

Markesteijn L, Poorter L. **2009**. Seedling root morphology and biomass allocation of 62 tropical tree species in relation to drought- and shade-tolerance. *Journal of Ecology* **97**: 311–325.

Mccarthy MC, Enquist BJ. **2007**. Consistency between an allometric approach and optimal partitioning theory in global patterns of plant biomass allocation. *Functional Ecology* **21**: 713–720.

Milla R, Matesanz S. **2017**. Growing larger with domestication: a matter of physiology, morphology or allocation? *Plant Biology* **19**: 475–483.

Milla R, Osborne CP, Turcotte MM, Violle C. **2015**. Plant domestication through an ecological lens. *Trends in Ecology & Evolution* **30**: 463–469.

Preece C, Livarda A, Christin P-A, Wallace M, Martin G, Charles M, Jones G, Rees M, Osborne CP. **2017**. How did the domestication of Fertile Crescent grain crops increase their yields? (A Brody, Ed.). *Functional Ecology* **31**: 387–397.

Preece C, Livarda A, Wallace M, Martin G, Charles M, Christin P-A, Jones G, Rees M, Osborne CP. **2015**. Were Fertile Crescent crop progenitors higher yielding than other wild species that were never domesticated? *New Phytologist* **207**: 905–913.

Rasmusson DC. **1987**. An Evaluation of Ideotype Breeding 1. *Crop Science* **27**: 1140–1146.

Reynolds MP, Balota M, Delgado MIB, Amani I, Fischer RA. **1994**. Physiological and Morphological Traits Associated With Spring Wheat Yield Under Hot, Irrigated Conditions. *Functional Plant Biology* **21**: 717–730.

Robertson BM, Waines JG, Gill BS. **1979**. Genetic variability for seedling root numbers in wild and domesticated wheats 1. *Crop Science* **19**: 843–847.

Smith JM. **1964**. Group selection and kin selection. *Nature* **201**: 1145–1147.

Smith BD. **2007**. Niche construction and the behavioral context of plant and animal domestication. *Evolutionary Anthropology: Issues, News, and Reviews* **16**: 188–199.

Virmani SS. **1996**. Hybrid Rice. In: Sparks DL, ed. Advances in Agronomy. Academic Press, 377–462.

Vos J, Evers JB, Buck-Sorlin GH, Andrieu B, Chelle M, de Visser PHB. **2010**. Functional–structural plant modelling: a new versatile tool in crop science. *Journal of Experimental Botany* **61**: 2101–2115.

Wang J, Zhang Z. **2021**. GAPIT Version 3: Boosting Power and Accuracy for Genomic Association and Prediction. *Genomics, Proteomics & Bioinformatics* **19**: 629–640.

Weiner J, Du Y-L, Zhang C, Qin X-L, Li F-M. **2017**. Evolutionary agroecology: individual fitness and population yield in wheat (Triticum aestivum). *Ecology* **98**: 2261–2266.

Williams RM, O'Brien L, Eagles HA, Solah VA, Jayasena V. **2008**. The influences of genotype, environment, and genotype× environment interaction on wheat quality. *Australian journal of agricultural research* **59**: 95–111.

Wright A, Schnitzer SA, Reich PB. **2014**. Living close to your neighbors: the importance of both competition and facilitation in plant communities. *Ecology* **95**: 2213–2223.

Yang J, Ferreira T, Morris AP, Medland SE, Consortium GI of AnT (GIANT), Consortium DiaGRAM (DIAGRAM), Madden PA, Heath AC, Martin NG, Montgomery GW. **2012**. Conditional and joint multiple-SNP analysis of GWAS summary statistics identifies additional variants influencing complex traits. *Nature genetics* **44**: 369–375.

Zohary D. **2004**. Unconscious selection and the evolution of domesticated Plants. *Economic Botany* **58**: 5–10.

(Wright *et al.*, 2014). Agriculture ecology theory tell us that individual fitness would benefit individual yield, but selfish behaviour harms population yield (Smith, 1964). This relationship is unimodal and the highest yielding populations come from varieties with moderate individual fitness (Weiner *et al.*, 2017). Therefore, our breeding target should be the phenotype that has better group yield, although its competitiveness might be decreased. How domestication changed the fitness of wheat is still controversial. Some opinions are that domestication increased wheat competitiveness because domesticated wheats always have larger seeds and bodies, which could provide advantages in light capture aboveground (Milla & Matesanz, 2017). However, another argument is that wild wheats have stronger roots adapting them to infertile soil environments (Robertson *et al.*, 1979). **Therefore, my fourth objective in Chapter 5 is to test if domestication increased or decreased wheat competitiveness.**

H5.1: Domestication increases wheat competitiveness. Domesticated wheats have higher competitiveness than wild wheats.

H5.2: Domestication decreases wheat competitiveness. Wild wheats have higher competitiveness than domesticated wheats.

1.2 Thesis overview

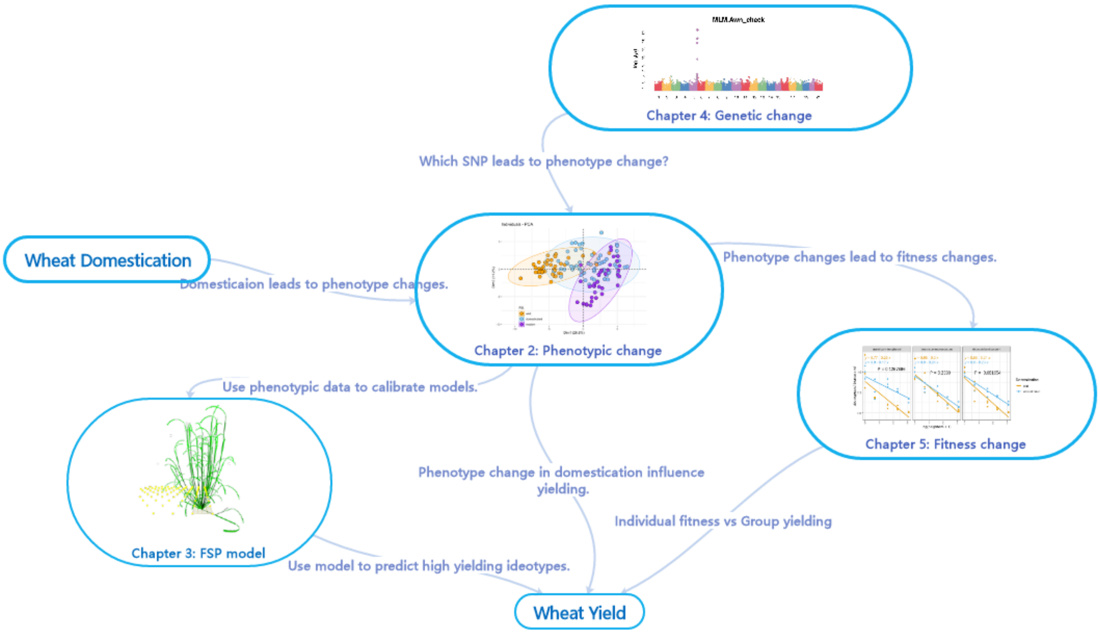


Figure 2: Schematic diagram demonstrating the relationships among domestication, phenotype and yielding that are investigated in this thesis (including chapter information).

1.2.1 Chapter 2: Morphological analysis of wheat diversity before and after domestication

In order to improve the yield of crops, we need to explore the potential variation in crop morphologies. The current trait values of wheats are limited because domestication influenced morphological diversity. My target in Chapter 2 is to test whether domesticated wheats have smaller morphospace than their wild progenitors. Moreover, wheat phenotypes have evolved over a long history, including polyploidy, domestication, landrace improvement (after domestication) and the Green Revolution. What changed at each historical stage and why they these changes occurred is still unclear.

I grew 142 wheat accessions with differing biological statuses (wild, domesticated, or modern), historical origins and geographical sources. During their growth, I measured their morphological data until they were harvested. By applying PCA (Principal component analysis) and mixed effects models, I compare their morphological variation.

I found that wild wheats have an overlapped morphospaces with that of domesticated wheats, but they occupy unique space too. Wheat phenotypic traits changed during all four historical periods, and at each stage, wheats developed different strategies to meet external requirements. Connecting our experiment data, yield improvement relies on finding proper trait values.

1.2.2 Chapter 3: The simulation of wheat ideotype to increase yield

I have found the existing domain of wheat phenotypic values. Is it possible to further optimise the wheat phenotype, e.g. by combining wild and domesticated traits to modern wheat, so as to improve yield? There is a need to test these in different morphological types of wheat. The current wheat morphology with the largest potential yield has been empirically established in our last experiment. If we want higher-yielding forms, we need to create new wheat morphologies that have not appeared globally. Some traits, identified in the morphological experiments in Chapter 2, have been linked to yield, such as leaf size, tiller number, seed weight, and plant height. If we modify these in a positive direction, will our yield in the FSP model increase or not? Based on the necessity to maintain source-sink balance, what is the potential for each trait to increase, and at what point (if any) does increasing size become detrimental, rather than beneficial, for yield? And, how realistic can the current FSP model be made in comparison with real plants?

In order to answer these questions, I calibrated an FSP (Functional Structural Plant) model using the wheat morphological data from Chapter 2. I then used sensitivity analysis and random forest methods to identify the key traits that contributed most to modelled yield. Then I applied a convex hull algorithm to explore the ideotype that combines the best trait values, and tested it at increased densities.

My ideotype achieves yield increases by recombining trait values within existing ranges. Among them, the increase of tillers, a height limit of 0.8-0.9m, and the reduction of blade insertion angle play important roles. However, the size of this ideotype is much larger than that of modern wheat. Moreover, it cannot maintain yield advantages in high-density farming, which made me reflect on whether the ideal modelled phenotype falls into the trap of gigantism.

1.2.3 Chapter 4: Association mapping identifies quantitative trait loci for wheat awns

After designing an ideotype for wheat *in silico*, the next step is to connect it to genotypes and test its farming performance. I therefore collected genetic and phenotypic data of domesticated wheat to investigate the genetic basis of morphological traits. The work compared the differences in key trait values among current landraces.

The SNPs data for a wheat landrace diversity panel were shared by collaborators at the University of York. I measured the phenotypic traits of 342 *T. aestivum* genotypes. These data were correlated with SNPs by applying GWAS analysis to identify the gene loci showing significant associations.

My work identified four important genetic loci at the chromosome 5A of *T. aestivum*, which controls awn appearance. SNPs that associated with plant height and spike number are also found, although the significance levels are not strong.

1.2.4 Chapter 5: Domestication increases wheat competitiveness

The modelling work presented in Chapter 3 serves as a reminder that individual ideotype performance does not necessarily equate to group yield. Agricultural ecology theory shows that achieving high population yield requires the inclusion of lower-fitness individuals, since their restrained competitive behaviours prevent detrimental effects on neighbouring plants. One interesting question is how the process of domestication impacts the individual competitiveness of wheat. Generally, domesticated wheats tend to exhibit greater aboveground biomass, which implies they might be stronger in competition. However, wild wheats possess more robust root systems that have proved adapted to wild competitive environments. Elucidating whether domestication amplifies or diminishes wheat competitiveness is important for refining breeding objectives.

To address this issue, I collected three distinct pairings of typical wild and domesticated wheat varieties, each highlighting different aspects of domestication effects, such as early vigour, plant height, and tillering. Employing a gradient density planting experiment, I put wild and domesticated wheat neighbours under varying neighbour densities to intensify resource competition. I evaluated their fitness under competition by assessing an array of performance traits, as well as the extent of decline exhibited when the densities of wild/domesticated neighbours were increased. Furthermore, I applied the FSP model to ask whether the effects of competition could be reproduced by simulating aboveground competition only, and used the model to ask whether biomass differences translated into fitness benefits.

The outcomes of this study were that domesticated wheats were less influenced by the presence of wild neighbours. In contrast, wild wheats experienced a significant detriment from competition with domesticated ones, with some instances of severe survival crisis. Certain wild wheats are very weak and struggle to survive and fail to fruitfully reproduce. The advantageous traits of early vigour and increased height confer benefits to domesticated wheats in competition. Our FSP modelling results support and reinforces these findings.

1.3 Reference

Adhikari S, Kumari J, Jacob SR, Prasad P, Gangwar OP, Lata C, Thakur R, Singh AK, Bansal R, Kumar S, *et al.* 2022. Landraces-potential treasure for sustainable wheat improvement. *Genetic Resources and Crop Evolution* **69**: 499–523.

Ashfaq M, KHAN A, Ali Z. **2003**. Association of Morphological Traits with Grain Yield in Wheat (Triticum aestivum L.).

Asif M, Iqbal M, Randhawa H, Spaner D. **2014**. *Managing and breeding wheat for organic systems: enhancing competitiveness against weeds*. Springer Science & Business Media.

Burnett AC, Rogers A, Rees M, Osborne CP. **2016**. Carbon source–sink limitations differ between two species with contrasting growth strategies. *Plant, cell & environment* **39**: 2460–2472.

Denison RF, Kiers ET, West SA. **2003**. Darwinian Agriculture: When Can Humans Find Solutions Beyond the Reach of Natural Selection? *The Quarterly Review of Biology* **78**: 145–168.

Diamond J. **2002**. Evolution, consequences and future of plant and animal domestication. *Nature* **418**: 700–707.

Donald CM. **1968a**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Donald CM. **1968b**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Döös BR. **2002**. Population growth and loss of arable land. *Global Environmental Change* **12**: 303–311.

Flint-Garcia SA. **2013**. Genetics and Consequences of Crop Domestication. *Journal of Agricultural and Food Chemistry* **61**: 8267–8276.

Gustafson P, Raskina O, Ma X, Nevo E. **2009**. Wheat evolution, domestication, and improvement. *Wheat: science and trade. Wiley, Danvers*: 5–30.

Henry RJ, Nevo E. **2014**. Exploring natural selection to guide breeding for agriculture. *Plant Biotechnology Journal* **12**: 655–662.

Jackson D, Buell CR. **2022**. Crop Domestication: Past, Present and Future. *Plant and Cell Physiology* **63**: 1527–1528.

Korte A, Farlow A. **2013**. The advantages and limitations of trait analysis with GWAS: a review. *Plant methods* **9**: 1–9.

Kovach M, McCouch S. **2008**. Leveraging natural diversity: back through the bottleneck. *Current Opinion in Plant Biology* **11**: 193–200.

Lopes MS, El-Basyoni I, Baenziger PS, Singh S, Royo C, Ozbek K, Aktas H, Ozer E, Ozdemir F, Manickavelu A. **2015**. Exploiting genetic diversity from landraces in wheat breeding for adaptation to climate change. *Journal of experimental botany* **66**: 3477–3486.

Loss SP, Siddique KHM. **1994**. Morphological and physiological traits associated with wheat yield increases in Mediterranean environments. *Advances in agronomy* **52**: 229–276.

Ma Y, Liu M, Stiller J, Liu C. **2019**. A pan-transcriptome analysis shows that disease resistance genes have undergone more selection pressure during barley domestication. *BMC Genomics* **20**: 12.

Markesteijn L, Poorter L. **2009**. Seedling root morphology and biomass allocation of 62 tropical tree species in relation to drought- and shade-tolerance. *Journal of Ecology* **97**: 311–325.

Mccarthy MC, Enquist BJ. **2007**. Consistency between an allometric approach and optimal partitioning theory in global patterns of plant biomass allocation. *Functional Ecology* **21**: 713–720.

Milla R, Matesanz S. **2017**. Growing larger with domestication: a matter of physiology, morphology or allocation? *Plant Biology* **19**: 475–483.

Milla R, Osborne CP, Turcotte MM, Violle C. **2015**. Plant domestication through an ecological lens. *Trends in Ecology & Evolution* **30**: 463–469.

Preece C, Livarda A, Christin P-A, Wallace M, Martin G, Charles M, Jones G, Rees M, Osborne CP. **2017**. How did the domestication of Fertile Crescent grain crops increase their yields? (A Brody, Ed.). *Functional Ecology* **31**: 387–397.

Preece C, Livarda A, Wallace M, Martin G, Charles M, Christin P-A, Jones G, Rees M, Osborne CP. **2015**. Were Fertile Crescent crop progenitors higher yielding than other wild species that were never domesticated? *New Phytologist* **207**: 905–913.

Rasmusson DC. **1987**. An Evaluation of Ideotype Breeding 1. *Crop Science* **27**: 1140–1146.

Reynolds MP, Balota M, Delgado MIB, Amani I, Fischer RA. **1994**. Physiological and Morphological Traits Associated With Spring Wheat Yield Under Hot, Irrigated Conditions. *Functional Plant Biology* **21**: 717–730.

Robertson BM, Waines JG, Gill BS. **1979**. Genetic variability for seedling root numbers in wild and domesticated wheats 1. *Crop Science* **19**: 843–847.

Smith JM. **1964**. Group selection and kin selection. *Nature* **201**: 1145–1147.

Smith BD. **2007**. Niche construction and the behavioral context of plant and animal domestication. *Evolutionary Anthropology: Issues, News, and Reviews* **16**: 188–199.

Virmani SS. **1996**. Hybrid Rice. In: Sparks DL, ed. Advances in Agronomy. Academic Press, 377–462.

Vos J, Evers JB, Buck-Sorlin GH, Andrieu B, Chelle M, de Visser PHB. **2010**. Functional–structural plant modelling: a new versatile tool in crop science. *Journal of Experimental Botany* **61**: 2101–2115.

Wang J, Zhang Z. **2021**. GAPIT Version 3: Boosting Power and Accuracy for Genomic Association and Prediction. *Genomics, Proteomics & Bioinformatics* **19**: 629–640.

Weiner J, Du Y-L, Zhang C, Qin X-L, Li F-M. **2017**. Evolutionary agroecology: individual fitness and population yield in wheat (Triticum aestivum). *Ecology* **98**: 2261–2266.

Williams RM, O'Brien L, Eagles HA, Solah VA, Jayasena V. **2008**. The influences of genotype, environment, and genotype× environment interaction on wheat quality. *Australian journal of agricultural research* **59**: 95–111.

Wright A, Schnitzer SA, Reich PB. **2014**. Living close to your neighbors: the importance of both competition and facilitation in plant communities. *Ecology* **95**: 2213–2223.

Yang J, Ferreira T, Morris AP, Medland SE, Consortium GI of AnT (GIANT), Consortium DiaGRAM (DIAGRAM), Madden PA, Heath AC, Martin NG, Montgomery GW. **2012**. Conditional and joint multiple-SNP analysis of GWAS summary statistics identifies additional variants influencing complex traits. *Nature genetics* **44**: 369–375.

Zohary D. **2004**. Unconscious selection and the evolution of domesticated Plants. *Economic Botany* **58**: 5–10.

Chapter 2: Diversification of quantitative morphological traits in wheat

---

Yixiang Shan & Colin Osborne

Plants, Photosynthesis and Soil, School of Biosciences, University of Sheffield, Sheffield S10 2TN, UK

2.1 Abstract

- **Background and aims**

The development and morphology of crop plants have been profoundly altered by evolution under cultivation, through a combination of unconscious selection without deliberate foresight, and later by directed breeding. Wild wheats remain an important potential source of variation for modern breeders, however, the sequence and timing of morphological changes during domestication are not fully resolved.

- **Methods**

We grew and measured 142 wheat accessions representing different stages in wheat evolution, including three independent domestication events, and compared their morphological traits to define the morphospace of each group.

- **Key results**

The results show that wild and domesticated wheats have overlapping morphospaces, but each also occupies a distinct area of morphospace from one another. Polyploid formation in wheat increased leaf biomass and seed weight but had its largest effects on tiller loss. Domestication continued to increase the sizes of wheat leaves and seeds, and made wheat grow taller with more erect architecture. These changes led to domesticated wheats generating more grains and achieving higher yields. Landrace improvement subsequently decreased tiller and spike numbers, to focus resource allocation to the main stem, accompanied by a thicker main stem and larger flag leaves. During the Green Revolution, wheat height was reduced to increase the harvest index and therefore yield. Modern wheats also have more erect leaves and larger flower biomass proportions than landraces.

- **Conclusions**

Quantitative trait history in wheat therefore differs by trait. Some trait values show progressive changes in the same direction (e.g. leaf size, grain weight), others change in a punctuated way at particular stages (e.g. canopy architecture), while other trait values switch directions during wheat evolution (e.g. plant height, flower biomass proportion). Agronomically valued domestication traits arose during different stages of wheat history, such that modern wheats are the product of 10,000 years of morphological evolution.

Key words: wheats, domestication, morphology, wheat (*Triticum aestivum* L.), polyploidy, selective breeding, Green Revolution, evolution.

2.2 Introduction

Wheat (*Triticum aestivum* L.) is one of the world's major crops, grown over a land area greater than any other crop (Milla & Osborne, 2019), and accounting for 20% of food calories globally (Erenstein *et al.*, 2022). The earliest evidence of wheat domestication comes from Neolithic archaeological sites in the western Fertile Crescent (Brown *et al.*, 2009). This ancient history makes wheat one of the oldest crops, and it was one of the species that underpinned the first agricultural economies (Abbo & Gopher, 2017) and later grain states (Zhao *et al.*, 2023a) in the Middle East. Both the genotype and phenotype of wheat have changed under domestication and subsequent evolution under selective breeding. Numerous studies have compared wild wheats with domesticated forms, finding a syndrome of traits associated with domestication, including non-brittle rachis, larger seeds and leaves (Evans, 1996), delayed flowering time (Cockram *et al.*, 2007), loss of dormancy (Harlan *et al.*, 1973), greater aboveground biomass (Roucou *et al.*, 2018) and faster growth (Gómez-Fernández *et al.*, 2022).

Many authors consider domestication to be a slow process, occurring across a broad geographic area, with domesticated forms first arising at low frequencies among cultivated stands of wild plants (Tanno & Willcox, 2006). In addition, several domestication traits are complex, presumably controlled by multiple loci, and arise gradually during wheat evolution. Examples of such quantitative traits include plant height (Peng *et al.*, 2003), tillering capacity (Peng *et al.*, 2011) and leaf size (Milla & Matesanz, 2017). All show marked differences in comparisons between wild and domesticated forms. However, there is considerable diversity among accessions and species, and the picture is complicated by changes in ploidy during wheat evolution that are classically associated with gigantism (Fuller, 2007). Therefore the extent to which quantitative morphological changes have arisen in wheat from polyploidy, domestication and selective breeding remains unclear (Li et al., 2014; Gui et al., 2021).

The diversity of modern wheat is well-characterised and provides a useful means to address these questions, and the specific effects of ploidy, domestication and selective breeding. These events happened at different historic time points and their effects may be inferred via comparisons of extant wheat species. Wild wheat *Triticum urartu* (AA) and *Triticum boeoticum* (AA) are regarded as the earliest diploid wheats (Johnson & Dhaliwal, 1976). The first polyploidisation event happened 300,000–500,000 years ago, when wild wheat *Triticum urartu* (AA) formed a natural hybrid with Aegilops (*Aegilops speltoides*, genome SS), the closest relative of Triticum (Abbo *et al.*, 2014). This hybridization created the wild progenitor of emmer wheat with the AABB genotype, named *Triticum dicoccoides* (Figure S1). Another wild relative, the tetraploid *Triticum araraticum* probably arose from an independent hybridisation of *Triticum urartu* with Aegilops (Figure S1), and has the AAGG genome (Badaeva *et al.*, 2022).

People started to cultivate those wild wheats in the Fertile Crescent around 10,000 years ago (Tanno & Willcox, 2006) (Faris, 2014). From this timepoint, there were three independent domestication trajectories (Figure S1): 1. Wild *Triticum boeoticum* was domesticated to *Triticum monococcum* (genome AmAm) (Heun *et al.*, 1997); 2. wild *Triticum araraticum* was domesticated to *Triticum timopheevii* (Oliveira *et al.*, 2020); and 3. wild *Triticum dicoccoides* was domesticated to *Triticum dicoccum* (genome AABB) (Peleg *et al.*, 2011). Domesticated emmer wheat, *Triticum dicoccum* underwent a second natural hybridization with another Aegilops species (*Aegilops tauschii*, genome DD) 9,000 years ago (Dvorak *et al.*, 2012). This event created hexaploid bread wheat (*Triticum aestivum*, genome AABBDD; Figure S1). Subsequent breeding under cultivation turned tetraploid emmer wheat into a landrace type, *Triticum durum* (genome AABB) (Figure S1; Bozzini 1988). Selection for free-threshing means that *T. durum* and *T. aestivum* have a low degree of glume tenacity, a fragile rachis and free-threshing habit, which distinguish them from hulled emmer wheat (Peng *et al.*, 2011). Both *T. aestivum* and *T. durum* were subsequently improved during the Green Revolution (Figure S1; Byerlee and Traxler 1995). Modern representatives of these two species are grown on large commercial scales today, while domesticated landraces of emmer and einkorn continue to be grown only on small scales as heritage varieties.

Here, we aim to determine how morphology has quantitatively changed during wheat evolution, and to attribute each change to either polyploidy, domestication, landrace improvement, or modern breeding during the Green Revolution. We compare a diverse range of wheat accessions in a common environment, and make four comparisons (Figure S2) to infer: i) the effects of polyploidy **pre-domestication** across two independent events (*urartu-dicoccoides, urartu-araraticum*); ii) **domestication** across three independent events (*boeoticum-monoccum*, *araraticum-timopheevii, dicoccoides-dicoccum*), **evolution of landraces after domestication** (*dicoccum*-landraces of *durum* or *aestivum*), and the **Green Revolution** (domesticated *aestivum*-modern *aestivum*, domesticated *durum*-modern *durum*). The novelty of this analysis comes from multiple independent comparisons (Figure S2), which sample a diversity of accessions. Our work shows that the pattern of variation in quantitative traits across the four stages differs by trait. Some trait values show progressive changes in the same direction (e.g. leaf size, shoot diameter), others change in a punctuated way at particular stages (e.g. leaf angle) while other trait values show changes in direction during wheat evolution (e.g. plant height, tiller numbers).

2.3 Methods

2.3.1 Plant material

We collected many accessions of wheat and cultivated them to measure their morphological characteristics. Sampling of the accessions was structured according to biological status and phylogeny. We first included the wild wheats, both diploid (*T. urartu*, *T.boeoticum*) and tetraploid (*T. dicoccoïdes*, *T. araraticum*) (Fig. 1). For domesticated landraces, we included diploid einkorn (*T. monococcum*), the tetraploid wheats (*T. timopheevii*, *T. dicoccum*, *T. durum*), and domesticated bread wheats (*T.aestivum*). For modern post-Green Revolution wheats we included durum (*T. durum*) and bread (*T. aestivum*) varieties. In total, there were therefore 11 wheat species in this experiment, representing the diversity of wild and domesticated forms (Figure S1).

Within this diversity, domesticated bread wheats were provided by Dr. Andrea Harper at York University. Modern bread wheats were collected from NIAB (National Institute of Agricultural Botany), and the others were bought from IPK Gatersleben Genebank (Stadt Seeland, Germany) and the US NPGS (National Plant Germplasm System). In order to sample the diversity for each of these wheat species, we obtained multiple accessions from the recognized wild progenitor and a cultivated variety, including the variation in geographical source, life history (spring or winter), seed cover (hulled or free-threshing). In total, we had 142 wheat accessions in our experiment, listed in Table S1. In the following analysis, we will combine and call their scientific name and bio-status. For example, the *T. urartu* in wild period will be given a wheat name as “urartu wild”. In total, we have 11 wheat names in Table S1.

2.3.2 Growth conditions

For each accession, up to ten seeds were selected randomly and put into the refrigerator at 4 °C for 24 hours. After that, the outer glumes were removed, and the seeds weighed to get their mass. Each accession of fresh seeds was germinated in a closed petri dish, with a wet filter paper put on the bottom (‘Introduction to Wheat

Growth', 2016), and kept in the following conditions in an incubator (versatile environmental test chamber, Panasonic, UK): 12 h dark, 12 h light, 20 ºC, photosynthetic photon flux density (PPFD) 300 µmol m^{-2} s^{-1} and 60% relative humidity (RH). Germination took different lengths of time in each accession and was recorded to the nearest day.

Germinated seeds were transplanted (one plant per pot) into trays (4*6 cells) containing high nutrient compost (M3, Levington Horticulture Ltd., Ipswich, UK), supplemented with perlite (Sinclair Nursery Stock Propagation, Levington Horticulture Ltd., Ipswich, UK) in a 3:1 ratio. These pots were labelled and moved into a new controlled-environment growth cabinet (Conviron BDW 40, Conviron, Winnipeg, Manitoba, Canada). This controlled environment, designed for vernalizing winter wheats, was: 12 h dark, 12 h light, 4 ºC, PPFD 300 µmol m^{-2} s^{-1} and 60% RHD. Spring wheats were treated in the same way, despite not requiring vernalization, to enable fair comparison of traits with the winter varieties. The vernalization lasted for 6 weeks. During the first week of May, 2021, the seedling wheat plants were transplanted into pots (15*15*20cm, 3.5ltr, LBS Horticulture, UK) with the same soil compost as mentioned above, and moved outdoors into an unshaded area of the Arthur Willis Environment Centre (AWEC) at the University of Sheffield, UK. For each wheat accession, we grew three individual plants, organised randomly and spaced in 5 x 5 plant blocks with 0.25 m distance between plants. In addition to rainwater inputs, the plants were watered as required to keep the soil wet.

2.3.3 Trait measurements

During wheat growth, we selected and measured some morphological traits that are recognized to influence yield (Table S2). Among them, plant biomass and mass measurement used one replicate plant for each accession, the final harvest measurement used another, and the third plant was a spare in case one of the others died. Other non-destructive trait measurements were taken in all three repeated samples and used to calculate an average for each accession. The wheat traits were named with the time when they were measured. In the following analysis and figures, we will use some of their replacement name to help understand. All the traits and their replacement names were listed in Table S2.

In addition, we used the measured traits to make predictions of yield, harvest index and the area of individual leaves. Expected yield (Y) was calculated using the grain weight on one spike ($WGS_{harvest}$) and spikelet number on one spike ($NST_{harvest}$) at harvest, and spikelet number in July (NST_{July}), flower biomass in July (BF_{July}) and one spike biomass in July (OBS_{July}), as follows:

$$Y = \frac{WGS_{harvest}}{NST_{harvest}} \times NST_{July} \times \frac{BF_{July}}{OBS_{July}}$$

Equation 1

Final yield (Y_f), calculated using the $NST_{harvest}$ and NST_{July}:

$$Y_f = Y \times \frac{NST_{harvest}}{NST_{July}}$$

Equation 2

Harvest index (HI) was calculated using leaf biomass (B_L), flower biomass (B_F) and shoot biomass (B_S) in July:

$$HI = \frac{Y_f}{FBL+BF+BS}$$ Equation 3

Expected leaf area (LA) followed Schrader *et al.* (2021), and was calculated using leaf length (LL_{July}) and leaf width (WL_{July}) in July:

$$= LL_{July} \times WL_{July} \times 0.75$$

Equation 4

Tiller loss proportion (LT) was calculated with tiller number in June (NT_{June}), spike number in July (NS_{July}) and spike number at harvest ($NS_{harvest}$):

$$LT = \left(Max\left(NT_{June},\ NS_{July}\right) - NS_{harvest}\right) / \left(Max\left(NT_{June},\ NS_{July}\right)\right.$$

Equation 5

In HI, Y and Y_f calculation, we removed samples ($n = 3$) in which HI was excess of 0.75, which were regarded as biologically implausible.

2.3.4 Statistical analysis

Replication in our experiment was at the level of wheat species, such that we could make comparisons among species, accounting for the diversity of accessions within each, but did not compare individual accessions. Data analysis was conducted using Microsoft Office, Excel (https://products.office.com/en-gb/get-started-with-office-2019) and R version 4.0.2 (https://www.r-project.org/). Variation within the dataset of morphological trait values was first described using principal components analysis (PCA) after scaling each trait to standardized values (mean = 0 and standard deviation = 1). We used “FactoMineR” package in R to run the PCA and visualise the resulting morphospace of wild and domesticated groups, then the “vegan” package in R was used to do the analysis. We fitted an Envfit model using the “rda” function to test whether biological status or polyploidy consistently influenced wheat morphologies.

To make the multiple planned comparisons outlined in Fig S2, we also applied mixed effects models using the “lme4” packages in R. We selected some of the traits that made high contributions to major axes in the PCA, and avoided repeating the analyses for strongly correlated traits. We used the four events described in Table 1 as fixed factors, and used wheat species as random effects to run the mixed effects models. Subsequent ANOVA tests on models were then done with the “lme4Test” package in R. For Domestication and Green-Revolution comparisons, we added the block as random effects too. When applying some of the traits as response variables, the model either failed to converge or converged to a parameter estimate at the boundary of parameter space. In these cases, we removed “species” as a random effect (only in Domestication and Green-Revolution cases). Finally, we applied the t-test to compare traits of wild *T. urartu* and modern *T. aestivum*, the results of which is used as the ultimate contrast between the most ancient species and the present wheat. We also applied the Tukey-HSD test to do pairwise comparison among wheat species using the “agricolae” package in R.

2.4 Results

2.4.1 Morphological variation

Since morphological traits are likely to be correlated, we began by using PCA to produce a morphospace showing the main axes of variation and important groupings of traits. The morphospace occupied by wild, domesticated and modern wheat species is distinct but overlapping. The species occupy a broad arc across the first two PC axes (Fig. 1A), such that the morphospace of wild forms overlaps with domesticated forms, and that of domesticated forms overlaps with modern wheats. However, there is no morphological overlap between wild and modern wheats. The main effect of domestication has been to increase values of dimension 1 in the PCA (Fig. 1A), which corresponds to greater size of plants, stems and leaves during the vegetative phase of development (Fig. S1). Alongside this, there is a diversification of low values in dimension 2 (Fig. 1A), which corresponds to shorter height at maturity (Fig. S1). Modern selective breeding has primarily acted to lower and diversify values of dimension 2 (Fig. 1A), to produce low stature varieties (Fig. S1). In broad terms, the results therefore confirm the known effects of domestication in producing gigantism, and modern breeding in shortening plants at maturity.

Within these broad patterns there are important differences among species. Polyploidy has had only modest effects on the sizes of plants and their organs in both *T. araraticum* and *T. dicoccoides* (dimension 1, Fig. 1B). However, the enlargement of plants during domestication is greater in the tetraploids (*T. dicoccum* and *T. timopheevi*) than in the diploid (*T. monococcum*) (dimension 1, Fig. 1B). Conversely, the final height increase associated with domestication is largely observed in *T. timopheevi*, with only limited or no height gains in *T. dicoccum* (emmer) and *T. monococcum* (einkorn) (dimension 2, Fig. 1B). The breeding of landraces from *T. dicoccum* has had more uniform effects in both *T. aestivum* and *T. durum*, with both showing size increases compared with *T. dicoccum* during the vegetative phase (dimension 1, Fig. 1B), but no reduction in final height (dimension 2, Fig. 1B). Finally, Green Revolution breeding has had limited effects on size during the vegetative phase (dimension 1, Fig. 1B), with a focus on shorter final height in *T. aestivum* but not *T. durum* (dimension 2, Fig. 1B).

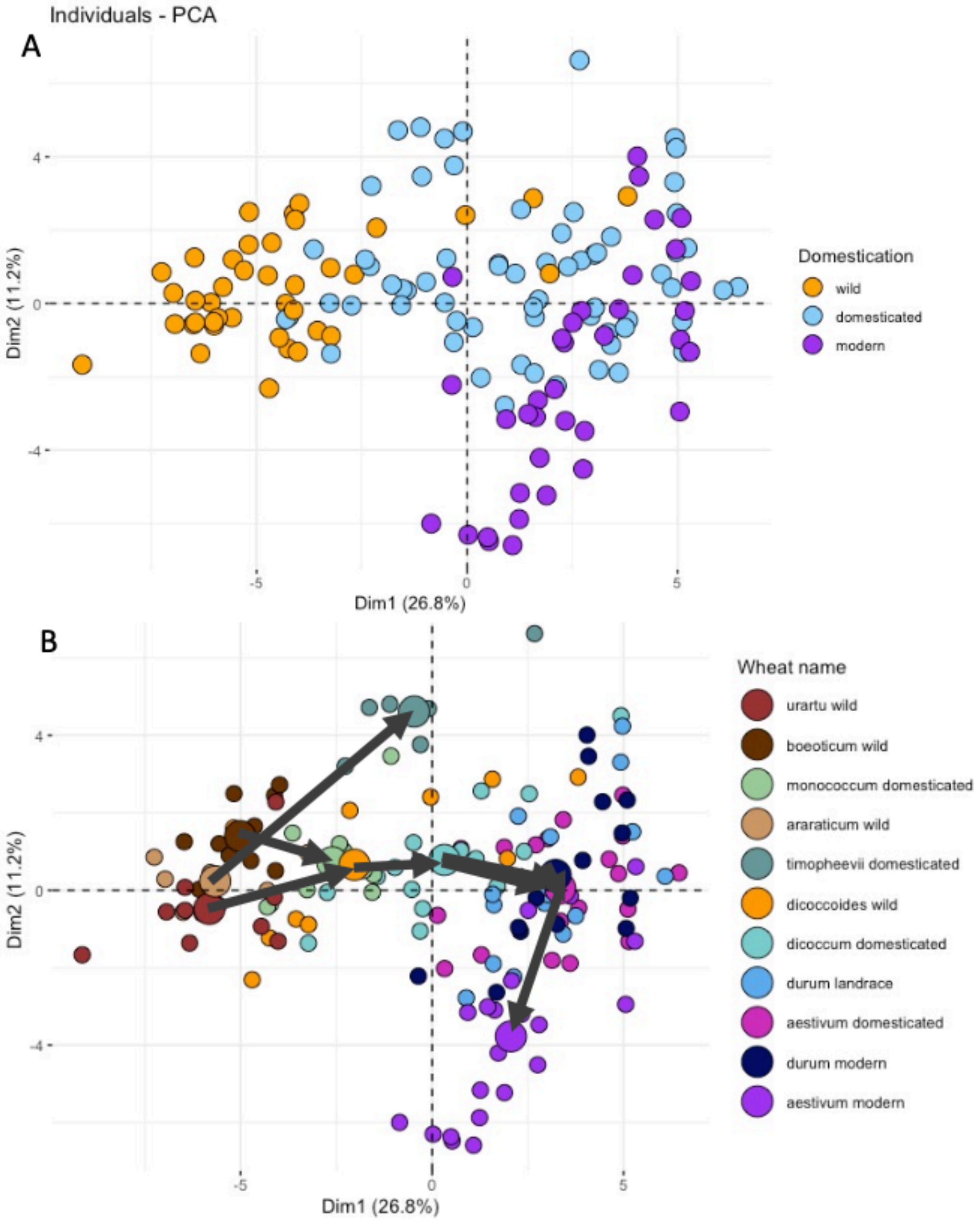


Figure 1: The morphospace occupied by wild and domesticated wheats, presented as a PCA for morphological traits during vegetative and reproductive phases. Points correspond to individual plants, while the colour coding in A distinguishes wild from domesticated and modern wheats, and in B. shows species, as indicated in the key. The black routes track the histories of three domesticated wheat lineages.

Table 1: Summary of trait changes during wheat evolution. The red arrows and shaded boxes indicate significant increases, while the green arrows and shaded boxes show significant decreases in trait values for the contrast indicated. The column of overall means the comparison of wild urartu and modern aestivum.

Category	Traits	Polyploid	Domestication	Landrace improvement	Modern breeding	Overall
Architecture traits	Initial plant height	-	-	-	↓	↑
	Final plant height	-	↑	-	↓	↓
	Stem diameter	-	-	↑	-	↑
	Leaf insertion angle	-	↓	-	↓	↓
Tillering strength	Max tiller number	-	-	↓	-	↓
	Final spike number	-	-	↓	-	↓
	Lost tiller proportion	↑	-	-	-	↑
Biomass allocation	Aboveground biomass	-	-	-	-	↑
	Shoot biomass	-	-	-	-	↑
	Leaf biomass	↑	-	-	-	↑
	Flower biomass	-	-	-	-	↑
	Flower biomass proportion	-	↓	-	↑	-
Leaf traits	Leaf length	-	↑	-	↓	↑
	Leaf width	-	-	-	-	↑
	Flag leaf length	-	-	↑	-	↑
	Flag leaf width	-	↑	↑	-	↑
	One leaf biomass	↑	↑	-	-	↑
	Expected leaf area	-	-	↑	-	↑
Yield related traits	One spike length	-	-	-	-	↑
	One spike biomass	-	-	-	-	↑

	Spikelet number per spike	-	↑	-	-	↑
	Grain number per spike	-	↑	-	↑	↑
	Grain weight per spike	-	↑	-	↑	↑
	Individual grain weight	↑	↑	-	-	↑
	Expected yielding with spike loss	-	↑	-	-	↑
	Harvest index	-	↑	-	-	↑

2.4.2 Architecture traits

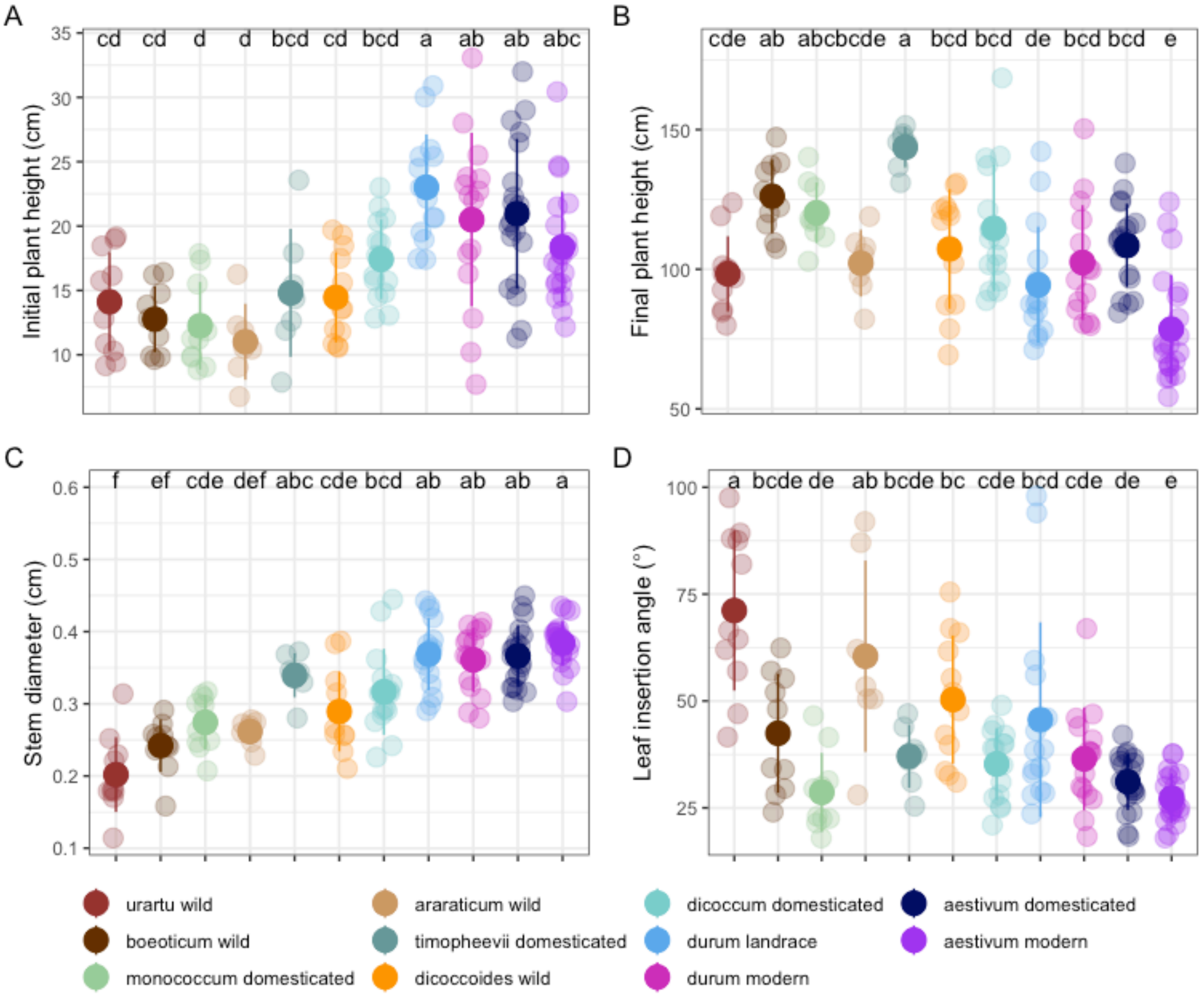


Figure 2: Diversity in morphology and architecture among wheat species. (A) initial plant height; (B) plant height at the end of vegetative growth; (C) main stem diameter at the end of vegetative growth; (D) leaf insertion angle on the main stem. Different letters above points indicate significant differences at p <0 .05 using the Tukey multiple comparison test.

Wheat diversification after domestication has been associated with progressive increases in height and stem diameter during the vegetative phase, such that there is up to a ten-fold variation in height among wild and domesticated forms during May (Fig. 2A). In contrast, although plant height at maturity varies more than three-fold after wheat diversification, the most prominent effects are associated with the short-stemmed modern cultivars of bread wheat released after the Green Revolution and the tall stature of *T. timopheevii* noted earlier (Fig. 2B).

Within the overall trends, substantial variation within groups means that finer-grained details are harder to resolve. Polyploidy has no effects on plant height in wild wheat species, such that there is no evidence of wild tetraploid wheats being taller during the vegetative phase than wild diploid species (Fig. 2A; Table 1) or at maturity (Fig. 2B; Table 1). Stem diameter was greater in *T. dicoccoides* than *T. uratu*, but the equivalent comparison for *T. araraticum* vs *T. uratu* was not significant (Fig. 2C; Table 1). Height and stem diameter were also generally unaffected across the three independent domestication events (Fig. 2A-B; Table 1), with the exception of height at maturity and stem diameter in *T. araraticum*-*T. timopheevii*, where the domesticated form is significantly taller with a thicker stem than the wild species (Fig. 2B; Table 1). Landrace diversification has resulted in taller forms of both durum and bread wheats, but the overall effect is only significant during the vegetative phase in durum (Figs. 2A-B; Table 1). However, stems are thicker in both cases (Fig. 2C; Table 1). Finally, as expected, modern breeding has typically shortened the height at maturity for bread wheat in comparison with its landraces (Fig. 2B; Table 1). This decreased height is only observed in *T. aestivum* and not in *T. durum* in our experiment.

Leaf insertion angle has also shown a progressive decrease during wheat evolution, to produce modern forms with much more erect, compact leaf canopies compared with the lax, spreading canopies of the wild ones (Fig. 2D; Table 1). As a consequence, there is no overlap in values between wild *T. uratu* and modern *T. aestivum* (Fig. 2D). The largest changes are observed across the three independent domestication events, while the difference between *T. aestivum* landraces and modern cultivars is not statistically significant (Fig. 2D).

2.4.3 Tillering strength

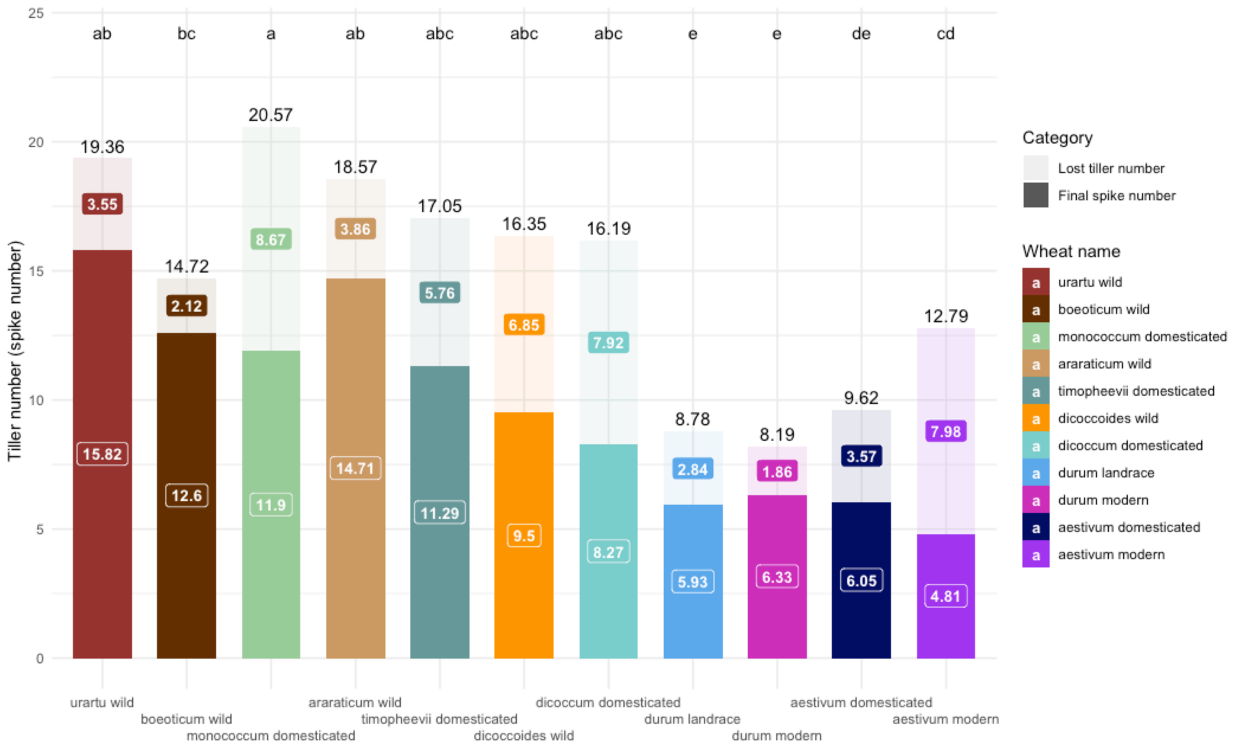


Figure 3: Diversity in tiller number and spike number among wheat species. For each species, the solid colour shows the final spike number at maturity, while the paler colour shows the maximum tiller number that we observed during development. The difference between these values gives tiller loss, highlighted in the coloured boxes. The numbers correspond to trait values. Different letters above points indicate significant differences at $p < 0.05$ using Tukey's multiple comparison test on the max tiller number.

Wild wheats tend to have strong tillering to occupy space and increase their reproductive potential. The polyploid formation has exacerbated spike loss so that larger proportions of tillers do not produce spikes (Table 1). Unexpectedly, we found no evidence of domestication having consistent impacts of tillering across the three domestication events (Table 1). However, tillering strength of einkorn (*T. boeoticum – T. monococcum*) increased after domestication (Fig 3), although subsequent tiller loss meant that final spike number of *T. monococcum* is not higher than that of its wild relatives. A reduced number of spikes at harvest after landrace improvement has arisen through a different mechanism. Selective breeding during landrace diversification has limited final spike number by decreasing the maximum number of tillers, without a change in the proportion of tillers that are lost without setting seeds (Fig. 3; Table 1). We found no evidence of further changes in tillering arising from modern breeding programmes. Overall, therefore, improved modern polyploid wheats produce fewer tillers and lose a greater proportion than wild diploid wheats, but these changes did not occur during either domestication or modern breeding.

2.4.4 Biomass allocation

There was no overall difference in aboveground vegetative biomass between the wild and modern varieties in our pot experiment, potentially reflecting the equal access to soil nutrients that each plant had available. However, we found evidence that the allocation of biomass between flowers, shoots and leaves at anthesis has changed during wheat evolution. Unexpectedly, domestication across three independent events has not brought an obvious increase in total flower biomass. Instead, the selective breeding of modern bread wheat

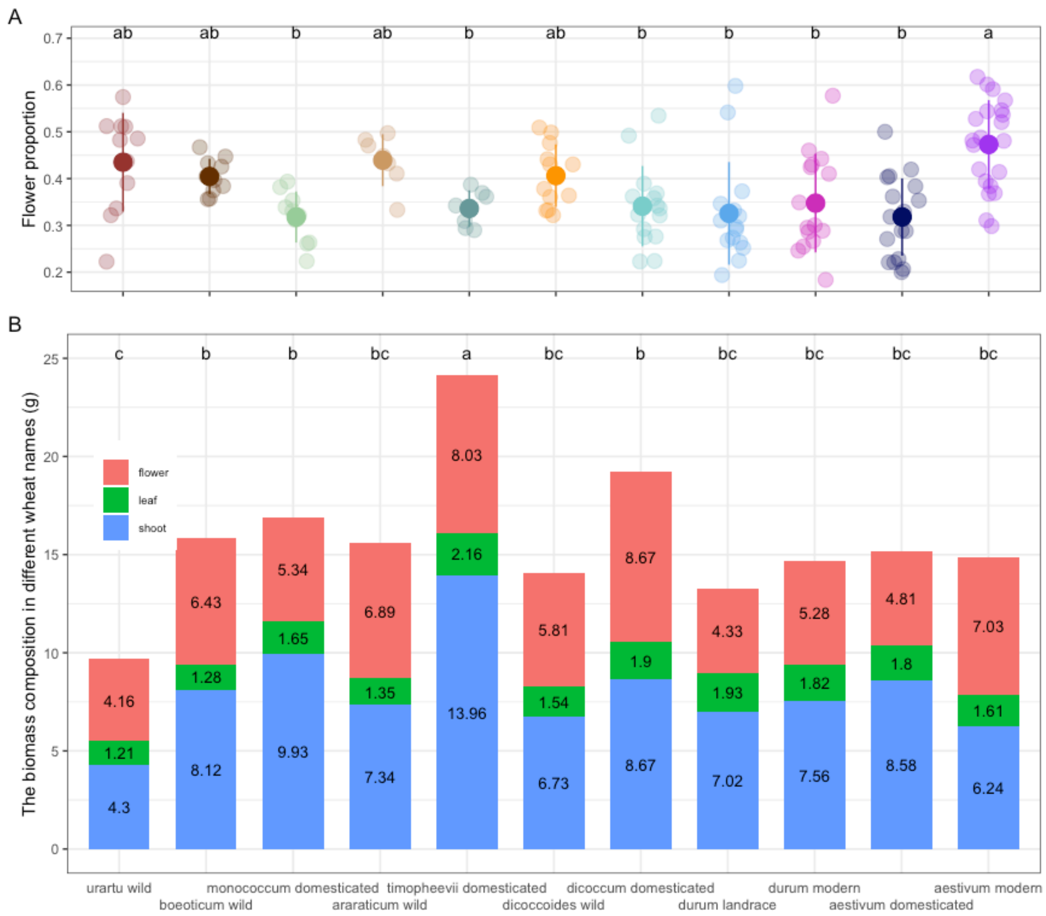


Figure 4: Diversity in flower proportion and biomass allocation at anthesis among wheat species. (A) flower biomass relative to the whole aboveground biomass. (B) biomass allocation to flower, leaf and shoot (stem and leaf sheaths) of wheat. The number shows the biomass value of each tissue. Different letters above points indicate significant differences at $p < .05$ using Tukey's multiple comparison test.

varieties during the Green Revolution is largely responsible for the greater flower biomass of modern in comparison with wild wheats, and its proportion relative to aboveground biomass (Fig. 4A; Table 1). Conversely, domestication across three independent events has decreased relative allocation of biomass to flowering (Table 1). At the same time, leaf biomass increased across these domestication events, continuing a pattern that started across the polyploidy events in wild wheats (Fig. 4B; Table 1). However, there have been no further changes during landrace diversification and modern breeding, and overall leaf biomass does not differ between wild and modern varieties (Fig. 4B; Table 1).

Domesticated wheats tend to have larger aboveground biomass than their wild relatives, although there are no statistically significant differences (Fig. 4B). Wheat has the largest aboveground biomass in domesticated *T. timopheevii*, which has larger shoot and leaf biomass than its wild progenitor, *T. araraticum* (Fig. 4B; Table 1). Meanwhile, *T.timopheevii* is also larger than the other domesticated wheats *T. dicoccum* and *T. monococ*

2.4.5 Leaf traits

Wheat evolution under cultivation has substantially altered leaf traits. In particular, maximum leaf length and flag leaf width were substantially increased during

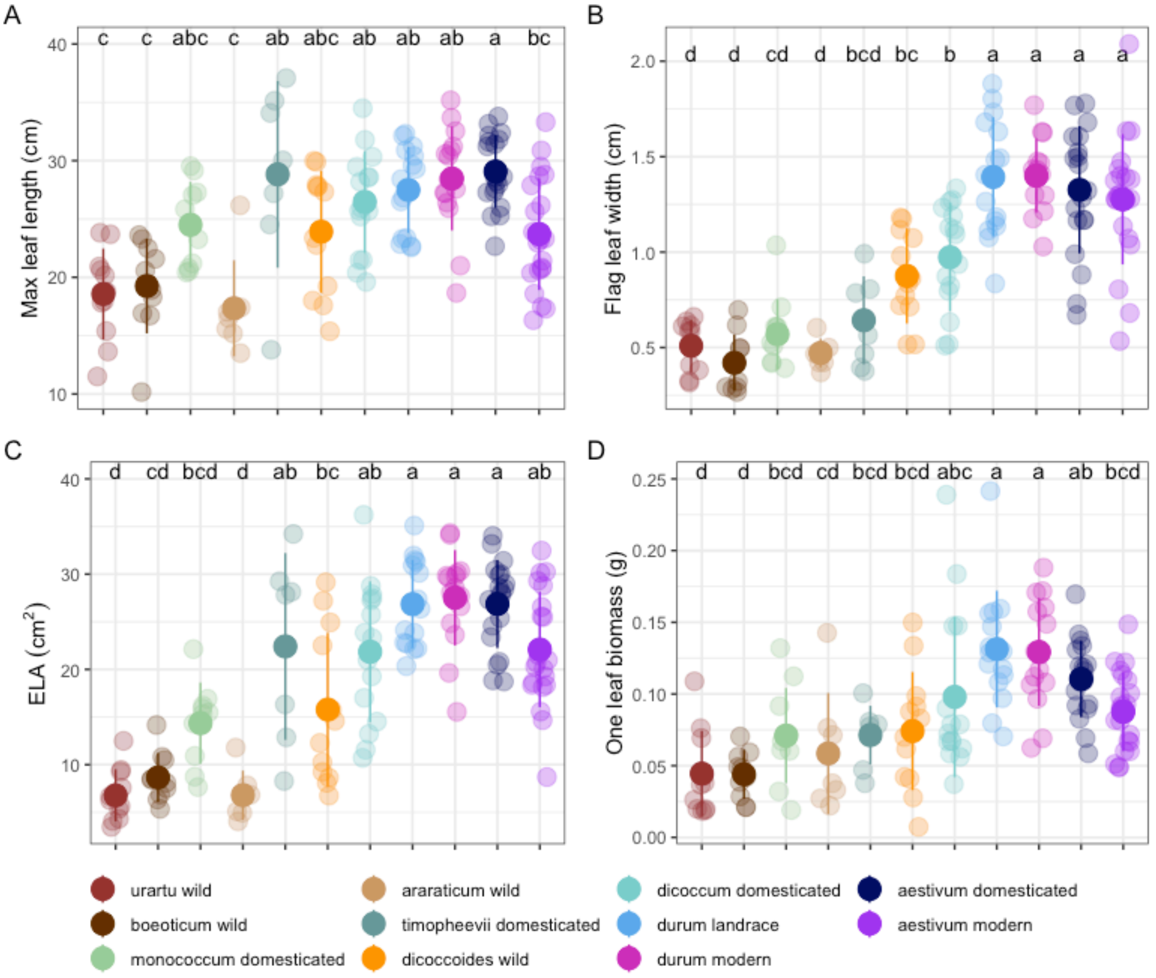


Figure 5: Diversity of leaf traits among wheat species. (A) maximum leaf length; (B) flag leaf width (C) individual leaf area, which is calculated using the maximum leaf length and width; (D) individual leaf biomass. Different letters above points indicate significant differences at p < .05 using Tukey's multiple comparison test.

domestication (Table 1). Fig 5A shows that leaf length increased most notably during the domestication of *T. araraticum* to *T. timopheevii*. Similarly, the width of the flag leaf was significantly increased during landrace improvement (Fig 5B, Table 1), enlarging individual leaves (Table 1). Although our analysis did not reveal a significant increase in leaf area during domestication (Table 1), the independently domesticated species *T. araraticum*-*T. timopheevii* showed a strong increase (Figure 5C). Mixed models found that individual leaf biomass increased continuously throughout both polyploid and domestication stages (Table 1), but the HSD test did not find significant differences among neighbouring individual wheat species (Fig 5D). Overall, leaf size showed a consistently increasing trend throughout the diversification of wheat, with the exception of modern varieties, which had shorter leaf lengths than *T. aestivum* landraces (Fig. 5A; Table 1). However, modern polyploid wheat leaves still have a much larger area than those of their ancient diploid progenitor, *T. urartu*.

2.4.6 Yield related traits

Yield related traits are of greatest concern from agronomic and economic perspectives. During domestication, the spikelet number increased significantly. Fig. 6A particularly shows large differences among wild and domesticated forms in the einkorn (*T. boeoticum – T. monococcum*) and emmer (*T. araraticum – T. timopheevii*, *T. dicoccoides – T. dicoccum*) groups. Grain number and grain weight also show an overall increasing trend throughout wheat diversification (Fig. 6B and 6C). In the analysis of wheat species, this increase is slow (Fig. 6B and 6C) and the huge gap between modern *T. aestivum* and wild *T. urartu* is formed gradually. However, mixed effects models point to two stages where changes are particularly pronounced, domestication and the Green Revolution (Table 1). The number of grains per spike, and the mass of individual grains, have both increased, with a consequent increase in the total grain mass per spike (Fig. 6B, 6C and 6D; Table 1). However, changes are not obvious at other stages (Fig. 6A, 6B and 6C; Table 1). Polyploid formation increases the individual grain weight significantly (Table 1), but in the contrasts among wheat species, the effects of polyploidy and landrace improvement are relatively small (Fig. 6D).

Domestication and selective breeding have brought higher yields in wheat, as expected. However, our experiment indicates that improvements have not been continuous, with the major change in yield being associated with domestication, as evidenced across three independent events (Table 1). In contrast, neither polyploidy in wild plants, nor landrace improvement and modern breeding, have had effects of an equivalent magnitude to those of domestication (Fig 6E; Table 1) under the conditions used in our study (individual plants grown in pots). The anticipated increase in harvest index associated with short stature plants after the Green Revolution is apparent in our data, but is not statistically significant due to substantial variation in this emergent trait within landraces and modern varieties of bread wheat (Fig. 6F; Table 1). In contrast, the statistical power associated with three domestication events shows statistically significant increases of harvest index in these cases (Fig. 6F; Table 1).

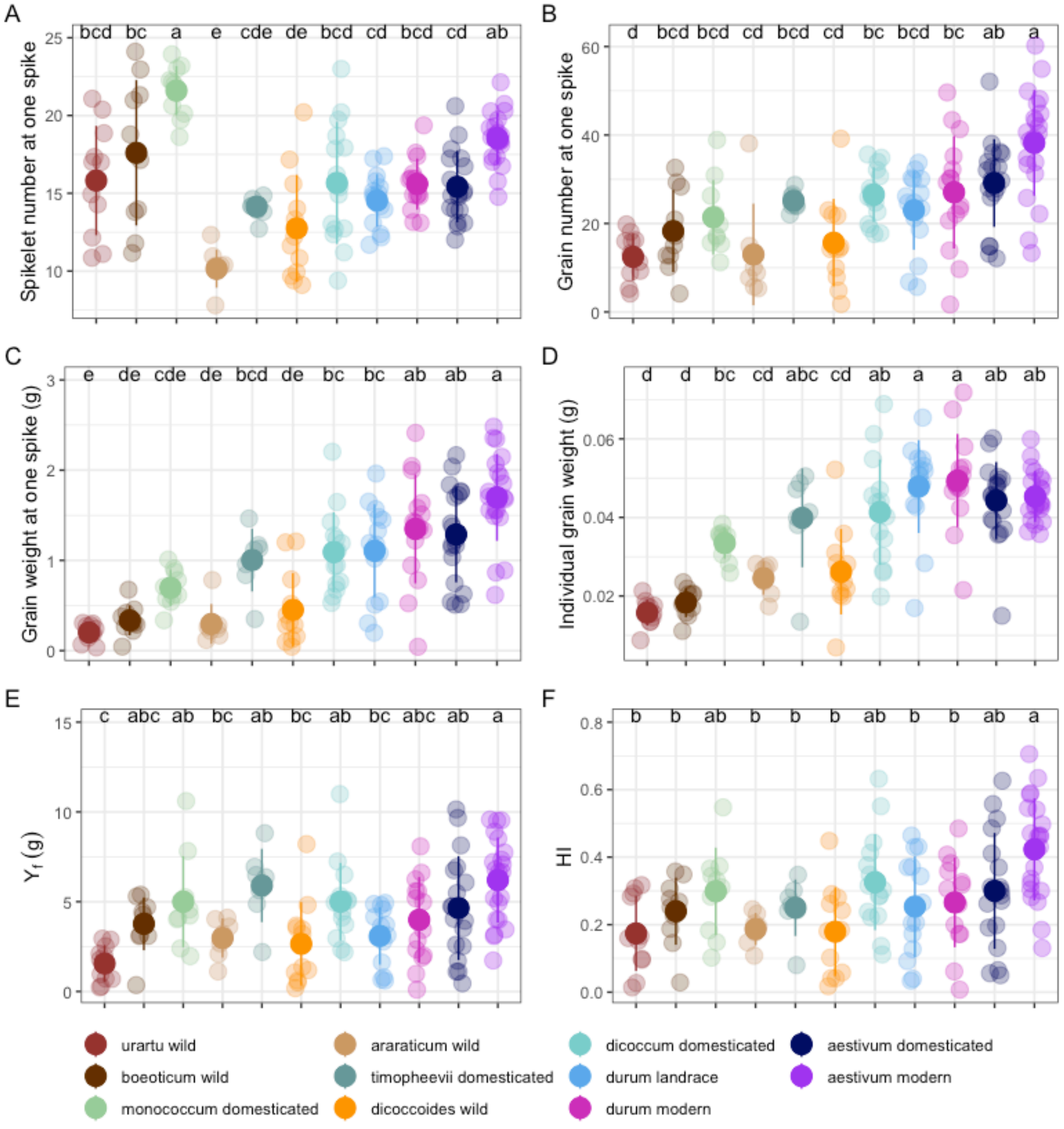


Figure 6: Diversity of yield-related traits among wheat species.(A) spikelet number on the largest spike; (B) grain number on the largest spike; (C) grain weight on the largest spike; (D) mean individual grain weight; (E) expected final yield for one plant, considering tiller loss; (F) expected harvest index for one wheat plant. Different letters above points indicate significant differences at $p < 0.05$ using Tukey’s multiple comparison test.

2.5 Discussions

In this study, we compared the morphological traits of wheat and investigated the stages of evolution at which they occurred. Our findings revealed that morphological changes during the evolution of wheat have been episodic, with different evolutionary trajectories for each trait. During each period, historical events caused wheat to improve its strategies for adapting to the external environment or to meet the artificial requirements of farmers.

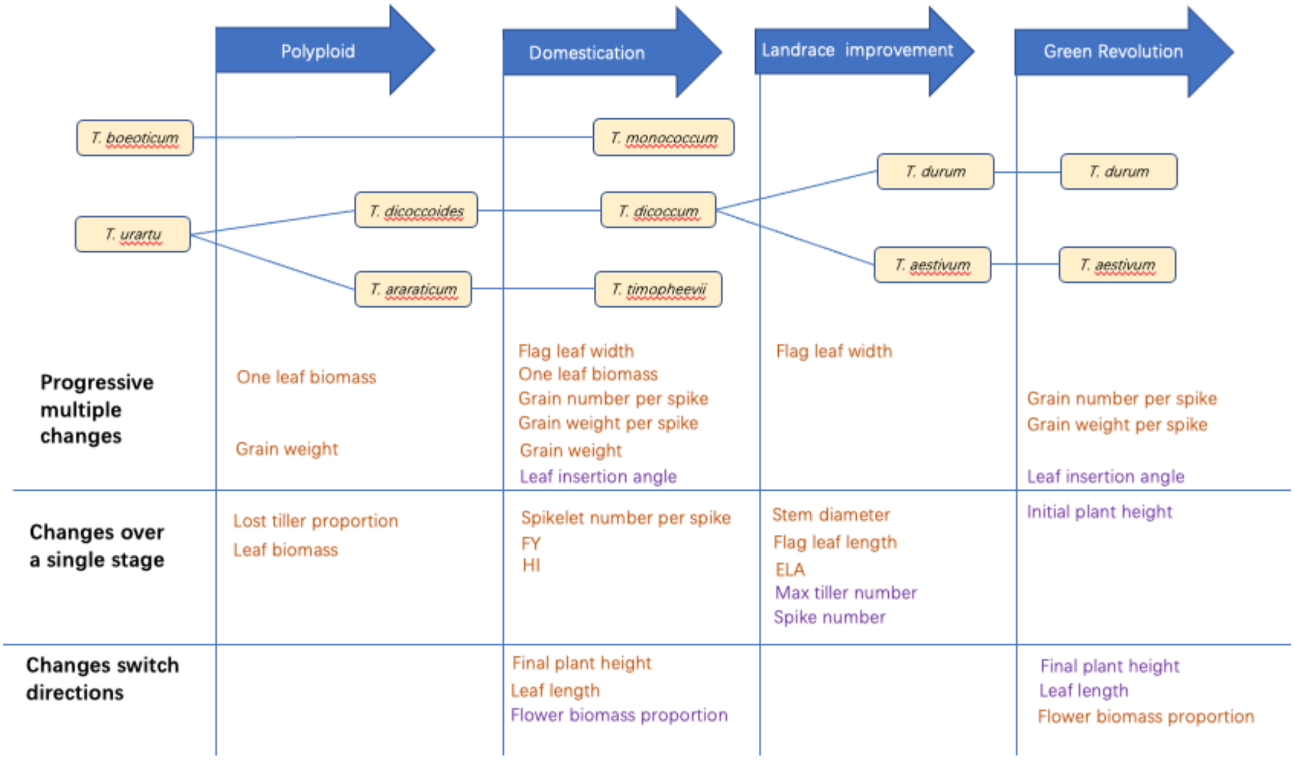


Figure 7: Conceptual diagram of wheat evolution, showing trait changes at four evolutionary stages (polyploid formation, domestication, landrace improvement and the Green Revolution). The traits with orange colour have increased values, whereas those with purple colour have decreased values.

2.5.1 Distinct patterns of phenotypic variation through history

The phenotypic variation observed in wheat reflects its growth strategies across the four examined periods (i.e., polyploid, domestication, landrace improvement, and the Green Revolution). For wild wheats, their main priority is to reproduce and survive. Genome doubling increases the genome sizes of wheats (Özkan *et al.*, 2010), allowing leaf size and seed size to increase. Our study is consistent with previous work, showing that tetraploid wheat (AABB, AAGG) has thicker leaves with more dry matter and chlorophyll per unit area than diploid ones (Kaminski *et al.*, 1990), suggesting that polyploidization promotes wheat photosynthesis as a source of increased vigour. The seed sizes of polyploids are typically larger than those of their diploid relatives (Dhawan & Lavania, 1996), and larger seeds provide competitive advantages in crop progenitors (Preece *et al.*, 2021). Compared with diploids, larger tetraploid seeds often result in greater growth vigour, as seen in muskmelons(Batra, 1952) and subterranean clover (Hutton & Peak, 1954). Larger seed and leaf biomass as characteristics of gigantism are considered typical features of polyploidy (Heslop-Harrison *et al.*, 2023), although neither is found with statistical significance in our study. This might be due to the slow growth speed of polyploids during the adult stage that has been observed previously (Bose & Choudhury, 1962). Further work supports this interpretation by comparing growth in diplod-tetraploid pairs of *Phlox drummondii*, finding that tetraploids tended to produce lower intrinsic rates of leaf growth, and fewer but larger flowers (Garbutt & Bazzaz, 1983). This finding may explain the increase in tiller loss we observed in polyploid wheat, even though tiller and spike numbers did not show significant variation. Therefore, we can infer that, although polyploidy influences early size and vigour, leaf size and tiller retention, it does not have obvious overall effects on growth.

Increased seed and leaf sizes continued through the process of domestication. In fact, the larger size of seeds may have strong positive relationships with larger leaves (Hodgson *et al.*, 2017) and they have been a crucial factor in species selection for cultivation (Preece *et al.*, 2015). During domestication, seed size is thought to have increased through selection on plant size and production, or natural selection for competitive ability, which indirectly selected for larger sizes of individual plant parts (Jones *et al.*, 2021). The nature of selection during domestication is controversial. In ancient cultivation, increased seed size might come from unconscious natural selection (Harlan *et al.*, 1973) by farmers because they lacked foresight of the potential for selective breeding (Kluyver *et al.*, 2017). In this case, the collection of plants from the wild or their cultivation in farming environments drove natural selection for traits that adapted crops for the new environment or harvest system (Zohary, 2004). However, Darwin believed that farmers were unconsciously selecting large seeds as a domestication trait by planting larger seeds each generation and discarded smaller ones (Darwin’s, 1859). This led to changes in the population without any deliberate planning (Darwin, 1868). Most recently, Jones argued that domesticated traits may be selected for by plant competition under anthropogenic environments (Jones *et al.* 2021). Our study cannot distinguish between these mechanisms, but did find that various traits including leaf size, plant height and grain mass all showed an increase consistent with previous ideas of domesticated plant morphology as gigantism (Fig. 7) (Milla & Matesanz, 2017; Gómez-Fernández *et al.*, 2022).

Our findings of a decrease in biomass allocation to flowers with domestication, despite the associated yield increase is at first sight a contradiction. However, they are consistent with previous work for emmer and einkorn wheat that showed reduced allocation to chaff (non-seed reproductive biomass) linked to domestication (Preece et al., 2017). Thus, seeds are favoured in domesticated wheats at the expense of other flowering structures.

Landrace improvement in wheat has led to reduced tillering and the promotion of main stem growth. Both tiller and spike numbers decrease but, at the same time, flag leaf size and stem diameter increase (Fig. 7). These changes reflect a classic trade-off between spike number and grain weight (Xie & Sparkes, 2021). In a field situation, fewer spikes per plant lead to higher yields, since decreased spike numbers can be compensated by high planting density (Li *et al.*, 2016). Previous work in rice has also suggested that decreased spike numbers would lead to sufficient grain filling and high starch content (Panigrahi *et al.*, 2019). However, our work does not find greater grain weight in landraces compared with less improved domesticated forms.

Our data for Green Revolution varieties show the well-known trade-off between investment in the stem and grains, seen as reduced plant height and improved yield. This variation has been mentioned in many studies (e.g. Würschum *et al.*, 2017; Hedden, 2003; Mann, 1997). Both initial plant height and final plant height are decreased. Investment in grain is promoted via increased flower proportion, grain number and weight (Fig. 7). Moreover, leaf size and insertion angle further decrease, meaning that intensive breeding has limited neighbour competition to favour investment in grains.

2.5.2 Continuity and opposition of trait change

Some trait values showed equivalent changes across multiple stages (Fig. 7). For example, leaf size increased during both polyploidy–domestication and domestication–landrace transitions. However, in wild plants the maximum leaf biomass increased, but in landrace improvement the flag leaf size increased. This may be because the flag leaf is more relevant to ear development (Sanchez-Bragado *et al.*, 2014), and is preferred by farmers or breeders. Domestication and Green Revolution both increased grain weight per spike and grain number per spike, which are more directly relevant to yielding. Moreover, the leaf insertion angle decreased at both these two stages. Leaf insertion angle, as one of the factors influencing wheat aboveground architecture, was thought to have changed during polyploidization (Li *et al.*, 2014). However, our work provides a wider range of wheat species at each polyploid and domestication level, and suggests that leaf insertion has been most influenced by the two farming stages. The increased density of farmed plants might have selected for more erect architectures, a conclusion supported by recent genetic evidence (Zhao *et al.*, 2023b).

However, there are some other traits showing opposite changes between domestication and the Green Revolution, indicating that modern breeding has in some respects needed to undo the effects of domestication. For example, both plant height and leaf length are important in early wheat improvement, but their reduction through selective breeding has improved flower biomass allocation. Thus, evolution during domestication led to trait combinations that are undesirable in modern agriculture. For example, selection for larger leaves and increased height helped to acquire aboveground resources (light and space) in early cultivated environments. However, these effects of gigantism in crops were detrimental for yields from the crop population as a whole. Crop plants need to cooperate, rather than compete, to maximise population yield (Anten & Vermeulen, 2016), such that crops with intermediate individual fitness have the highest yield per unit area (Weiner *et al.*, 2017).

2.5.3 Further development in phenotypic work and how phenotype benefits yield

Due to time and cost limitations, our phenotypic study was unable to study wheat root phenotypes, which may play an important role in wheat evolution. For example, domestication increases biomass allocation to the shoot instead of the root (Qin *et al.*, 2012), and the Green Revolution further decreased root biomass in elite wheat varieties (Waines & Ehdaie, 2007). As fertilizer applications increased under cultivation, wheats needed to allocate fewer resource to roots, to acquire water and nitrogen (Gioia *et al.*, 2015). We would therefore expect the individual competitiveness of modern wheat to decrease below ground.

Phenotyping of diverse wheat accessions has high current relevance, due to the focus on traits from wild progenitors in modern breeding programmes (Skovmand *et al.*, 2001) (Leigh *et al.*, 2022). Wheat germplasm diversity is generally thought to have decreased through artificial selection (Reif *et al.*, 2005) (Kilian *et al.*, 2010) (Haudry *et al.*, 2007). However, our work has shown that in some respects this loss has been associated with the diversification of trait values. The wild morphospace does not cover the domesticated one completely because new trait values were generated during wheat evolution. Crop diversification compensates for domestication bottlenecks by capturing part of the genetic diversity of its progenitors and by generating new diversity at a relatively fast pace (Dubcovsky & Dvorak, 2007). Thus, domesticated and modern morphospaces expand beyond that of the wild species, which represents valuable trait diversity available to breeders.

2.6 Conclusions

In conclusion, our study shows that wheat phenotypic evolution is a long, and complex process. Some traits have been continuously changed in the same directions through crop history, while other traits have changed in opposite directions during two or more periods. Differences between wild and modern wheats are therefore the product of multiple phases of historical change, in which natural and artificial selection have been variously important. This long history of crop diversification has generated valuable traits for using in today’s breeding work. Understanding the trajectory of wheat phenotypic evolution can therefore promote agricultural and germplasm improvement.

2.7 Reference

Abbo S, Gopher A. **2017**. Near Eastern Plant Domestication: A History of Thought. *Trends in Plant Science* **22**: 491–511.

Abbo S, Pinhasi van-Oss R, Gopher A, Saranga Y, Ofner I, Peleg Z. **2014**. Plant domestication versus crop evolution: a conceptual framework for cereals and grain legumes. *Trends in Plant Science* **19**: 351–360.

Anten NPR, Vermeulen PJ. **2016**. Tragedies and Crops: Understanding Natural Selection To Improve Cropping Systems. *Trends in Ecology & Evolution* **31**: 429–439.

Badaeva ED, Konovalov FA, Knüpffer H, Fricano A, Ruban AS, Kehel Z, Zoshchuk SA, Surzhikov SA, Neumann K, Graner A, *et al.* 2022. Genetic diversity, distribution and domestication history of the neglected GGAtAt genepool of wheat. *Theoretical and Applied Genetics* **135**: 755–776.

Batra S. **1952**. Induced tetraploidy in muskmelons. *Journal of Heredity* **43**: 141–148.

Bose RB, Choudhury JK. **1962**. A Comparative Study of the Cytotaxonomy, Pallynology, Physiology of ‘Diploid’ and ‘Polyploid’ Plants of Ocimum Kilimandscharicum Guerke and their Yield of Raw Material and Volatile Contents. *Caryologia* **15**: 435–454.

Bozzini A. **1988**. Origin, distribution, and production of durum wheat in the world. *Durum wheat: chemistry and technology*: 1–16.

Brown TA, Jones MK, Powell W, Allaby RG. **2009**. The complex origins of domesticated crops in the Fertile Crescent. *Trends in Ecology & Evolution* **24**: 103–109.

Byerlee D, Traxler G. **1995**. National and International Wheat Improvement Research in the Post-Green Revolution Period: Evolution and Impacts. *American Journal of Agricultural Economics* **77**: 268–278.

Cockram J, Jones H, Leigh FJ, O'Sullivan D, Powell W, Laurie DA, Greenland AJ. **2007**. Control of flowering time in temperate cereals: genes, domestication, and sustainable productivity. *Journal of Experimental Botany* **58**: 1231–1244.

Darwin C. **1868**. *The Variation of Animals and Plants Under Domestication*. J. Murray.

Darwin's C. **1859**. On the origin of species. *published on* **24**: 1.

Dhawan OP, Lavania UC. **1996**. Enhancing the productivity of secondary metabolites via induced polyploidy: a review. *Euphytica* **87**: 81–89.

Dubcovsky J, Dvorak J. **2007**. Genome Plasticity a Key Factor in the Success of Polyploid Wheat Under Domestication. *Science* **316**: 1862–1866.

Dvorak J, Deal KR, Luo M-C, You FM, von Borstel K, Dehghani H. **2012**. The Origin of Spelt and Free-Threshing Hexaploid Wheat. *Journal of Heredity* **103**: 426–441.

Erenstein O, Jaleta M, Mottaleb KA, Sonder K, Donovan J, Braun H-J. **2022**. Global Trends in Wheat Production, Consumption and Trade. In: Reynolds MP, Braun H-J, eds. Wheat Improvement: Food Security in a Changing Climate. Cham: Springer International Publishing, 47–66.

Evans LT. **1996**. *Crop evolution, adaptation and yield*. Cambridge university press.

Faris JD. **2014**. Wheat Domestication: Key to Agricultural Revolutions Past and Future. In: Tuberosa R, Graner A, Frison E, eds. Genomics of Plant Genetic Resources: Volume 1. Managing, sequencing and mining genetic resources. Dordrecht: Springer Netherlands, 439–464.

Fuller DQ. **2007**. Contrasting Patterns in Crop Domestication and Domestication Rates: Recent Archaeobotanical Insights from the Old World. *Annals of Botany* **100**: 903–924.

Garbutt K, Bazzaz FA. **1983**. Leaf Demography, Flower Production and Biomass of Diploid and Tetraploid Populations of Phlox Drummondii Hook. on a Soil Moisture Gradient. *New Phytologist* **93**: 129–141.

Gioia T, Nagel KA, Beleggia R, Fragasso M, Ficco DBM, Pieruschka R, De Vita P, Fiorani F, Papa R. **2015**. Impact of domestication on the phenotypic architecture of durum wheat under contrasting nitrogen fertilization. *Journal of Experimental Botany* **66**: 5519–5530.

Gómez-Fernández A, Osborne CP, Rees M, Palomino J, Ingala C, Gómez G, Milla R. **2022**. Disparities among crop species in the evolution of growth rates: the role of distinct origins and domestication histories. *New Phytologist* **233**: 995–1010.

Gui Y, Sheteiwy MS, Zhu S, Zhu L, Batool A, Jia T, Xiong Y. **2021**. Differentiate responses of tetraploid and hexaploid wheat (Triticum aestivum L.) to moderate and severe drought stress: a cue of wheat domestication. *Plant Signaling & Behavior* **16**: 1839710.

Harlan JR, de Wet JMJ, Price EG. **1973**. Comparative Evolution of Cereals. *Evolution* **27**: 311–325.

Haudry A, Cenci A, Ravel C, Bataillon T, Brunel D, Poncet C, Hochu I, Poirier S, Santoni S, Glémin S, *et al.* **2007**. Grinding up Wheat: A Massive Loss of Nucleotide Diversity Since Domestication. *Molecular Biology and Evolution* **24**: 1506–1517.

Hedden P. **2003**. The genes of the Green Revolution. *Trends in Genetics* **19**: 5–9.

Heslop-Harrison JS (Pat), Schwarzacher T, Liu Q. **2023**. Polyploidy: its consequences and enabling role in plant diversification and evolution. *Annals of Botany* **131**: 1–10.

Heun M, Schäfer-Pregl R, Klawan D, Castagna R, Accerbi M, Borghi B, Salamini F. **1997**. Site of Einkorn Wheat Domestication Identified by DNA Fingerprinting. *Science* **278**: 1312–1314.

Hodgson JG, Santini BA, Montserrat Marti G, Royo Pla F, Jones G, Bogaard A, Charles M, Font X, Ater M, Taleb A, *et al.* **2017**. Trade-offs between seed and leaf size (seed–phytomer–leaf theory): functional glue linking regenerative with life history strategies … and taxonomy with ecology? *Annals of Botany* **120**: 633–652.

Hutton WM, Peak JW. **1954**. The effect of autotetraploidy in five varieties of subterranean clover (Trifolium subterraneum L.). *Australian Journal of Agricultural Research* **5**: 356–364.

Introduction to Wheat Growth. **2016**. *Wheat Training*.

Johnson BL, Dhaliwal HS. **1976**. Reproductive Isolation of Triticum Boeoticum and Triticum Urartu and the Origin of the Tetraploid Wheats. *American Journal of Botany* **63**: 1088–1094.

Jones G, Kluyver T, Preece C, Swarbrick J, Forster E, Wallace M, Charles M, Rees M, Osborne CP. **2021**. The origins of agriculture: Intentions and consequences. *Journal of Archaeological Science* **125**: 105290.

Kaminski ANN, Austin RB, FORD MA, Morgan CL. **1990**. Flag leaf anatomy of Triticum and Aegilops species in relation to photosynthetic rate. *Annals of Botany* **66**: 359–365.

Kilian B, Martin W, Salamini F. **2010**. Genetic Diversity, Evolution and Domestication of Wheat and Barley in the Fertile Crescent. In: Glaubrecht M, ed. Evolution in Action: Case studies in Adaptive Radiation, Speciation and the Origin of Biodiversity. Berlin, Heidelberg: Springer, 137–166.

Kluyver TA, Jones G, Pujol B, Bennett C, Mockford EJ, Charles M, Rees M, Osborne CP. **2017**. Unconscious selection drove seed enlargement in vegetable crops. *Evolution Letters* **1**: 64–72.

Leigh FJ, Wright TIC, Horsnell RA, Dyer S, Bentley AR. **2022**. Progenitor species hold untapped diversity for potential climate-responsive traits for use in wheat breeding and crop improvement. *Heredity* **128**: 291–303.

Li P-F, Cheng Z-G, Ma B-L, Palta JA, Kong H-Y, Mo F, Wang J-Y, Zhu Y, Lv G-C, Batool A, *et al.* **2014**. Dryland Wheat Domestication Changed the Development of Aboveground Architecture for a Well-Structured Canopy. *PLOS ONE* **9**: e95825.

Li Y, Cui Z, Ni Y, Zheng M, Yang D, Jin M, Chen J, Wang Z, Yin Y. **2016**. Plant Density Effect on Grain Number and Weight of Two Winter Wheat Cultivars at Different Spikelet and Grain Positions. *PLOS ONE* **11**: e0155351.

Mann C. **1997**. Reseeding the Green Revolution. *Science* **277**: 1038–1043.

Milla R, Matesanz S. **2017**. Growing larger with domestication: a matter of physiology, morphology or allocation? *Plant Biology* **19**: 475–483.

Oliveira HR, Jacocks L, Czajkowska BI, Kennedy SL, Brown TA. **2020**. Multiregional origins of the domesticated tetraploid wheats. *PLOS ONE* **15**: e0227148.

Özkan H, Tuna M, Kilian B, Mori N, Ohta S. **2010**. Genome size variation in diploid and tetraploid wild wheats. *AoB PLANTS* **2010**: plq015.

Panigrahi R, Kariali E, Panda BB, Lafarge T, Mohapatra PK. **2019**. Corrigendum to: Controlling the trade-off between spikelet number and grain filling: the hierarchy of starch synthesis in spikelets of rice panicle in relation to hormone dynamics. *Functional Plant Biology* **46**: 595–595.

Peleg Z, Fahima T, Korol AB, Abbo S, Saranga Y. **2011**. Genetic analysis of wheat domestication and evolution under domestication. *Journal of Experimental Botany* **62**: 5051–5061.

Peng J, Ronin Y, Fahima T, Röder MS, Li Y, Nevo E, Korol A. **2003**. Domestication quantitative trait loci in Triticum dicoccoides, the progenitor of wheat. *Proceedings of the National Academy of Sciences* **100**: 2489–2494.

Peng JH, Sun D, Nevo E. **2011**. Domestication evolution, genetics and genomics in wheat. *Molecular Breeding* **28**: 281.

Preece C, Jones G, Rees M, Osborne CP. **2021**. Fertile Crescent crop progenitors gained a competitive advantage from large seedlings. *Ecology and Evolution* **11**: 3300–3312.

Preece C, Livarda A, Wallace M, Martin G, Charles M, Christin P-A, Jones G, Rees M, Osborne CP. **2015**. Were Fertile Crescent crop progenitors higher yielding than other wild species that were never domesticated? *New Phytologist* **207**: 905–913.

Qin X, Niklas KJ, Qi L, Xiong Y, Li F. **2012**. The effects of domestication on the scaling of below- vs. aboveground biomass in four selected wheat (Triticum; Poaceae) genotypes. *American Journal of Botany* **99**: 1112–1117.

Reif JC, Zhang P, Dreisigacker S, Warburton ML, van Ginkel M, Hoisington D, Bohn M, Melchinger AE. **2005**. Wheat genetic diversity trends during domestication and breeding. *Theoretical and Applied Genetics* **110**: 859–864.

Roucou A, Violle C, Fort F, Roumet P, Ecarnot M, Vile D. **2018**. Shifts in plant functional strategies over the course of wheat domestication. *Journal of Applied Ecology* **55**: 25–37.

Sanchez-Bragado R, Elazab A, Zhou B, Serret MD, Bort J, Nieto-Taladriz MT, Araus JL. **2014**. Contribution of the ear and the flag leaf to grain filling in durum wheat inferred from the carbon isotope signature: Genotypic and growing conditions effects. *Journal of Integrative Plant Biology* **56**: 444–454.

Schrader J, Shi P, Royer DL, Peppe DJ, Gallagher RV, Li Y, Wang R, Wright IJ. **2021**. Leaf size estimation based on leaf length, width and shape. *Annals of Botany* **128**: 395–406.

Skovmand B, Reynolds MP, Delacy IH. **2001**. Mining Wheat Germplasm Collections for Yield Enhancing Traits. In: Bedö Z, Láng L, eds. Developments in Plant Breeding. Wheat in a Global Environment: Proceedings of the 6th International Wheat Conference, 5–9 June 2000, Budapest, Hungary. Dordrecht: Springer Netherlands, 761–771.

Tanno K, Willcox G. **2006**. How Fast Was Wild Wheat Domesticated? *Science* **311**: 1886–1886.

Waines JG, Ehdaie B. **2007**. Domestication and Crop Physiology: Roots of Green-Revolution Wheat. *Annals of Botany* **100**: 991–998.

Weiner J, Du Y-L, Zhang C, Qin X-L, Li F-M. **2017**. Evolutionary agroecology: individual fitness and population yield in wheat (Triticum aestivum). *Ecology* **98**: 2261–2266.

Würschum T, Langer SM, Longin CFH, Tucker MR, Leiser WL. **2017**. A modern Green Revolution gene for reduced height in wheat. *The Plant Journal* **92**: 892–903.

Xie Q, Sparkes DL. **2021**. Dissecting the trade-off of grain number and size in wheat. *Planta* **254**: 3.

Zhao X, Guo Y, Kang L, Yin C, Bi A, Xu D, Zhang Z, Zhang J, Yang X, Xu J, *et al.* **2023a**. Population genomics unravels the Holocene history of bread wheat and its relatives. *Nature Plants* **9**: 403–419.

Zhao L, Zheng Y, Wang Y, Wang S, Wang T, Wang C, Chen Y, Zhang K, Zhang N, Dong Z, *et al.* 2023b. A HST1-like gene controls tiller angle through regulating endogenous auxin in common wheat. *Plant Biotechnology Journal* **21**: 122–135.

Zohary D. **2004**. Unconscious selection and the evolution of domesticated Plants. *Economic Botany* **58**: 5–10.

2.8 Supporting information

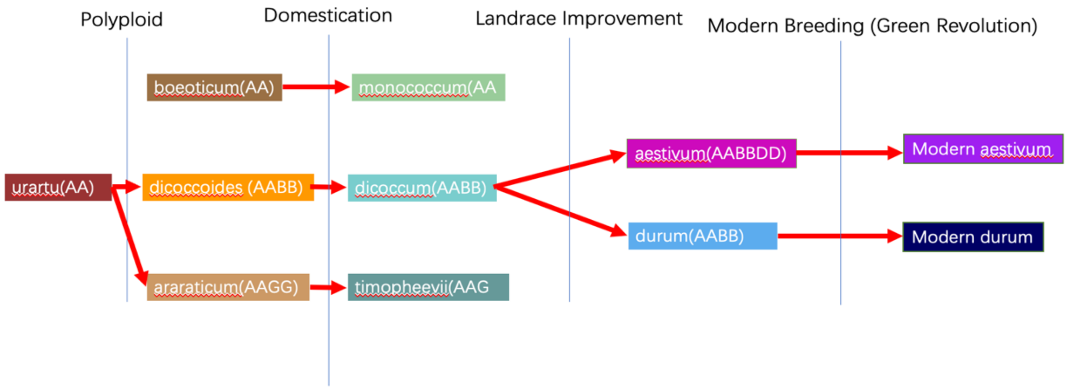
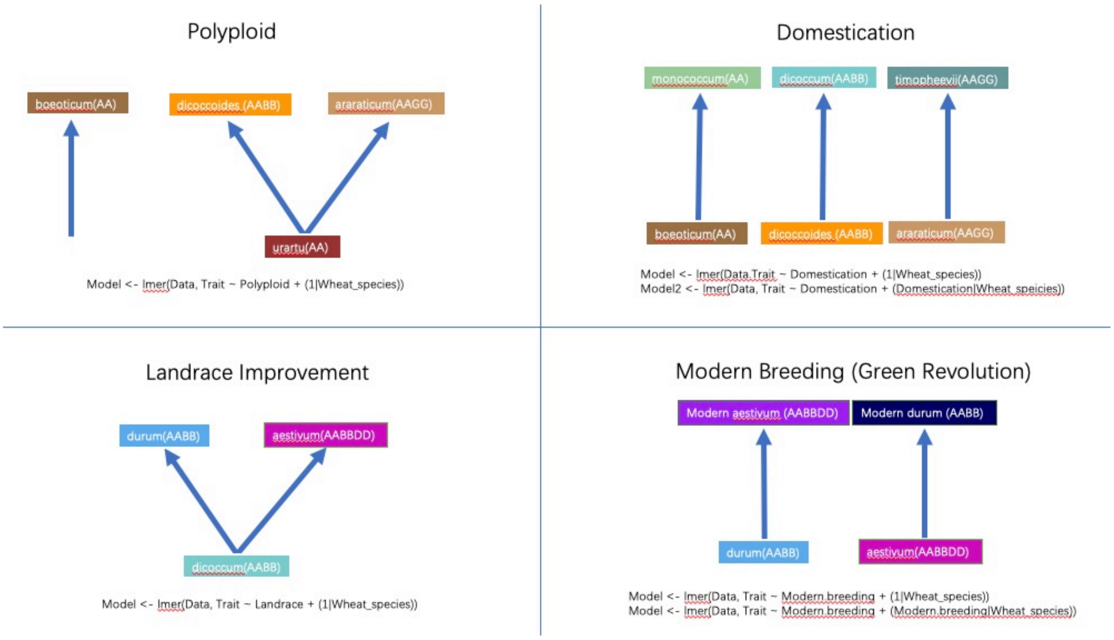


Figure S 1: the wheat evolution history and relations.



```
Model <- lmer(Data, Trait ~ Polyploid + (1|Wheat_species))
```

```
Model <- lmer(Data,Trait ~ Domestication + (1|Wheat_species))
Model2 <- lmer(Data, Trait ~ Domestication + (Domestication|Wheat_speicies))
```

```
Model <- lmer(Data, Trait ~ Landrace + (1|Wheat_species))
```

```
Model <- lmer(Data, Trait ~ Modern.breeding + (1|Wheat_species))
Model <- lmer(Data, Trait ~ Modern.breeding + (Modern.breeding|Wheat_species))
```

Figure S 2: the wheat accessions and event timepoint in wheat evolution. The statistical method applied a mixed effects model. The four big events are regarded as fixed factors respectively. The wheat species are random effects.

Table S 1: all wheat accessions used in this experiments.

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
York 102+aestivum25	domesticated	hexaploid	aestivum domesticated	aestivum	York 102	University of York
York 198+aestivum27	domesticated	hexaploid	aestivum domesticated	aestivum	York 198	University of York
York 209+aestivum4	domesticated	hexaploid	aestivum domesticated	aestivum	York 209	University of York
York 229+aestivum29	domesticated	hexaploid	aestivum domesticated	aestivum	York 229	University of York
York 239+aestivum17	domesticated	hexaploid	aestivum domesticated	aestivum	York 239	University of York
York 246+aestivum28	domesticated	hexaploid	aestivum domesticated	aestivum	York 246	University of York
York 271+aestivum5	domesticated	hexaploid	aestivum domesticated	aestivum	York 271	University of York
York 286+aestivum16	domesticated	hexaploid	aestivum domesticated	aestivum	York 286	University of York
York 297+aestivum30	domesticated	hexaploid	aestivum domesticated	aestivum	York 297	University of York
York 299+aestivum6	domesticated	hexaploid	aestivum domesticated	aestivum	York 299	University of York
York 302+aestivum11	domesticated	hexaploid	aestivum domesticated	aestivum	York 302	University of York

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
York 310+aestivum13	domesticated	hexaploid	aestivum domesticated	aestivum	York 310	University of York
York 311+aestivum7	domesticated	hexaploid	aestivum domesticated	aestivum	York 311	University of York
York 312+aestivum12	domesticated	hexaploid	aestivum domesticated	aestivum	York 312	University of York
York 321+aestivum15	domesticated	hexaploid	aestivum domesticated	aestivum	York 321	University of York
York 328+aestivum10	domesticated	hexaploid	aestivum domesticated	aestivum	York 328	University of York
York 334+aestivum9	domesticated	hexaploid	aestivum domesticated	aestivum	York 334	University of York
York 335+aestivum31	domesticated	hexaploid	aestivum domesticated	aestivum	York 335	University of York
York 75+aestivum23	domesticated	hexaploid	aestivum domesticated	aestivum	York 75	University of York
TRI 10324+dicoccum4	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 10324	IPK
TRI 13158+dicoccum15	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 13158	IPK
TRI 14077+dicoccum5	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 14077	IPK
TRI 14734+dicoccum13	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 14734	IPK

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
TRI 16880+dicoccum7	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 16880	IPK
TRI 17038+dicoccum6	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 17038	IPK
TRI 17634+dicoccum8	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 17634	IPK
TRI 19232+dicoccum14	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 19232	IPK
TRI 19294+dicoccum16	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 19294	IPK
TRI 2215+dicoccum9	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 2215	IPK
TRI 28049+dicoccum17	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 28049	IPK
TRI 2884+dicoccum12	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 2884	IPK
TRI 29820+dicoccum11	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 29820	IPK
TRI 6141+dicoccum10	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 6141	IPK
TRI 9542+dicoccum3	domesticated	tetraploid	dicoccum domesticated	dicoccum	TRI 9542	IPK
CItr 14712+durum3	domesticated	tetraploid	durum landrace	durum	CItr 14712	IPK
CItr 14978+durum4	domesticated	tetraploid	durum landrace	durum	CItr 14978	IPK

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
CItr 15024+durum5	domesticated	tetraploid	durum landrace	durum	CItr 15024	IPK
CItr 5083+durum1	domesticated	tetraploid	durum landrace	durum	CItr 5083	IPK
TRI 10513+durum15	domesticated	tetraploid	durum landrace	durum	TRI 10513	IPK
TRI 14570+durum22	domesticated	tetraploid	durum landrace	durum	TRI 14570	IPK
TRI 14690+durum16	domesticated	tetraploid	durum landrace	durum	TRI 14690	IPK
TRI 1542+durum9	domesticated	tetraploid	durum landrace	durum	TRI 1542	IPK
TRI 26410+durum20	domesticated	tetraploid	durum landrace	durum	TRI 26410	IPK
TRI 26511+durum8	domesticated	tetraploid	durum landrace	durum	TRI 26511	IPK
TRI 2721+durum12	domesticated	tetraploid	durum landrace	durum	TRI 2721	IPK
TRI 2928+durum13	domesticated	tetraploid	durum landrace	durum	TRI 2928	IPK
TRI 29588+durum19	domesticated	tetraploid	durum landrace	durum	TRI 29588	IPK
TRI 5508+durum14	domesticated	tetraploid	durum landrace	durum	TRI 5508	IPK
W 2604+durum24	domesticated	tetraploid	durum landrace	durum	W 2604	IPK
PI 418583+monococcum8	domesticated	diploid	monococcum domesticated	monococcum	PI 418583	NPGS
PI 428159+monococcum9	domesticated	diploid	monococcum domesticated	monococcum	PI 428159	NPGS
TRI 19406+monococcum10	domesticated	diploid	monococcum domesticated	monococcum	TRI 19406	IPK

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
TRI 28132+monococcum15	domesticated	diploid	monococcum domesticated	monococcum	TRI 28132	IPK
TRI 28139+monococcum11	domesticated	diploid	monococcum domesticated	monococcum	TRI 28139	IPK
TRI 28142+monococcum17	domesticated	diploid	monococcum domesticated	monococcum	TRI 28142	IPK
TRI 28145+monococcum14	domesticated	diploid	monococcum domesticated	monococcum	TRI 28145	IPK
TRI 28175+monococcum13	domesticated	diploid	monococcum domesticated	monococcum	TRI 28175	IPK
TRI 28176+monococcum12	domesticated	diploid	monococcum domesticated	monococcum	TRI 28176	IPK
TRI 28186+monococcum16	domesticated	diploid	monococcum domesticated	monococcum	TRI 28186	IPK
CItr 15205+timopheevii1	domesticated	diploid	timopheevii domesticated	timopheevii	CItr 15205	IPK
PI 119442+timopheevii2	domesticated	diploid	timopheevii domesticated	timopheevii	PI 119442	NPGS

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
PI 221421+timopheevii9	domesticated	diploid	timopheevii domesticated	timopheevii	PI 221421	NPGS
PI 272530+timopheevii4	domesticated	diploid	timopheevii domesticated	timopheevii	PI 272530	NPGS
PI 282932+timopheevii5	domesticated	diploid	timopheevii domesticated	timopheevii	PI 282932	NPGS
PI 352512+timopheevii6	domesticated	diploid	timopheevii domesticated	timopheevii	PI 352512	NPGS
TRI 4349+timopheevii8	domesticated	diploid	timopheevii domesticated	timopheevii	TRI 4349	IPK
ALCHEMY14	modern	hexaploid	aestivum modern	modern_wheat	ALCHEMY	NIAB
BANCO3	modern	hexaploid	aestivum modern	modern_wheat	BANCO	NIAB
BERSEE18	modern	hexaploid	aestivum modern	modern_wheat	BERSEE	NIAB
BROMPTON19	modern	hexaploid	aestivum modern	modern_wheat	BROMPTON	NIAB
CLAIRE22	modern	hexaploid	aestivum modern	modern_wheat	CLAIRE	NIAB
COPAIN2	modern	hexaploid	aestivum modern	modern_wheat	COPAIN	NIAB
CORDIALE7	modern	hexaploid	aestivum modern	modern_wheat	CORDIALE	NIAB
FLAMINGO11	modern	hexaploid	aestivum modern	modern_wheat	FLAMINGO	NIAB
GLADIATOR15	modern	hexaploid	aestivum modern	modern_wheat	GLADIATOR	NIAB

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
HEREWARD6	modern	hexaploid	aestivum modern	modern_wheat	HEREWARD	NIAB
HOLDFAST10	modern	hexaploid	aestivum modern	modern_wheat	HOLDFAST	NIAB
KLOKA20	modern	hexaploid	aestivum modern	modern_wheat	KLOKA	NIAB
MARIS FUNDIN4	modern	hexaploid	aestivum modern	modern_wheat	MARIS FUNDIN	NIAB
RIALTO12	modern	hexaploid	aestivum modern	modern_wheat	RIALTO	NIAB
ROBIGUS9	modern	hexaploid	aestivum modern	modern_wheat	ROBIGUS	NIAB
SLEPNER8	modern	hexaploid	aestivum modern	modern_wheat	SLEPNER	NIAB
SOISSONS1	modern	hexaploid	aestivum modern	modern_wheat	SOISSONS	NIAB
SPARK21	modern	hexaploid	aestivum modern	modern_wheat	SPARK	NIAB
STEADFAST16	modern	hexaploid	aestivum modern	modern_wheat	STEADFAST	NIAB
STETSON17	modern	hexaploid	aestivum modern	modern_wheat	STETSON	NIAB
XI 19/13	modern	hexaploid	aestivum modern	modern_wheat	XI 19/13	NIAB
TRI 10271+durum23	modern	tetraploid	durum modern	durum	TRI 10271	IPK
TRI 16641+durum27	modern	tetraploid	durum modern	durum	TRI 16641	IPK
TRI 19047+durum28	modern	tetraploid	durum modern	durum	TRI 19047	IPK
TRI 19241+durum39	modern	tetraploid	durum modern	durum	TRI 19241	IPK
TRI 26968+durum41	modern	tetraploid	durum modern	durum	TRI 26968	IPK
TRI 2930+durum33	modern	tetraploid	durum modern	durum	TRI 2930	IPK
TRI 3216+durum30	modern	tetraploid	durum modern	durum	TRI 3216	IPK

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
TRI 3615+durum31	modern	tetraploid	durum modern	durum	TRI 3615	IPK
TRI 6328+durum29	modern	tetraploid	durum modern	durum	TRI 6328	IPK
TRI 6998+durum25	modern	tetraploid	durum modern	durum	TRI 6998	IPK
TRI 7662+durum38	modern	tetraploid	durum modern	durum	TRI 7662	IPK
TRI 880+durum26	modern	tetraploid	durum modern	durum	TRI 880	IPK
TRI 9776+durum36	modern	tetraploid	durum modern	durum	TRI 9776	IPK
TRI 9836+durum42	modern	tetraploid	durum modern	durum	TRI 9836	IPK
TRI 9936+durum34	modern	tetraploid	durum modern	durum	TRI 9936	IPK
PI 361859+araraticum1	wild	tetraploid	araraticum wild	araraticum	PI 361859	NPGS
PI 427998+araraticum2	wild	tetraploid	araraticum wild	araraticum	PI 427998	NPGS
TRI 11345+araraticum6	wild	tetraploid	araraticum wild	araraticum	TRI 11345	IPK
TRI 11354+araraticum4	wild	tetraploid	araraticum wild	araraticum	TRI 11354	IPK
TRI 18515+araraticum3	wild	tetraploid	araraticum wild	araraticum	TRI 18515	IPK
TRI 18534+araraticum5	wild	tetraploid	araraticum wild	araraticum	TRI 18534	IPK
TRI 7388+araraticum8	wild	tetraploid	araraticum wild	araraticum	TRI 7388	IPK

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
PI 352276+boeoticum2	wild	diploid	boeoticum wild	boeoticum	PI 352276	NPGS
PI 352503+boeoticum3	wild	diploid	boeoticum wild	boeoticum	PI 352503	NPGS
PI 352505+boeoticum4	wild	diploid	boeoticum wild	boeoticum	PI 352505	NPGS
PI 355522+boeoticum5	wild	diploid	boeoticum wild	boeoticum	PI 355522	NPGS
PI 407640+boeoticum7	wild	diploid	boeoticum wild	boeoticum	PI 407640	NPGS
PI 418580+boeoticum8	wild	diploid	boeoticum wild	boeoticum	PI 418580	NPGS
PI 427447+boeoticum9	wild	diploid	boeoticum wild	boeoticum	PI 427447	NPGS
PI 427465+boeoticum10	wild	diploid	boeoticum wild	boeoticum	PI 427465	NPGS
PI 427466+boeoticum11	wild	diploid	boeoticum wild	boeoticum	PI 427466	NPGS
PI 427637+boeoticum12	wild	diploid	boeoticum wild	boeoticum	PI 427637	NPGS
PI 256029+dicoccoides1	wild	tetraploid	dicoccoides wild	dicoccoides	PI 256029	NPGS
PI 266841+dicoccoides2	wild	tetraploid	dicoccoides wild	dicoccoides	PI 266841	NPGS

Wheat accession	**Domestication**	**Genome**	**Wheat name**	**Scientifc name**	**Wheat code**	**Source**
PI 352323+dicoccoides4	wild	tetraploid	dicoccoides wild	dicoccoides	PI 352323	NPGS
PI 352325+dicoccoides5	wild	tetraploid	dicoccoides wild	dicoccoides	PI 352325	NPGS
PI 352326+dicoccoides6	wild	tetraploid	dicoccoides wild	dicoccoides	PI 352326	NPGS
PI 362036+dicoccoides7	wild	tetraploid	dicoccoides wild	dicoccoides	PI 362036	NPGS
PI 428016+dicoccoides8	wild	tetraploid	dicoccoides wild	dicoccoides	PI 428016	NPGS
TRI 14095+dicoccoides15	wild	tetraploid	dicoccoides wild	dicoccoides	TRI 14095	IPK
TRI 18505+dicoccoides14	wild	tetraploid	dicoccoides wild	dicoccoides	TRI 18505	IPK
TRI 18530+dicoccoides10	wild	tetraploid	dicoccoides wild	dicoccoides	TRI 18530	IPK
TRI 18539+dicoccoides9	wild	tetraploid	dicoccoides wild	dicoccoides	TRI 18539	IPK
TRI 9865+dicoccoides16	wild	tetraploid	dicoccoides wild	dicoccoides	TRI 9865	IPK
PI 401411+urartu1	wild	diploid	urartu wild	urartu	PI 401411	NPGS
PI 427328+urartu2	wild	diploid	urartu wild	urartu	PI 427328	NPGS
PI 487271+urartu3	wild	diploid	urartu wild	urartu	PI 487271	NPGS
PI 662225+urartu4	wild	diploid	urartu wild	urartu	PI 662225	NPGS

Wheat accession	Domestication	Genome	Wheat name	Scientifc name	Wheat code	Source
TRI 17119+urartu7	wild	diploid	urartu wild	urartu	TRI 17119	IPK
TRI 17122+urartu8	wild	diploid	urartu wild	urartu	TRI 17122	IPK
TRI 17128+urartu6	wild	diploid	urartu wild	urartu	TRI 17128	IPK
TRI 17129+urartu5	wild	diploid	urartu wild	urartu	TRI 17129	IPK
TRI 17148+urartu11	wild	diploid	urartu wild	urartu	TRI 17148	IPK
TRI 17161+urartu12	wild	diploid	urartu wild	urartu	TRI 17161	IPK
TRI 6735+urartu14	wild	diploid	urartu wild	urartu	TRI 6735	IPK

Table S 2: the traits that we measured in this experiment.

Measuring Time	Trait	Age ref (days)	Explanantion
Apr-21	Seed_weight	0	individual seed weight, g
Apr-21	Germination_delay	10	how many days that seeds sprout need, days
May-21	Plant_height_May	40	shown as [Initial plant height]; choose the main, strech it and measure the length, cm
May-21	Architecture_height_May	40	plant height in narual states, cm
May-21	Leaf_number_May	40	leaf number at one plant in May
May-21	Tiller_number_May	40	tiller number in May
May-21	Leaf_length_May	40	the maxium leaf length in May, cm
Jun-21	Plant_height_June	70	plant height in June, cm
Jun-21	Architecture_height_June	70	plant height in natrual states, cm
Jun-21	Leaf_number_onestem_June	70	leaf number on the largest stem
Jun-21	Leaf_length_June	70	length of the largest leaf at one plant in June, cm
Jun-21	Leaf_width_June	70	width of the largest leaf at one plant in June, cm
Jun-21	Leaf_position_June	70	location on the leaf where width is maximal, ratio

Measuring Time	Trait	Age ref (days)	Explanantion
Jun-21	Leaf_insertion_June	70	Shown as [Leaf insertion angle]; insertion angle of leaves, angle
Jun-21	Leaf_curtivation_June	70	leaf curvature - angle between the bottom and top of leaf blade, angle
Jun-21	Shoot_hair_June	70	If shoot has white hair, Yes = 1, No = 0
Jun-21	Weed_June	70	If the pot has weeds. Yes= 1, No =0
Jun-21	Tiller_number_June	70	branch number in June
Jul-21	Spike_number_July	100	spike number in July
Jul-21	Spike_length_July	100	length of the largest spike, cm
Jul-21	Node_number_July	100	node number on the main stem
Jul-21	Stem_diameter_July	100	Shown as [Stem diameter]; largest stem diameter on the main stem, cm
Jul-21	Peduncle_length_July	100	peduncle length in July, cm
Jul-21	Plant_height_July	100	Shown as [Final plant height]; plant height in July, cm
Jul-21	Architecture_height_July	100	plant height at natural states, cm
Jul-21	Flag_leaf_length_July	100	leaf length of the flag leaf on the main stem, cm
Jul-21	Flag_leaf_width_July	100	Shown as [Flag leaf width]; leaf width of the flag leaf on the main stem, cm
Jul-21	Awn_length_July	100	the longest awn length, cm
Jul-21	One_leaf_length_July	100	Shown as [Max leaf length]; length of the largest leaf (not include flag leaf) in July, cm
Jul-21	One_leaf_width_July	100	width of the largest leaf (not include flag leaf) in July, cm
Jul-21	One_leaf_mass_July	100	mass of the largest leaf (not include flag leaf) in July, cm
Jul-21	Flower_mass_July	100	mass of all the spike at one plant, g
Jul-21	Leaf_mass_July	100	mass of all the leaves at one plant, g
Jul-21	Shoot_mass_July	100	mass of all the shoots at one plant, g
Jul-21	Leaf_biomass_July	100	biomass of all the leaves at one plant, g
Jul-21	Shoot_biomass_July	100	biomass of all the shoots at one plant, g
Jul-21	Flower_biomass_July	100	biomass of all the spike at one plant, g
Jul-21	One_leaf_biomass_July	100	Shown as [One leaf biomass]; biomass of the largest leaf on the main stem, g
Jul-21	Spikelet_number_July	100	spikelet number of the largest spike on the main stem

Measuring Time	Trait	Age ref (days)	Explanantion
Jul-21	One_spike_biomass_July	100	biomass of the largest spike on the main stem, g
Jul-21	Internode_biomass_July	100	biomass of the second internode the main stem, g
Jul-21	Peduncle_biomass_July	100	biomass of the peduncle on the main stem, g
Sep-21	Spike_number_harvest	160	spike number at one plant in harvest (consider spike loss)
Sep-21	Spikelet_number_onespike_harvest	160	Shown as [Spikelet number at one spike]; spikelet number of the largest spike in harvest
Sep-21	Spike_length_harvest	160	length of the largest spike in harvest, cm
Sep-21	Plant_height_harvest	160	plant height in harvest
Sep-21	Leaf_cur_angle_harvest	160	angle between consecutive leaves along a stem for the lower phytomers
Sep-21	Spike_ratio_harvest	160	raito of the spike harvest to the largest tiller number
Sep-21	Leafpetiole_ratio_harvest	160	fraction of leaf biomass partioned to the sheath
Sep-21	Flag_leafpetiole_ratio_harvest	160	fraction of flag leaf biomass partioned to the sheath
Sep-21	Grain_number_onespike_harvest	160	Shown as [Grain number at one spike]; grain number of the largest spike on the main stem
Sep-21	Grain_weight_onespike_harvest	160	Shown as [Grain weight at one spike]; average yielding of the lragest spike on the main stem, g
Sep-21	Grain_weight	160	Shown as [Individual grain wegiht]; individual grain weight from harvest, g

Chapter 3: Exploring wheat ideotypes using a Functional-Structural Plant Model

Yixiang Shan & Colin Osborne

Plants, Photosynthesis and Soil, School of Biosciences, University of Sheffield, Sheffield S10 2TN, UK;

3.1 Abstract

Wheat has undergone long-term adaptation to cultivated environments, and its phenotypes have changed to meet farmers' needs. The yield improvements driven by phenotype changes proved successful during domestication and the Green Revolution. However, yield improvements seem to have encountered a bottleneck, with a slowing of progress since the 1990s, motivating innovation in research towards new ideotypes. Here, we examined how the diversity in phenotypic traits among ancient and modern wheat accessions influence yield, and how the existing trait diversity might be combined in novel configurations to improve yield. We parameterised an FSP (Functional Structural Plant) model using empirical data for wheat morphology to explore ideotypes. We optimized groups of traits using two different methods, and tested the effects of density on these ideotypes. The first method using biomass traits found ideotypes that achieved a new balance in shoot, leaf, and flower allocation, to improve yield. The second method optimized leaf insertion angle, seed weight, and stem diameter, resulting in a change to ideotype architecture. The ideotypes based on an average historical wheat plant have been reproduced by modern breeding to increase flower and leaf biomass and stem diameter, but decrease plant height, internode biomass and leaf insertion angle. The ideotypes based on modern accessions would require the introduction of wild traits, including decreasing flower biomass, stem diameter and leaf insertion angle. Both ideotypes increased branch number and leaf sizes. However, in high-density farming, these ideotypes could not maintain their yield advantages. New optimized ideotypes were therefore developed for high density planting, by increasing flower biomass and stem diameter, but decreasing seed weight, leaf biomass, and branches, to become more group friendly. When ideotypes were optimized for high density planting, yield gains from trait optimisation are no longer evident. The results provide references to breeders and help them consider

which phenotypes are worth pursuing in wheat. The ideotypes identified will benefit crop production and agricultural progress.

3.2 Introduction

The imperative of addressing population growth and climate change necessitates a 70% increase in crop yield by 2050 to ensure food security (Tester & Langridge, 2010). Past enhancements in crop yield are attributed to domestication and the Green Revolution (Evenson & Gollin, 2003; Meyer *et al.*, 2012). Taking wheat as an example, domestication has significantly influenced yield through modifications in key traits such as spike number (Peng *et al.*, 2011), seed size (Fuller, 2007) and spike weight (Peng *et al.*, 2003). Likewise, the Green Revolution's impact on yield is notable, achieved by reducing wheat plant height and adjusting biomass allocation (Würschum *et al.*, 2017). These changes in phenotypic traits have collectively contributed to variation in crop yield.

Even before the elucidation of genetic mechanisms, ancient plant breeders and farmers practised selection based on observable phenotypic traits (Araus & Cairns, 2014). Donald played a pioneering role in highlighting the significance of wheat phenotype as a driving force in the breeding process (Donald, 1968). He introduced two primary breeding methodologies: (1) defect elimination and (2) selection for yield (Donald, 1968). These approaches involve mating elite progenitors to produce divergent populations, from which high-yielding individuals are selected and perpetuated (Sedgley, 1991). Defect elimination operates as a complement to yield-centric selection, eliminating traits known to impede yield. Its disadvantage is to prioritize yield or a singular trait, sometimes overlooking the interactions of correlated traits and their effects (Litrico & Violle, 2015). That means that wheat evolution has taken opposite directions at different times, e.g. plant height increased during domestication but decreased in the Green Revolution (Hedden, 2003).

The concept of the ideotype in breeding also originates with Donald (1968). In contrast to conventional breeding methodologies, Donald's approach to the ideotype concept employs a comprehensive system-wide modelling framework. The initial step in constructing an ideotype model involves defining the traits of interests, which are determined by the project objectives. The ideotype is then meticulously crafted to align with these defined goals. For instance, Donald's original ideal wheat type was underpinned by the objective of minimizing plant competition within a crop community (Donald, 1968). Furthermore, ideotypes geared towards disease control have gained traction as effective breeding strategies (Andrivon *et al.*, 2013). For this ideotype breeding strategy, yielding becomes the result of multiple phenotypic traits (Fischer & Edmeades, 2010). Wild genetic resources then need to be explored in order to achieve these new ideotypes (Kulwal *et al.*, 2022).

The advancement of computer science has facilitated the exploration of ideotypes through crop modelling (Rötter *et al.*, 2015). Notable instances of ideotype modeling abound in the literature. Semenov, for example, used the Sirius model to devise wheat ideotypes that adapt to varying European weather conditions (Semenov & Stratonovitch, 2013). Senapati then used the same Sirius model to assess the yield potential of wheat across diverse geographical locations (Senapati *et al.*, 2019) (Senapati & Semenov, 2019a) (Senapati & Semenov, 2020) (Senapati *et al.*, 2022). Bogard also applied a phenology model of winter wheat, called ARCWHEAT (Weir et al., 1984) to design ideotypes to improve their avoidance of abiotic stress (Bogard *et al.*, 2021). Beyond wheat, ideotype optimization has found application in other domains. In other investigations, optimization of leaf blade characteristics was carried out for sunflower and apple trees (Picheny *et al.*, 2017a). Maize and peanut ideotypes were improved to obtain high yield with APSIM (https://www.apsim.info/) under specific climate, soil and management practices ((Suriharn *et al.*, 2011)) (Xiao *et al.*, 2020). APSIM was also instrumental in simulating future barley ideotypes tailored to the Boreal and Mediterranean climatic zones (Tao *et al.*, 2017). Several specialized models have emerged catering to particular plant species. SIMPLE is a model to simulate germination and emergence, which has been applied in *Medicago truncatula* ideotype breeding (Brunel-Muguet *et al.*, 2011). The ARMOSA model provided a method to predict a maize ideotype with improved drought adaptations (Perego *et al.*, 2014). The SUNFLO model is specific to sunflower with an algorithm for the optimization of black-box models with uncertain climatic inputs (Picheny *et al.*, 2017b). The model named DSSAT (https://dssat.net/) produced in the USA, was commonly used in multiple crops, such as wheat (Li *et al.*, 2023), maize (Kothari *et al.*, 2022), cotton (Kothari *et al.*, 2021) and sorghum (Nagaleekara *et al.*, 2022).

Our study focused on wheat morphology, so we selected an FSP (Functional Structural Plant) model to simulate wheat growth (Vos *et al.*, 2010), because of its explicit consideration of organ sizes and plant branching architecture. FSP models are simulation models that simulate plant growth and development in time and three-dimensional (3-D) space. Two defining properties of all FSP models are: (1) the plant structure, i.e. the topological and/or 3-D geometric features of the plant, are explicitly considered as model input or output; treated as a separate entity (Evers *et al.*, 2018). These features support us to edit wheat morphological traits and then test their impacts on growth through modelling. We are able to combine yielding-friendly traits in one FSP wheat ideotype. Our objective is to optimize wheat ideotypes using phenotypic data from our previous wheat experiment.

We were interested in testing how the diversity in phenotypic traits among ancient and modern wheat accessions influences yield, and how the existing trait diversity might be combined in novel configurations to improve yield. We applied the wheat phenotypic data that we got in our previous experiment to calibrate two wheat models. The first was based on average trait values across the whole previous experiment – i.e.

an ”average” wheat, including wild species and landraces. In developing an ideotype from this baseline, we expected to reproduce some of the changes associated with the Green Revolution. The second model was based on average trait values for modern wheat. In optimizing an ideotype based on this baseline, we wanted to explore the potential for the unrealized remaining potential to improve modern wheats via morphological changes. After parameterizing baseline models, we changed trait values or parameters in those models to explore ideotypes with improved yields compared with the baseline cases. Finally, we test planting density effects on ideotypes and check if different ideotypes optimizations are adapted to increased densities.

3.3 Methods

3.3.1 FSP model development

Here, we applied an FSP (Functional Structural Plant) model of cereals, mainly including organ development and radiation modules, which was developed in the GroIMP platform (www.sourceforge.net/projects/groimp). In order to parameterise the model for wheat, we used the phenotypic dataset from the previous chapter (Chapter 2). In that experiment, morphologies were measured for 114 wheat accessions, spanning the diversity of wild, domesticated and improved varieties, and including *T. urartu*, *T. boeoticum*, *T. araraticum*, *T. dicoccoides*, *T. dicoccum*, *T. timopheevii*, *T. monococcum*, *T. durum*, *T. aestivum*, modern *T. durum* and modern *T. aestivum*. How to convert the wheat phenotyping data from Chapter 2, into input parameters for the FSP model in this chapter, can be found in Tables S1 and S2. In addition to phenotypic data, we also set the planting density as 25 plants/m^2 to match our previous wheat setup in Chapter 2. We first focused on modern *T. aestivum* and fit its phenotypic data to model parameters, generating a modern wheat in FSP as our first wheat baseline case. We also calculated the mean values of all 114 wheat morphological traits and parameterised a virtual average wheat as the second baseline case. These two basic wheat models served as the starting points for optimization.

3.3.2 Two methods for determining which traits to optimize

Optimising all parameters within the FSP model was unfeasible computationally. We therefore applied two methods to decide which traits might best be optimised. The first method is based on a sensitivity analysis of the parameterised model. We listed all the traits in the average wheat model that had been derived from quantitative empirical values measured in Chapter 2 (Table S1 and S2). Next, we varied each one from a 20% decrease to a 20% increase in 10% increments, recording how these changes influenced yield. The result was that, of the traits recorded in Chapter 2, only the maximum potential biomass of spikes (flower biomass), internodes (internode biomass) and leaves (leaf biomass) showed strong relationships with yields. These three traits are specified and coded in the model and are listed in the Table S1. These biomass capacities represent the maximum, genetically determined potential size of individual organs that can be achieved if enough carbon is supplied through photosynthesis. The potential spike and leaf biomasses showed positive relationships with yields but internode biomass capacity had a negative relationship. We therefore tested the maximum internode, leaf and flower biomass as traits for optimization.

As an alternative method for identifying the most influential input parameters for yield, we also applied a RF (random forest) algorithm to our wheat morphological dataset. I use the expected yield (Chapter 2) as the Y value and all the other traits as predictor variables. The result is shown in Figure 1. I chose three traits that ranked highly and translated directly into FSP parameters. At the same time, however, I had to filter out values that could not find a corresponding parameter in the model, even though they may have been ranked higher, such as [Leaf_biomass_July], [Leaf_mass_July] and [Shoot_mass_July]. After eliminating these parameters that

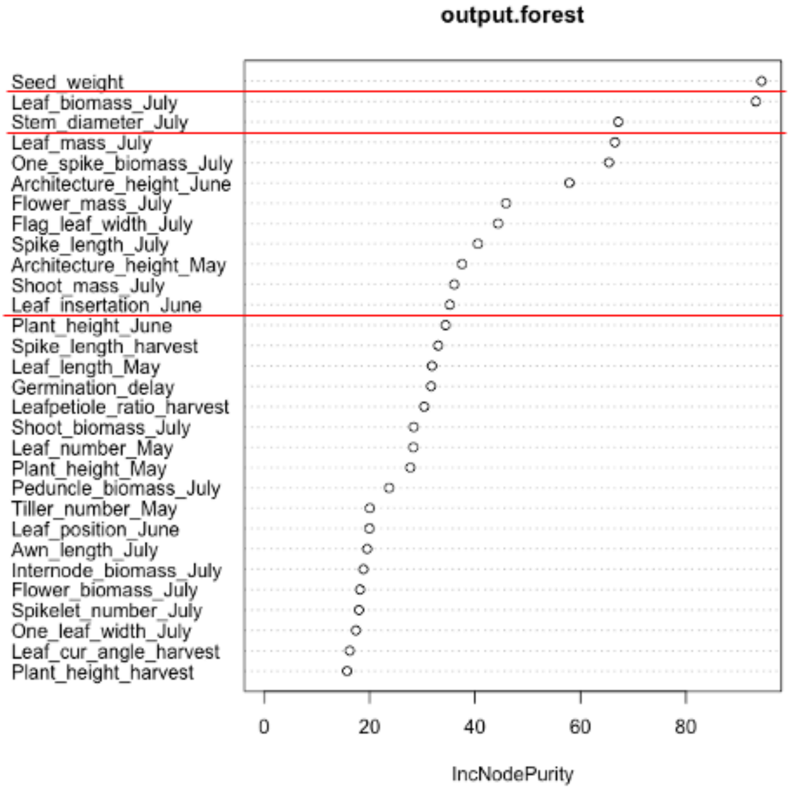


Figure 1: The output of random forest modelling. The traits underlined in red are what we picked for optimization.

could not be entered in the FSP model, I obtained three trait parameters: [Seed Weight], [Stem diameter] and [Leaf insert angle]. In this paper, we will call them “seed weight”, “stem diameter” and “leaf insert angle” to make our descriptions easier. They are the second series of traits/RF traits for optimization.

3.3.3 Accounting for trait correlations

Before picking the best trait value combination from their data range, we first needed to account for correlations among traits that indicate trade-offs. For example, we cannot pick the largest flower biomass and the smallest internode biomass, since this trait combination would mean that shoots are too mechanically weak to support heavy spikes. Considering this limitation, we applied a convex hull algorithm to account for the trait combinations that occurred across the diversity of wheat accessions surveyed in Chapter 2. We then only considered these trait combinations in our optimization procedure.

The specific method is illustrated in Figure 2. We used the wheat experimental data to create a convex hull for biomass and RF traits respectively (Fig. 2A, B &C). For each trait, we chose the maximum and minimum values and divided the value range between them into ten equal parts. After that, we used the method of permutation and combination to permutate and combine the ten values of flower, internode and leaf biomass to form a three-digit matrix of 10*10*10 trait combinations (Fig. 2D). The matrix was then filtered using the convex hull (Fig. 2E). The points outside the convex hull were excluded as being unfeasible in reality, and the points inside were listed as having relationships within the envelope of natural variation (Fig 2F). We then input all the saved data points into the FSP base wheat model and simulated wheat growth for each combination. We recorded the combination of traits producing the highest yield among the model outputs. The corresponding trait values represent the optimized wheat ideotype. For RF traits, we used the same method to get an optimised ideotype.

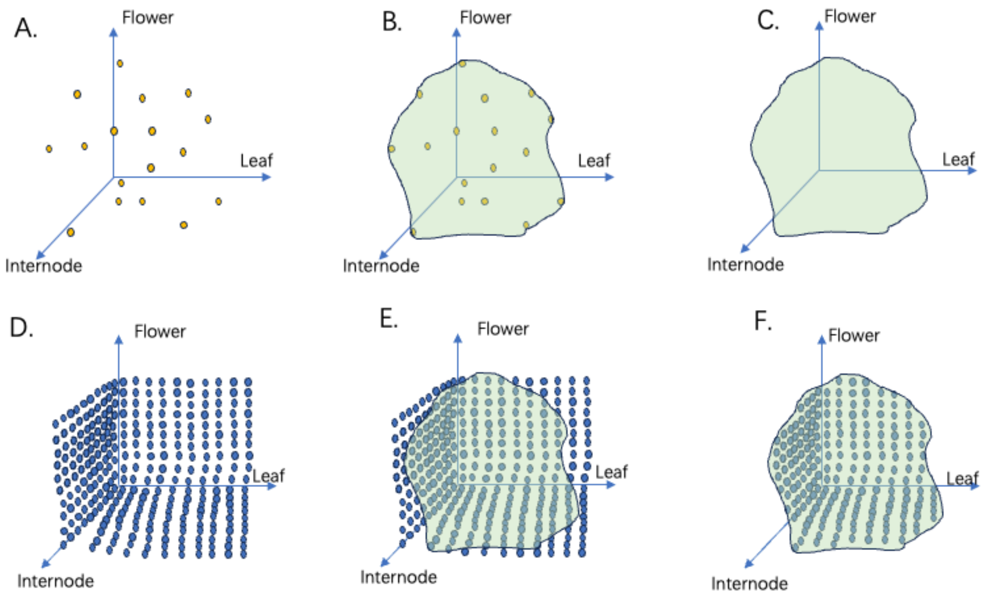


Figure 2: the process of filtering traits by convex hull (using biomass traits as examples).

3.3.4 Ideotype analysis in different densities.

We also used the FSP model to test whether the ideotype we found is adapted well for agronomic planting densities. Our Chapter 2 wheat experiment applied 25 plants/m^2, but most UK wheat are farmed at a density of 200 – 400 plants/m^2. We changed the planting distance but kept the plant number the same at 5 x 5. Additionally, we repeated the ideotype exploration at increased densities (100 plants/m^2, 400 plants/m^2 and 1600 plants/m^2) in the FSP model, to test whether the optimized trait combination depended on planting density. In these cases, we obtained new ideotypes based on average and modern wheat base models, optimized by biomass and RF traits respectively. To test whether the ideotype changed the traits compared with the original wheat bases, we carried out t-tests for each trait in R programming.

3.4 Results

3.4.1 Calibration of two original models

We classified and summarized wheat data from our previous wheat growth experiment (Chapter 2) according to their respective species, and calculated the trait values for each. We then used these FSP model parameters for wheat as a baseline, to identify which traits that we could use to modify wheat phenotypes (Table. S1). We selected the traits that exist both in our wheat experiment and FSP models (Table. S2). We input the true trait mean values into the FSP model, and then ran the model to get the phenotype in each case. We then compared the simulated wheat with real wheat data, mainly comparing height and tiller numbers. Then, keeping the values of other traits unchanged, we tuned the apical dominance parameter multiple times, until height and tiller numbers approached the observed values (within one standard error). Finally, we calibrated the wheat FSP model to multiple wheat accessions (Table. S3).

Table 1: The parameters of FSP models, which are set for default model, average wheat and modern wheat. The parameters with a blue background are what we calibrated. All values are rounded as required by the model.

FSP model parameters	**Reference value**	**average wheat**	**modern wheat**
nrRows	5	5	5
nrPlants	1	5	5
rowDistance	0.15	0.25	0.25
plantDistance	0.15	0.25	0.25
delay	0	6	7
harvest	110	110	110
hexa	false	false	false
offspotIntraRow	0.025	0.025	0.025
offspotInterRow	0.05	0.05	0.05
determinate	TRUE	TRUE	TRUE
plastochron	43	43	43
phyllochron	86	86	86
finalPhytNum	10	9	9
nrShortInternodes	4	4	5
wmaxRoot	2000	2000	2000
wmaxFlower	3000	1009	1609
wmaxInt	266	455	533

FSP model parameters	Reference value	average wheat	modern wheat
wmaxLeaf	266	240	150
teRoot	1800	1800	1800
teFlower	800	800	800
teInt	182	182	182
teLeaf	220	220	220
maxWidthInt	0.005	0.0032	0.0038
specificInternodeLength	0.6	0.6221	0.376
amax	25	25	25
eff	0.06	0.06	0.06
C4	FALSE	FALSE	FALSE
nitro	0.0543	0.0543	0.0543
LMA	4.6	4.6	4.6
leafLife	4	4	4
lwRatio	27	27.0533	20.007
maxWidth	0.7249	0.0496	0.0515
shapeCoeff	0.2027	0.2027	0.2027
leafCurve	46	117.266	142.8333
rankLower	3	3	3
leafAngleLower	40	40.1466	27.2698

FSP model parameters	Reference value	average wheat	modern wheat
leafAngleUpper	40	40.1466	27.2698
nrLeafletsLower	1	1	1
nrLeafletsUpper	1	1	1
petioleFraction	0.3	0.6315	0.6384
petioluleFraction	0	0	0
specificPetioleLength	2.5	2.5	2.5
specificPetioluleLength	5	5	5
nrLeavesLower	1	1	1
nrLeavesUpper	1	1	1
phyllotaxisLower	180	73.6546	59.8095
phyllotaxisUpper	137	73.6546	59.8095
varDelay	0	10	10
seedMass	25	39	53
SASextend	TRUE	TRUE	TRUE
branching	TRUE	TRUE	TRUE
tillersOnly	TRUE	TRUE	TRUE
dominance	0	4.75	5.5
srAbortThresh	0.5	0.5	0.5
tb	0	0	0

We applied the same method to create a virtual wheat, termed “average wheat”. All its traits were obtained by taking the average value across all wild and landrace wheat accessions. The FSP model parameters of this average wheat and modern *T. aestivum* are listed in Table 1. Both these two wheats were created at 25 plants/m^2, which is the same as the experiment setting in Chapter 2.

3.4.2 Wheat yield was improved in ideotypes

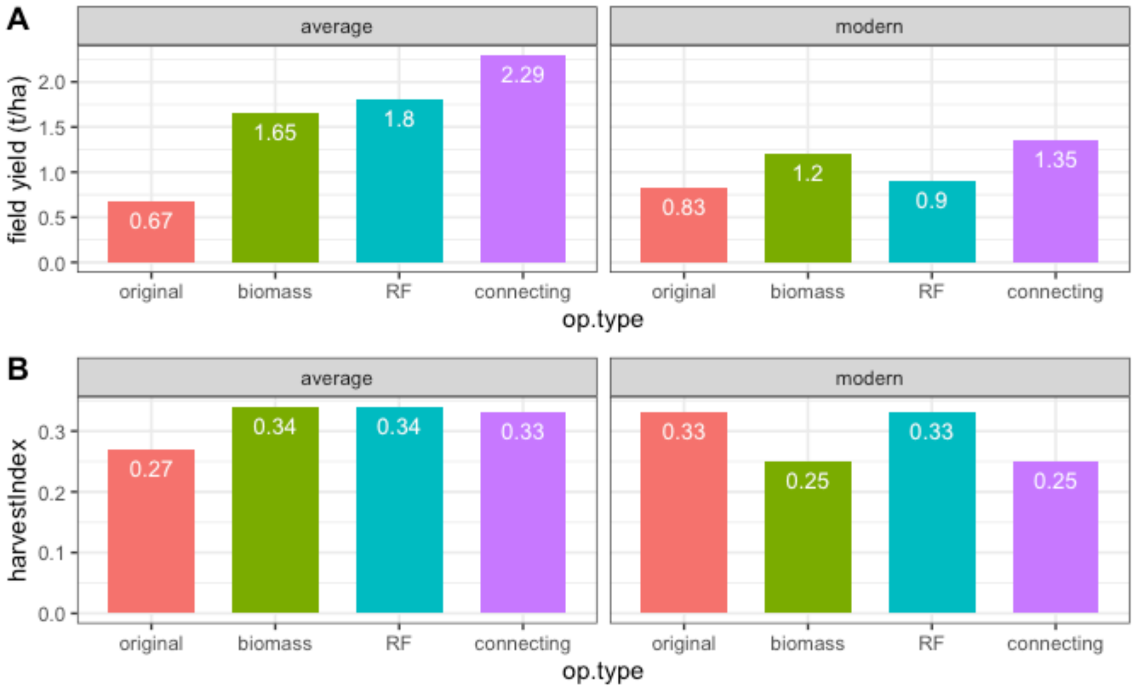


Figure 3: Yield and harvest performance of ideotypes. (A) the yield improvement based on average and modern wheat models, comparing the original baseline simulation, the biomass optimized ideotype, the RF optimized ideotype and their combined ideotypes; (B) the field harvest index for average and modern wheat models, comparing original baseline wheat, biomass optimized ideotype, RF optimized ideotype and their connecting ideotypes.

The FSP model incorporates the simulation of our ideotype obtained from optimization, demonstrating a significant increase in yield compared to the baseline model simulations for an average wheat (Fig. 3A). Because the density (25 plants/m^2) that we set for simulation is lower than normal farming (400 plants/m^2), the predicted yield is not as high as real farming. Notably, the inclusion of RF traits in average wheat led to greater yield improvements compared to potential biomass traits. Conversely, in modern wheat, biomass re-allocation appeared to play a more crucial role in enhancing yields than RF traits. However, in comparison with both wheat baseline cases, changes to biomass and RF traits resulted in improved yields. The average ideotype achieved through this connected optimization approach yielded 2.29 t/ha, surpassing the yield of the modern ideotype. Analysis of the harvest index did not show significant improvements in modern wheat (Fig. 3B). Nonetheless, all three average ideotypes resulting from optimization exhibited higher harvest indexes.

3.4.3 Ideotype traits optimized to maximize yield potential.

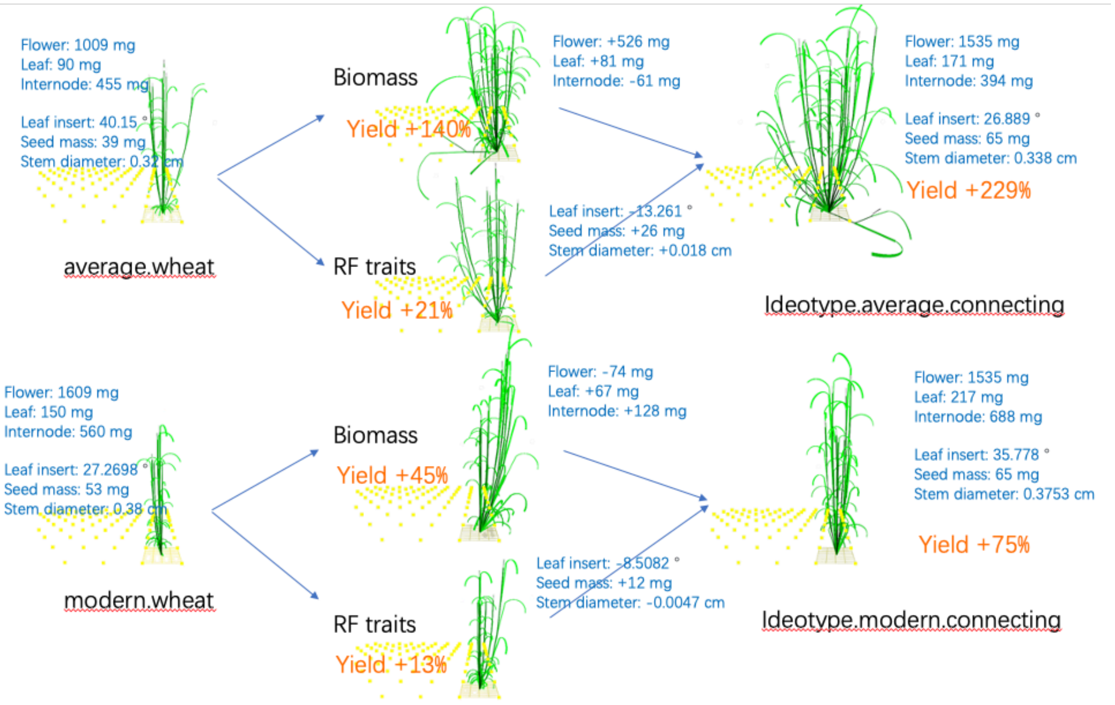


Figure 4: Summary of wheat optimization and yield improvement. The plots of wheat are screenshotted from FSP at a fixed scale. The black words are the names or status of wheat models. Blue words show the original trait values and their optimized variation. The orange words show the proportion of yield increases in ideotype compared with their original wheat.

The variation in wheat morphology resulting from ideotype optimization is depicted in Figure 4. The overall finding is that ideotypes are much larger in size than the original wheat baseline cases. Specifically in average wheat, the biomass ideotype increases the potential flower biomass by 526 mg and potential leaf biomass by 81 mg as inputs, while the potential internode biomass decreases by 61 mg. This allocation pattern directs more carbohydrate to carbon source tissue (leaf) and yield tissue (flower), which leads to a 140% increase in yield (Fig. 4). It is worth noting that all these three traits are not the minimum or maximum values in our data set, although their values each have linear relationships with yields. Instead, the biomass allocation is constrained by trade-offs to achieve the best yield.

For the RF ideotype based on average wheat, the leaf insertion angle decreased by 13.3º, which led to a more erect canopy, minimizing shading of neighbouring plants and the interception of light for photosynthesis at low sun angles. Seed weight and stem diameter are also both improved in the RF optimization, increasing yield in comparison with the baseline case by 21%. When both optimized biomass and RF traits are combined to create an ideotype based on average wheat, the yield experiences a remarkable enhancement of 229%. This combined ideotype is characterized by maximum individual spike biomass of 1535 mg, maximum leaf biomass of 171 mg and maximum internode biomass of 394 mg (Fig. 4). Its optimized traits also included leaf insertion angle of 26.9º, seed mass of 65 mg and stem diameter of 0.338 cm (Fig. 4). Computer optimisation of ideotypes based on average wheat is in reality the same as modern breeding phenotypic modifications of ancient wheat in some aspects, such as increasing flower biomass, decreasing leaf insertion angle and increasing main stem thickness.

In contrast, ideotype optimization on a baseline of modern wheat showed different patterns (Fig. 4). Its maximum flower biomass decreased by 74 mg, with the lost biomass transferred to maximum leaf biomass (+ 67 mg) and maximum internode biomass (+128 mg), which together bring a 45% yield increase (Fig. 4). RF traits are also changed in the ideotypes based on modern wheat. Leaf insertion angle and stem diameter decreased only a little, implying that they are already close to their optimum values. However, the seed mass of the modern ideotype was increased to 65 mg, which represents the largest seed mass value in our experimental dataset, and the same as that in the average ideotype. The modern combined ideotype has maximum biomasses for flower : leaf : internode of 1525 : 217 : 688, leaf insertion angle of

35.8º and stem diameter of 0.3753 cm. The overall yield of the modern combined ideotype is 75% more than the original modern wheat baseline.

In terms of both biomass and RF traits, trait optimisation produced yield increases for both original and modern wheats. Biomass traits optimization caused larger yield improvements than RF traits (Fig. 4). Their connection did not reduce the optimization effect, but enhanced the yield increase.

3.4.4 Phenotypic variation in ideotypes

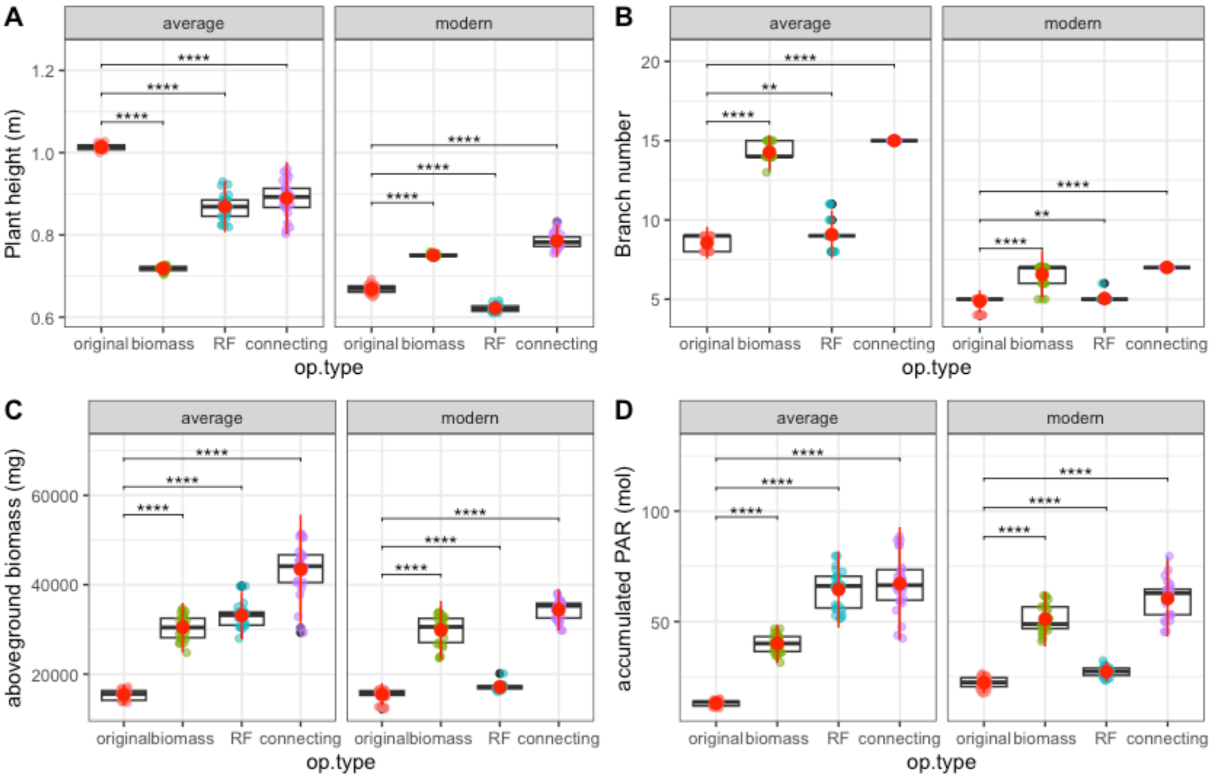


Figure 5: Phenotypic variation in traits involved in ideotype and original wheat baselines. (A) plant height variation among different ideotypes; (B) branch number variation among different ideotypes; (C) aboveground biomass variation among different ideotypes; (D) accumulated PAR variation among different ideotypes. For every plot, the left panel shows the wheat models based on average wheat. The right panel shows the wheat model based on modern wheat. All plots show that the presence of three asterisks (***) in the figure denotes statistical significance, specifically indicating that the observed findings are significant at a significance level of $p < 0.05$.

In addition to yield variation, we also examined specific plant phenotypic traits that underwent emergent changes during the optimization process. Plant height was one of the important traits that was focused on during the Green Revolution. In our optimization, we find plant height does not show stable increasing or decreasing trends. Based on average wheat, all the three ideotypes are shorter than the original wheat baseline (Fig. 5A). The average combined ideotypes grew to a height of about 0.9 m (Fig. 5A). Moreover, in RF optimization and combined optimization, ideotypes show huge variance in individual traits (Fig. 5A). The modern combined ideotypes shows the similar emergent properties, producing heights slightly greater than 0.8m (Fig. 5A) and a final average of 0.8 m, which is significantly taller than modern wheats.

Regarding the branch number, ideotypes all increased tillering strength at the low densities simulated (Fig. 5B), although our optimized traits (biomass and RF) did not specifically target tillering-related traits. Potential biomass allocation to individual organs contributed to the branch increases against both average and modern wheat baselines (Fig. 5B). It made the tillers of average wheat increase from approximately 8 to almost 15, and modern wheats from about 5 to nearly 7 (Fig. 5B). These effects were also shown in combined ideotypes. RF traits also had a noticeable impact on branch development but the effects were not as large as those of the biomass optimization. As one of the yield component traits, branching increases may be a key factor to improving yield in ideotypes.

FSP model also calculated the accumulated PAR (Photosynthetically Active Radiation), which represented the total light absorbed by leaves during the lifetime of the crop (Nobel & Hartsock, 1983). The aboveground biomass and accumulated PAR showed similar patterns in ideotypes (Fig. 5C and D). Both biomass and RF traits improved all their values in the optimization. That confirms the ideotypes had heavier and larger bodies than their original wheat baselines. This led to increased accumulated PAR so that ideotypes have better interception and conversion of light energy into carbohydrates. However, we noticed that both average and modern combined ideotypes have large individual differences in aboveground biomass and

PAR in the FSP model (Fig. 5C and D). That might be because large plant body size causes competition among individuals in the field.

3.4.5 Density effects on ideotypes

In order to test if ideotypes with larger sizes will cause greater competition, we increased planting density in the FSP model and re-tested ideotype growth. The result is shown in Figure 6. Average ideotypes and modern ideotypes showed different reactions. In the average panel, the original average wheat had the smallest yield with increasing density. The biomass and combined ideotypes had the largest yields, reaching close to 10 t/ha (Fig. 6). This suggests that the ideotypes based on an average wheat baseline maintained their advantages in high-density farming conditions.

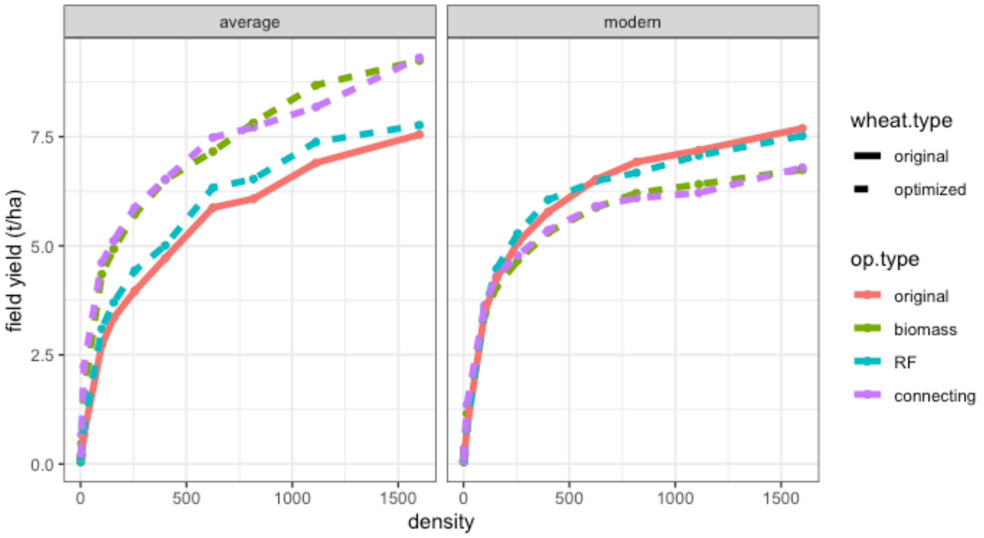


Figure 6: the field yield of ideotypes when farming density increases. The left panel shows the wheat models based on average wheat. The right panel shows the wheat model based on modern wheat. The solid line shows the original wheat bases of average and modern ones. The dotted line shows the ideotypes with optimized. The optimized method is coloured and pointed in legend.

However, for the modern wheat baseline, we observed that the original wheat case outperformed the ideotypes in terms of yield. The yields of original wheats reached more than 7.5t/ha (Fig. 6). However, its ideotypes did not maintain their yield advantages when density increased.

3.4.6 Ideotype requirements change with increased densities

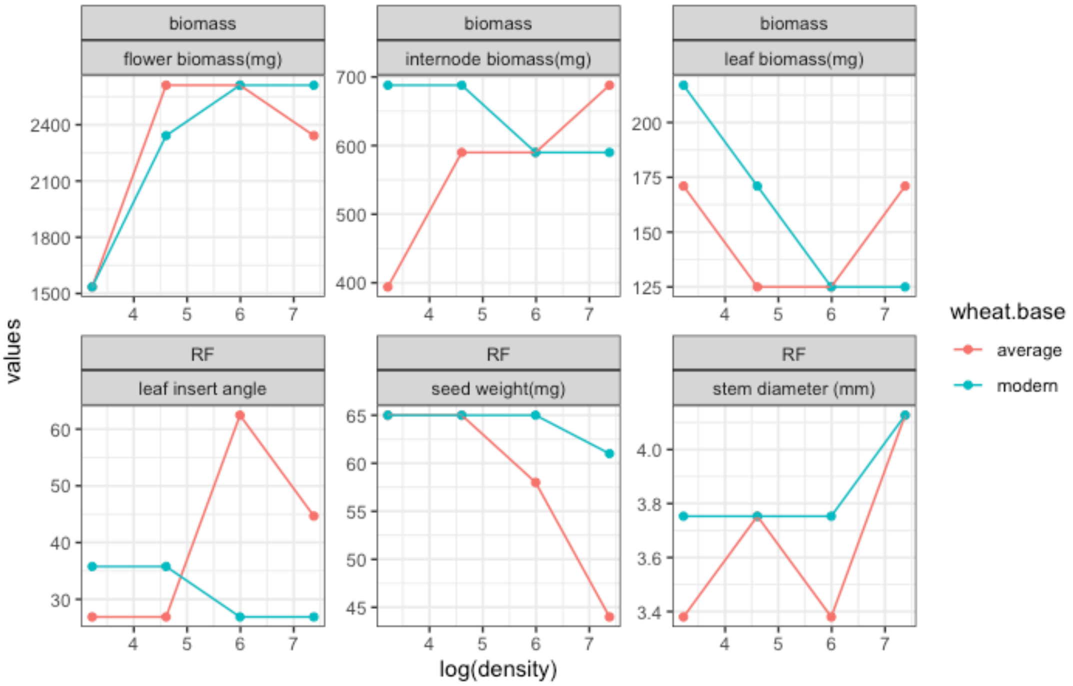


Figure 7: Comparison of the input trait value variation for ideotype optimization in response to increased densities.

The ideotypes developed for modern wheat at low planting densities were limited under increased densities. This result encouraged us to try exploring ideotypes based on high densities. Therefore, we repeated the ideotype determination by FSP models at 25 plants/m^2, 100 plants/m^2, 400 plants/m^2 and 1600 plants/m^2. The resulting ideotypes at higher densities were distinct from those at 25 plants/m^2. We extracted

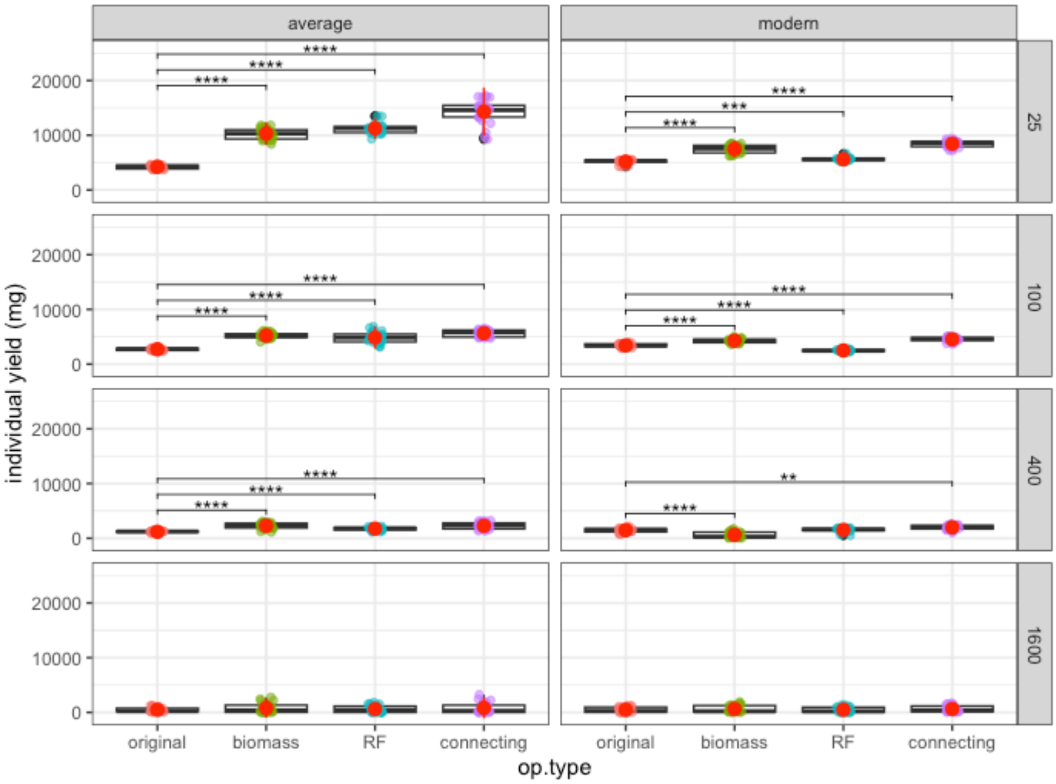


Figure 8: the individual plant yield of ideotypes optimized on different densities. The right panel shows the average wheat baseline and the right panel shows the modern wheat baseline. In all plots, the presence of three asterisks (***)denotes statistical significance at a level of $p < 0.05$.

the trait input values for the ideal phenotype at each density and compared them in Figure 7. It is obvious that, as density increases, the modern ideotype is more likely to increase the maximum potential flower biomass (2611 mg) and reduce the potential leaf biomass (125 mg) (Fig. 7). For modern wheat, the maximum potential internode biomass experienced a small decease to 590 mg with increasing density (Fig. 7). In contrast, the ideotypes based on an average wheat kept internode biomass capacity increasing with density to reach a maximum (688 mg). At the highest density of 1600 plants/m^2, ideotypes based on the average wheat incorporated a rise in maximum leaf biomass and a fall in flower biomass, leading to sub-extreme value selections (flower – 2342 mg and leaf – 171 mg) (Fig. 7).

In RF traits, the variation shows a greater difference between modern and average wheat baselines. The leaf insertion angle of the ideotype based on an average wheat even reached 62.44º at 400 plants/m^2, which is the largest value in these traits (Fig. 7). The modern ideotype had a much steadier leaf angle decrease with density from 35.78º to 26.89º (Fig. 7). For seed weight, with increasing density, both average and modern ideotypes trended towards smaller seed mass. However, the decline of average ideotype was largest, from 65 mg to 44 mg (Fig. 7). The optimization of stem diameter showed an upward trend in the overall value, and both average and modern ideotypes chose the largest value (4.1 mm) at 1600 plants/m^2 (Fig. 7). Similarly, the change in the average group is more drastic, and there is even a sharp drop at 400 plants/m^2 densities.

As density increases, our modelled yield per unit area improves. However, the role of the two optimisation models in this becomesno longer significant. At 1600 plants/m^2 density, there was no significant yield difference between the original wheat and the three optimised wheats (Fig. 8). With the density increases, the RF ideotypes firstly do not show significant increases in plant yield at 400 plants/m^2 (Fig. 8). When density is increased to 1600 plants/m^2, none of the ideotype optimizations showed significant improvements over their original wheat bases (Fig. 8). This is especially relevant to aboveground biomass and accumulated PAR, because their optimized effects also disappear at 1600 plants/m^2 density (Fig. S4). High density farming might be thought disable biomass and RF optimization.

3.5 Discussions

Phenotypic measurements and simulation-based optimization using existing cultivar populations allow us to virtually recombine plant traits to identify an optimal set of phenotypes that maximize performance and viability. The model-based analysis highlighted the morphological advantages to redesigning the ideotype of wheat, and tested the ideotype differences at individual and population levels.

3.5.1 Possible methodological limitations in trait selection and modelling

This work is a computational approach to the prediction of realistic wheat. There are therefore differences between the ideotype and what we breed in real world wheat. This point is reflected in our approach to trait selection, which plays an important role in our ideotype optimizations. Our approaches were based on two basic concepts. Sensitivity analysis is totally based on the FSP model. The features of the model therefore decide the key traits that we selected to optimise yield. However, other models use other assumptions and parameterizations, allowing models with different assumptions to acceptably simulate plants (Tardieu *et al.*, 2020). Therefore, sensitivity analysis performed using a given model is largely a direct translation of the choices made when the model was constructed. The parameters of maximum potential leaf, internode and flower biomass might not be the most important parameters in real wheat plants. In contrast, RF traits come from the morphological data in our empirical experiment. Random Forest combines the output of multiple decision trees to reach a single result, although it may show some instability (Fox *et al.*, 2017). From the point of view of model effects, biomass trait optimization definitely had larger effects than the RF traits (Fig. 4). However, their mixed effects created a cooperative effect rather than conflicts, which resulted in the highest yield improvement (+229% based on average wheat and +75% based on modern wheat) (Fig. 4).

The second point is that there is a gap between ideal wheat and realistic breeding, arising from omissions in the model. Our FSP model does not simulate wind and lodging characteristics, and resistance to collapse (via dwarfing) is precisely the trait that was selected for during the Green Revolution in wheat (Foulkes *et al.*, 2011). Our ideal wheat, on the other hand, has increased height, and this may be an artefact of using the FSP model, which does not simulate lodging. Similarly, we found a decrease in stem biomass and an increase in flower biomass in our high-density ideotype optimisation. In the real world, wheat stems too thin to support the weight of the flowers can also make wheat lodge (Zhang *et al.*, 2020). In wild wheat, this is common. But agricultural cultivation of wheat requires care to avoid this. Our model allows us to reduce stem biomass and increase flower biomass, but this strategy may not work in agricultural breeding.

3.5.2 Is the ideotype equivalent to gigantism?

The increased yield in our ideotypes comes as a result of gigantism. Overall, our ideotypes were bigger plants than their original templates (Fig. 4), with no obvious harvest index increases in ideotypes (Fig. 3B). These heavier wheats led us to suspect that our ideotypes may be trapped in a tragedy of the commons (Hardin, 1968), in which the plants do not perform well in high densities. However, our density tests on ideotypes show that average-based wheat and modern-based wheat behave differently. The average ideotypes with larger sizes maintained their production at high densities, while the modern ideotypes with smaller sizes were not as good as the plants before optimization (Fig. 6). This latter result conflicts with our initial hypothesis because modern wheats after the Green Revolution are regarded as better than older varieties in high-density environments (Hedden, 2003). When comparing individual plants within our simulations, we found that average ideotypes had higher standard error than modern ideotypes in yield, aboveground biomass and plant height (Table S1). It is possible that average ideotypes compete with and kill some of their neighbours. However, these strong-fitness individuals grow up healthy and make up for the loss of some individuals with their high yield.

However, this high competition strategy is inefficient in high density farming, where seed is wasted if there is self-thinning in the crop stand. When we set the density first and then explored ideotypes, we found that the optimization strategy was different in comparison with low densities (Fig. 7). Ideotypes trended towards cooperative strategies, including decreased seed weight and leaf biomass as inputs, transferring this resource into yield traits (i.e. flower biomass) (Fig. 7). The plant height and branch number were both decreased in each version of the ideotype with density increasing (Fig. S1 and S2). The competitive characters were only shown in average ideotypes. Their internode biomass, leaf insertion angle and stem diameter input were selected to increase as density increased (Fig. 7). In contrast, these traits in modern ideotypes generally decreased. Therefore, we find average wheats still retain some competitive characters, but modern wheats are much more cooperative. Our simulated results align with the agricultural ecology perspective (Weiner *et al.*, 2010). The gigantism or high fitness ideotype will achieve high yields, but as density increases, group-friendly ideotypes are more productive.

3.5.3 Comparison with other wheat ideotypes

Compared with other modelling ideotypes, our wheat ideotypes focus more on morphology. The Sirius wheat models optimize canopy architecture, grain filling and cumulative intercepted solar radiation to adapt to the climate, achieving yields of 15-

19 t/ha^{-1}, which represent 39-57% improvements (Senapati & Semenov, 2019). The common points of our two optimizations are that the crop in both cases has larger aboveground biomass. However, the harvest index of the Sirius wheat models is increased as well. A similar trait optimization was carried out in the Greenlab maize model, which reallocated the cob, stem and leaf biomass (Qi *et al.*, 2010). It gave the best simulated ratio of leaf-shoot vs cob tissues, which achieved 2% yield increases. This supports our biomass trait optimization which showed that we could not increase single tissue biomass to a maximum due to source-sink limitation, but we could optimize the ratio of biomass allocation to benefit plant growth (Burnett *et al.*, 2018). The model of SUNFLO in apple trees similarly selected branch angle, shoot diameter and leaf sizes to optimize yield (Picheny *et al.*, 2017). The results are also similar to ours, showing that 80° insertion angle and larger leaf sizes would benefit plant yield. Another model of maize, simulated by ARMOSA, decreased the underground biomass input, to optimize drought-resistance, maintaining high yield in maize under less irrigation (Perego *et al.*, 2014). Root system optimization is one aspect we lack in our study, although it shows an important role in wheat evolution (Waines & Ehdaie, 2007). However, root modules has been added into FSP recently and will be applied in crop studies soon (de Vries *et al.*, 2021).

3.5.4 Improvements to the optimization approach

Although our optimization using a convex hull has provided appropriate ranges of trait values, its dimensions could increase more (Nemirko & Dulá, 2021). Our work only picks three dimensions (leaf, internode and flower biomass; or leaf insertion angle, stem diameter and seed mass), but there are still more traits that we could optimize from real values. That means we could add the optimized variables and apply a convex hull for multiple dimensions in our wheat phenotypic data. In addition, there are also some alternative optimization examples based on FSP models that have been developed. For example, Xu integrated a FSP model with a workflow based on a Mixed Particle Swarm Optimization (MPSO) algorithm, to optimize the best planting distance in rice (Xu *et al.*, 2020). de Vries proposed an evolutionary modelling approach, connecting an FSP model of plant growth in a 3D light climate with a model of natural selection, to optimize the competition input of plants (de Vries *et al.*, 2020). These algorithm codes are programmed into GroIMP, the modelling platform for FSP models. It may therefore be possible to get better optimized effects in the ideotype of our wheat morphological data.

3.5.5 Future developments in ideotype breeding

The ideotype results from our FSP modelling are valuable for breeding, ecology and plant physiology. We explored the potential for using wild traits in modern wheat improvement, identifying which traits are key to yield and modifying morphology. The ideotype optimization that started with an average wheat reproduces the path of the Green Revolution, including decreasing height and leaf insertion angle, increasing flower biomass and seed mass input (Würschum *et al.*, 2017b). In the modern wheat baseline simulations, wild traits become important optimized resources. This was mainly seen in internode biomass and plant height improvement at the cost of flower biomass reduction. In addition, both average and modern ideotypes emphasized leaf biomass and branch number increases, which leads to improved PAR interception to increase source strength (Burnett *et al.*, 2016). However, for high-density farming, the flower biomass needed to be improved again with leaf and internode biomass decreasing. The lower leaf insertion angle and the stronger stem could be encouraged continuously to adapt to group farming. These changes in high densities in our FSP support current modern breeding strategies (Reynolds *et al.*, 1999).

Crop individual performance and group farming might be contradictory. We therefore tested the hypothesis of ecological agriculture, that ideotypes may be equal or opposite to high fitness. We found in the ideotype optimization that the increase in fitness due to large body size only increased population production at low densities, but did not significantly optimise the effect at high densities, but instead caused the death of some individuals. Future work is expected to concentrate on how wheat root and fitness change in domestication. It would be exciting to test if they could contribute into improvement using wheat modelling.

3.6 Conclusions

- Both groups of traits were proven to achieve ideal types through optimization. In biomass optimization, none of the three maximum potential tissue biomasses was optimal at the largest value in our data range. Instead, they achieved a three-way balance at a certain value of tissue biomass allocation. The RF optimization did not have effects as large as those of biomass. Seed mass increases were always associated with improved yield.
- The ideotype optimization of average wheat followed the path taken by the Green Revolution. This involved reducing stem biomass to allocate more resources to flowers and leaves, decreasing plant height and leaf insertion angle, and increasing plant stem thickness. Conversely, the ideotype optimization of modern wheat incorporated more features from wild traits, such as reducing flower biomass to increase internode length and enhancing leaf insertion angle. Both of these ideotypes led to increased numbers of branches and leaf biomass.
- At the low original simulated planting density, the ideotype exhibited different strategies as density increased. We aimed to explore ideotypes at various density levels. At high densities representing modern agricultural planting, we observed an increase in flower biomass and stem diameter, but a decrease in leaf biomass and seed weight. Both internode biomass and leaf insertion angle show different responses to optimization in modern and average wheat varieties. The optimization decreased individual fitness to increase group efficiency. However, the optimized effects brought diminishing benefits as the density increases.

3.7 Reference

Andrivon D, Giorgetti C, Baranger A, Calonnec A, Cartolaro P, Faivre R, Guyader S, Lauri PE, Lescourret F, Parisi L, *et al.* 2013. Defining and designing plant architectural ideotypes to control epidemics? *European Journal of Plant Pathology* **135**: 611–617.

Araus JL, Cairns JE. **2014**. Field high-throughput phenotyping: the new crop breeding frontier. *Trends in Plant Science* **19**: 52–61.

Bogard M, Hourcade D, Piquemal B, Gouache D, Deswartes J-C, Throude M, Cohan J-P. **2021**. Marker-based crop model-assisted ideotype design to improve avoidance of abiotic stress in bread wheat. *Journal of Experimental Botany* **72**: 1085–1103.

Brunel-Muguet S, Aubertot J-N, Dürr C. **2011**. Simulating the impact of genetic diversity of Medicago truncatula on germination and emergence using a crop emergence model for ideotype breeding. *Annals of Botany* **107**: 1367–1376.

Burnett AC, Rogers A, Rees M, Osborne CP. **2016**. Carbon source–sink limitations differ between two species with contrasting growth strategies. *Plant, Cell & Environment* **39**: 2460–2472.

Burnett AC, Rogers A, Rees M, Osborne CP. **2018**. Nutrient sink limitation constrains growth in two barley species with contrasting growth strategies. *Plant Direct* **2**: e00094.

Donald CM. **1968**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Evenson RE, Gollin D. **2003**. Assessing the Impact of the Green Revolution, 1960 to 2000. *Science* **300**: 758–762.

Evers JB, Letort V, Renton M, Kang M. **2018**. Computational botany: advancing plant science through functional–structural plant modelling. *Annals of Botany* **121**: 767–772.

Fischer RA (Tony), Edmeades GO. **2010**. Breeding and Cereal Yield Progress. *Crop Science* **50**: S-85-S-98.

Foulkes MJ, Slafer GA, Davies WJ, Berry PM, Sylvester-Bradley R, Martre P, Calderini DF, Griffiths S, Reynolds MP. **2011**. Raising yield potential of wheat. III. Optimizing partitioning to grain while maintaining lodging resistance. *Journal of experimental botany* **62**: 469–486.

Fox EW, Hill RA, Leibowitz SG, Olsen AR, Thornbrugh DJ, Weber MH. **2017**. Assessing the accuracy and stability of variable selection methods for random forest modeling in ecology. *Environmental monitoring and assessment* **189**: 1–20.

Fuller DQ. **2007**. Contrasting Patterns in Crop Domestication and Domestication Rates: Recent Archaeobotanical Insights from the Old World. *Annals of Botany* **100**: 903–924.

Hardin G. **1968**. The Tragedy of the Commons. *Science* **162**: 1243–1248.

Hedden P. **2003**. The genes of the Green Revolution. *Trends in Genetics* **19**: 5–9.

Kothari K, Ale S, Bordovsky JP, Munster CL, Singh VP, Nielsen-Gammon J, Hoogenboom G. **2021**. Potential genotype-based climate change adaptation strategies for sustaining cotton production in the Texas High Plains: A simulation study. *Field Crops Research* **271**: 108261.

Kothari K, Ale S, Marek GW, Munster CL, Singh VP, Chen Y, Marek TH, Xue Q. **2022**. Simulating the climate change impacts and evaluating potential adaptation strategies for irrigated corn production in Northern High Plains of Texas. *Climate Risk Management* **37**: 100446.

Kulwal PL, Mir RR, Varshney RK. **2022**. Efficient Breeding of Crop Plants. In: Yadava DK, Dikshit HK, Mishra GP, Tripathi S, eds. Fundamentals of Field Crop Breeding. Singapore: Springer Nature, 745–777.

Li Y, Tao F, Hao Y, Tong J, Xiao Y, Zhang H, He Z, Reynolds M. **2023**. Linking genetic markers with an eco-physiological model to pyramid favourable alleles and design wheat ideotypes. *Plant, Cell & Environment* **46**: 780–795.

Litrico I, Violle C. **2015**. Diversity in Plant Breeding: A New Conceptual Framework. *Trends in Plant Science* **20**: 604–613.

Meyer RS, DuVal AE, Jensen HR. **2012**. Patterns and processes in crop domestication: an historical review and quantitative analysis of 203 global food crops. *New Phytologist* **196**: 29–48.

Nagaleekara B, Kg S, Patil R, Kubsad V. **2022**. Sorghum hybrid (CSH-16) ideotype to cope with projected climate of North Interior Karnataka. **34**: 441–445.

Nemirko AP, Dulá JH. **2021**. Machine learning algorithm based on convex hull analysis. *Procedia Computer Science* **186**: 381–386.

Nobel PS, Hartsock TL. **1983**. Relationships between Photosynthetically Active Radiation, Nocturnal Acid Accumulation, and CO2 Uptake for a Crassulacean Acid Metabolism Plant, Opuntia ficus-indica. *Plant Physiology* **71**: 71–75.

Peng J, Ronin Y, Fahima T, Röder MS, Li Y, Nevo E, Korol A. **2003**. Domestication quantitative trait loci in Triticum dicoccoides, the progenitor of wheat. *Proceedings of the National Academy of Sciences* **100**: 2489–2494.

Peng JH, Sun D, Nevo E. **2011**. Domestication evolution, genetics and genomics in wheat. *Molecular Breeding* **28**: 281–301.

Perego A, Sanna M, Giussani A, Chiodini ME, Fumagalli M, Pilu SR, Bindi M, Moriondo M, Acutis M. **2014**. Designing a high-yielding maize ideotype for a changing climate in Lombardy plain (northern Italy). *Science of The Total Environment* **499**: 497–509.

Picheny V, Casadebaig P, Trépos R, Faivre R, Da Silva D, Vincourt P, Costes E. **2017a**. Using numerical plant models and phenotypic correlation space to design achievable ideotypes. *Plant, Cell & Environment* **40**: 1926–1939.

Picheny V, Trépos R, Casadebaig P. **2017b**. Optimization of black-box models with uncertain climatic inputs—Application to sunflower ideotype design. *PLOS ONE* **12**: e0176815.

Qi R, Ma Y, Hu B, de Reffye P, Cournède P-H. **2010**. Optimization of source–sink dynamics in plant growth for ideotype breeding: A case study on maize. *Computers and Electronics in Agriculture* **71**: 96–105.

Reynolds MP, Rajaram S, Sayre KD. **1999**. Physiological and Genetic Changes of Irrigated Wheat in the Post–Green Revolution Period and Approaches for Meeting Projected Global Demand. *Crop Science* **39**: 1611–1621.

Rötter RP, Tao F, Höhn JG, Palosuo T. **2015**. Use of crop simulation modelling to aid ideotype design of future cereal cultivars. *Journal of Experimental Botany* **66**: 3463–3476.

Sedgley RH. **1991**. An appraisal of the Donald ideotype after 21 years. *Field Crops Research* **26**: 93–112.

Semenov MA, Stratonovitch P. **2013**. Designing high-yielding wheat ideotypes for a changing climate. *Food and Energy Security* **2**: 185–196.

Senapati N, Semenov MA. **2019a**. Assessing yield gap in high productive countries by designing wheat ideotypes. *Scientific Reports* **9**: 5516.

Senapati N, Semenov MA. **2019b**. Assessing yield gap in high productive countries by designing wheat ideotypes. *Scientific Reports* **9**: 5516.

Senapati N, Semenov MA. **2020**. Large genetic yield potential and genetic yield gap estimated for wheat in Europe. *Global Food Security* **24**: 100340.

Senapati N, Semenov MA, Halford NG, Hawkesford MJ, Asseng S, Cooper M, Ewert F, van Ittersum MK, Martre P, Olesen JE, *et al.* 2022. Global wheat production could benefit from closing the genetic yield gap. *Nature Food* **3**: 532–541.

Senapati N, Stratonovitch P, Paul MJ, Semenov MA. **2019**. Drought tolerance during reproductive development is important for increasing wheat yield potential under climate change in Europe. *Journal of Experimental Botany* **70**: 2549–2560.

Suriharn B, Patanothai A, Boote KJ, Hoogenboom G. **2011**. Designing a Peanut Ideotype for a Target Environment Using the CSM-CROPGRO-Peanut Model. *Crop Science* **51**: 1887–1902.

Tao F, Rötter RP, Palosuo T, Díaz-Ambrona CGH, Mínguez MI, Semenov MA, Kersebaum KC, Nendel C, Cammarano D, Hoffmann H, *et al.* 2017. Designing future barley ideotypes using a crop model ensemble. *European Journal of Agronomy* **82**: 144–162.

Tardieu F, Granato ISC, Van Oosterom EJ, Parent B, Hammer GL. **2020**. Are crop and detailed physiological models equally 'mechanistic' for predicting the genetic variability of whole-plant behaviour? The nexus between mechanisms and adaptive strategies. *in silico Plants* **2**: diaa011.

Tester M, Langridge P. **2010**. Breeding Technologies to Increase Crop Production in a Changing World. *Science* **327**: 818–822.

Vos J, Evers JB, Buck-Sorlin GH, Andrieu B, Chelle M, de Visser PHB. **2010**. Functional–structural plant modelling: a new versatile tool in crop science. *Journal of Experimental Botany* **61**: 2101–2115.

de Vries J, Evers JB, Kuyper TW, van Ruijven J, Mommer L. **2021**. Mycorrhizal associations change root functionality: a 3D modelling study on competitive interactions between plants for light and nutrients. *New Phytologist* **231**: 1171–1182.

de Vries J, Evers JB, Poelman EH, Anten NPR. **2020**. Optimal plant defence under competition for light and nutrients: an evolutionary modelling approach. *in silico Plants* **2**: diaa008.

Waines JG, Ehdaie B. **2007**. Domestication and crop physiology: roots of green-revolution wheat. *Annals of botany* **100**: 991–998.

Weiner J, Andersen SB, Wille WK-M, Griepentrog HW, Olsen JM. **2010**. Evolutionary Agroecology: the potential for cooperative, high density, weed-suppressing cereals. *Evolutionary Applications* **3**: 473–479.

Weir AH, Bragg PL, Porter JR, Rayner JH. **1984**. A winter wheat crop simulation model without water or nutrient limitations. *The Journal of Agricultural Science* **102**: 371–382.

Würschum T, Langer SM, Longin CFH, Tucker MR, Leiser WL. **2017a**. A modern Green Revolution gene for reduced height in wheat. *The Plant Journal* **92**: 892–903.

Würschum T, Langer SM, Longin CFH, Tucker MR, Leiser WL. **2017b**. A modern Green Revolution gene for reduced height in wheat. *The Plant Journal* **92**: 892–903.

Xiao D, Liu DL, Wang B, Feng P, Waters C. **2020**. Designing high-yielding maize ideotypes to adapt changing climate in the North China Plain. *Agricultural Systems* **181**: 102805.

Xu L, Huang Z, Yang Z, Ding W, Buck-Sorlin GH. **2020**. Optimization study on spatial distribution of rice based on a virtual plant approach. *PLOS ONE* **15**: e0243717.

Zhang H, Li T, Liu H, Mai C, Yu G, Li H, Yu L, Meng L, Jian D, Yang L, *et al.* **2020**. Genetic progress in stem lodging resistance of the dominant wheat cultivars adapted to Yellow-Huai River Valleys Winter Wheat Zone in China since 1964. *Journal of Integrative Agriculture* **19**: 438–448.

3.8 Supplements

Table S 1: The parameters in the FSP model and their definitions.

FSP model parameters	**Term used in the article**	**Explanation**
nrRows		number of rows
nrPlants		number of plants in a row
rowDistance		distance between rows
plantDistance		distance between plants in a row
delay	Germination delay	germination delay after start of simulation (in days, to represent late sowing)
harvest		duration, i.e. harvest/removal time after emergence (in days)
hexa		true: hexagonal layout, rectangular otherwise
offspotIntraRow		fraction of plant distance the plant seed is off-spot
offspotInterRow		fraction of row distance the plant seed is off-spot
determinate		TRUE = determinate, FALSE = indeterminate
plastochron		time between creation of two phytomers (dd)
phyllochron		time between appearance of two leaves (dd)
finalPhytNum		final number of main stem vegetative phytomers
nrShortInternodes		number of bottom internodes that should not elongate and have no mass
wmaxRoot		maximum root system biomass
wmaxFlower	flower biomass	maximum flower/fruit biomass
wmaxInt	internode biomass	maximum internode biomass
wmaxLeaf	(one) leaf biomass	maximum leaf biomass
teRoot		root growth duration
teFlower		flower/fruit growth duration
teInt		internode growth duration
teLeaf		leaf growth duration
maxWidthInt	internode width	maxium internode width

FSP model parameters	**Term used in the article**	**Explanation**
specificInternodeLength		internode ratio length / biomass (mm/mg)
amax		max photosynthesis rate
eff		initial light use efficiency (initial slope of light response curve)
C4		false: C3, true: C4 (parameter only valid when FvCB is true)
nitro		leaf nitrogen mass fraction at top of canopy
LMA		leaf mass per unit area (mg/cm2)
leafLife		life span of a leaf since appearance (expressed as X times its growth duration (te))
lwRatio		ratio between leaf blade length and width
maxWidth		location on the leaf where width is maximal (fraction of length)
shapeCoeff		leaf shape coefficient (0 = rectangular, high value = pinched)
leafCurve	leaf insertion angle	leaf curvature - angle between bottom and top of leaf blade (0 = flat)
rankLower		final phtyomer that has properties of lower phytomers (e.g. nr of leaflets, leaf angle, etc)
leafAngleLower		insertion angle of lower leaves (90 = horizontal)
leafAngleUpper		insertion angle of upper leaves (90 = horizontal)
nrLeafletsLower		number of leaflets per leaf for the lower phytomers
nrLeafletsUpper		number of leaflets per leaf for the upper phytomers
petioleFraction		fraction of biomass partitioned to the petiole
petioluleFraction		fraction of biomass partitioned to the petiolule
specificPetioleLength		specific petiole length (mm/mg)
specificPetioluleLength		specific petiolule length (mm/mg)
nrLeavesLower		number of leaves per phytomer for the lower phytomers
nrLeavesUpper		number of leaves per phytomer for the upper phytomers
phyllotaxisLower		angle between consecutive leaves along a stem for the lower phytomers

FSP model parameters	**Term used in the article**	**Explanation**
phyllotaxisUpper		angle between consecutive leaves along a stem for the upper phytomers
varDelay		max variation in germination delay (in days, 0 = simultaneous germination)
seedMass	seed weight / seed mass	seed endosperm mass in mg
SASextend		toggle internode SAS extention response
branching		toggle branching
tillersOnly		true: bud break only if parent internode has length 0 (= tillering)
dominance		minimum dominance, so maximal branching phytomer distance, at infinitely large source/sink ratio (no neighbours)
srAbortThresh		threshold sink/source ratio for branch abortion
tb		base temperature for thermal time calculation

Table S 2: The parameters that we calibrated in the FSP model and how we calculate them with real values from the wheat experiment in Chapter 2.

Input parameters	**Corresponding values or calculations in actual experiments**
nrRows = 5;	
nrPlants = 5;	
rowDistance = 0.25;	
plantDistance = 0.25;	
delay = 0;	[Germination_delay]
harvest = 110;	
hexa = false;	
offspotIntraRow = 0.025;	
offspotInterRow = 0.05;	
// plant parameters	
determinate = true;	
plastochron = 43;//45;	
phyllochron = 86;//90;	
finalPhytNum = 10;	[Node_number_July]--------esimate; set the final number as 9
nrShortInternodes = 4;	[Node_number_July]--------esimate; set the final number as 9, and minus node number
wmaxRoot = 3000;	
wmaxFlower = 3000;	[One_spike_biomass_July]
wmaxInt = 400	[Internode_biomass_July]/[Peduncle_biomass_July]
wmaxLeaf = 400	One_leaf_biomass_July
teRoot = 1800;	
teFlower = 800;	
teInt = 182;	
teLeaf = 220;	
maxWidthInt = 0.005;	[Stem_diameter_July]
specificInternodeLength = 0.6;	[Peduncle_length_July], [Peduncle_biomass_July] -----calculate
amax = 25;	
eff = 0.06;	
C4 = false;	
nitro = 2.5;	
LMA = 4.6;//3.5;	
leafLife = 3;//2;	
lwRatio = 27;	[Leaf_length_July], [Leaf_width_July]---------calculate
maxWidth = .7249;	[Leaf_position_June]
shapeCoeff = 0.2027;//0.7552;	

leafCurve = 46;//;	[Leaf_curtivation_June]
rankLower = 3;	
leafAngleLower = 40:	[Leaf_insertation_June]
leafAngleUpper = 40;	[Leaf_insertation_June]
nrLeafletsLower = 1;	
nrLeafletsUpper = 1;	
petioleFraction = 0.3;	[Leafpetiole_ratio_harvest]
petioluleFraction = 0;	
specificPetioleLength = 2.5;	
specificPetioluleLength = 5.0;	
nrLeavesLower = 1;	
nrLeavesUpper = 1;	
phyllotaxisLower = 180;	[Leaf_cur_angle_harvest]
phyllotaxisUpper = 137;	[Leaf_cur_angle_harvest]
varDelay = 2;	[Germination_delay]
seedMass = 15;	[Seed_weight/Grain_weight]
SASextend = true;	
branching = true;	
tillersOnly = true;	
dominance = 2;	Estimate; run the model until the branch number and plant hegiht are right to real values.
srAbortThresh = 0.5;	
tb = 0;	
output parameters (plant level)	Corresponding values or calculations in actual experiments
nrBranches	Select the max tiller number from [Tiller_number_June] and [Spike_number_July]
leafArea(m2)	
fpar	
accumulated PAR(mol)	
rfr	
biom(mg)	
yield(mg)	[Grain_weight_onespike_hravest], [Spikelet_number_harvest], [Spikelet_number_July], [Spike_number_July], [Spike_number_harvest] -------- calculate expected yielding
leafMass(mg)	[Leaf_mass_July]
stemMass(mg)	[Shoot_mass_July]

rootMass(mg)	
shootRootRatio(mg)	
aboveBiom(mg)	[Leaf_biomass_July], [Shoot_biomass_July], [Flower_biomass_July] --------- calculate
Nsource(mg)	
Total N uptake(mg)	
Root length(m)	
Plant height	[Plant_height_July]
Nphoto(mg)	
Nstem(mg)	
Ngrain(mg)	
Nroots(mg)	
bladeMass(mg)	

Table S3: Wheat FSP models calibrated by their real values in the wheat experiment based on different accessions.

Wheat names	Parameters	T. urartu	T. dicoccoides	T. dicoccum	T. durum landrace	T. durum modern	T. aestivum landrace	T. aestivum modern
delay	input	3.43	4.67	5.00	5.93	6.33	7.95	7.43
finalPhyNum	input	9.00	9.00	9.00	9.00	9.00	9.00	9.00
nrShortInternodes	input	6.14	5.67	4.80	5.13	5.20	5.26	5.76
wmaxFlower	input	497.14	973.33	1017.33	923.33	1105.33	1035.79	1609.05
wmaxInt	input	195.71	416.67	445.33	502.67	529.33	618.95	533.81
wmaxleaf	input	110.00	150.00	240.00	240.00	190.00	170.00	150.00
maxWidthInt	input	0.00	0.00	0.00	0.00	0.00	0.00	0.00
specificInternodeLength2	input	1.35	0.76	0.59	0.44	0.45	0.39	0.38
lwRatio	input	46.94	30.13	25.43	21.45	22.49	24.07	20.01
maxWidth	input	0.04	0.06	0.05	0.05	0.06	0.04	0.05
leafCurve	input	79.86	102.35	119.90	102.00	110.76	123.69	142.83
LeafAngle	input	75.36	50.33	35.27	45.61	36.48	31.11	27.27
petioleFraction	input	0.64	0.64	0.60	0.65	0.64	0.63	0.64
phyllotaxis	input	51.00	76.58	66.13	78.93	94.48	82.53	59.81
varDelay	input	5.00	6.00	7.00	10.00	8.00	10.00	10.00
seedMass	input	13.47	35.13	43.15	52.58	52.25	36.96	53.08
dominance	input	1	4.0000	5.5000	6.7400	6.6000	6.3600	5.5000
Plant_height (cm)	output	95.96	107.26	114.65	94.41	102.41	108.51	78.55
Spike_number	output	18.00	9.50	8.27	5.93	6.33	6.05	4.81

Table S 4: the traits of ideotypes in density tests.

density (plants/m2)	wheat.base	op.type	mean.yield (mg)	se.yield	mean.height (m)	se.height	mean.branches	se.branches	mean.aboveground biomass (mg)	se.abbiomass
1.00	average	original	3965.5	119.6	1.0421	0.0030	7.48	0.23	14166	2833
1.00	average	biomass	9773.2	283.5	0.7645	0.0065	11.88	0.28	28294	5659
1.00	average	RF	5077.0	71.1	0.9314	0.0052	9.44	0.13	18290	3658
1.00	average	connecting	15278.1	224.1	0.8101	0.0146	15.00	0.00	46079	9216
1.00	modern	original	4351.8	92.1	0.7141	0.0050	3.96	0.09	12658	2532
1.00	modern	biomass	6317.2	258.0	0.7842	0.0073	5.28	0.22	24517	4903
1.00	modern	RF	4579.2	105.6	0.7083	0.0057	4.08	0.10	13348	2670
1.00	modern	connecting	6094.9	140.0	0.7881	0.0051	5.08	0.13	23275	4655
1.56	average	original	4501.2	52.8	1.0290	0.0021	8.64	0.13	16364	3273
1.56	average	biomass	10868.6	294.2	0.7450	0.0039	12.84	0.24	31672	6334
1.56	average	RF	5362.0	73.6	0.9051	0.0040	9.96	0.16	19443	3889
1.56	average	connecting	15767.3	221.3	0.8458	0.0132	15.00	0.00	47745	9549
1.56	modern	original	4860.3	117.7	0.6909	0.0037	4.36	0.10	14358	2872
1.56	modern	biomass	6927.5	160.0	0.7680	0.0020	5.80	0.15	27210	5442
1.56	modern	RF	4583.6	98.6	0.7057	0.0048	4.04	0.09	13443	2689
1.56	modern	connecting	6887.6	146.5	0.7758	0.0033	5.80	0.13	27035	5407
2.78	average	original	4507.7	60.3	1.0115	0.0023	8.72	0.09	16480	3296
2.78	average	biomass	12082.7	223.8	0.7212	0.0016	14.36	0.11	35749	7150
2.78	average	RF	5757.8	88.0	0.8781	0.0036	10.52	0.20	20947	4189
2.78	average	connecting	17261.1	182.5	0.9949	0.0108	15.00	0.00	52378	10476
2.78	modern	original	5486.7	75.0	0.6619	0.0028	4.88	0.07	16645	3329
2.78	modern	biomass	7928.0	148.2	0.7591	0.0014	6.60	0.10	32057	6411

density (plants/m2)	wheat.base	op.type	mean.yield (mg)	se.yield	mean.height (m)	se.height	mean.branches	se.branches	mean.aboveground biomass (mg)	se.abbiomass
2.78	modern	RF	5185.9	116.7	0.6732	0.0032	4.56	0.10	15560	3112
2.78	modern	connecting	7878.7	166.9	0.7597	0.0008	6.44	0.12	31611	6322
6.25	average	original	4302.4	54.6	1.0173	0.0022	8.40	0.10	15681	3136
6.25	average	biomass	11491.1	219.6	0.7197	0.0014	14.36	0.11	33963	6793
6.25	average	RF	5528.6	78.6	0.8862	0.0024	10.28	0.16	19946	3989
6.25	average	connecting	16377.4	187.0	0.9136	0.0084	15.00	0.00	49599	9920
6.25	modern	original	5062.1	95.4	0.6708	0.0023	4.68	0.10	15283	3057
6.25	modern	biomass	7711.8	136.4	0.7536	0.0009	6.64	0.10	31096	6219
6.25	modern	RF	4980.5	100.1	0.6780	0.0018	4.48	0.10	14860	2972
6.25	modern	connecting	7483.1	138.3	0.7556	0.0005	6.36	0.10	29937	5987
25.00	average	original	4055.2	55.9	1.0139	0.0017	8.40	0.10	14698	2940
25.00	average	biomass	8853.1	267.7	0.7144	0.0011	14.44	0.10	26528	5306
25.00	average	RF	5013.5	61.2	0.8842	0.0014	10.20	0.12	17997	3599
25.00	average	connecting	11814.9	518.5	0.8583	0.0103	15.00	0.00	36135	7227
25.00	modern	original	5037.5	82.2	0.6678	0.0023	4.84	0.07	15214	3043
25.00	modern	biomass	6652.7	145.6	0.7486	0.0007	6.36	0.15	26604	5321
25.00	modern	RF	4866.3	106.5	0.6771	0.0019	4.60	0.10	14581	2916
25.00	modern	connecting	6399.0	135.8	0.7517	0.0009	5.84	0.16	25206	5041
100.00	average	original	2659.8	52.1	1.0154	0.0015	7.08	0.06	9686	1937
100.00	average	biomass	4300.8	97.8	0.7287	0.0042	9.68	0.28	12736	2547
100.00	average	RF	3025.5	61.8	0.8956	0.0024	8.92	0.06	11103	2221
100.00	average	connecting	4677.1	143.8	0.6969	0.0043	12.96	0.26	14986	2997

density (plants/m2)	wheat.base	op.type	mean.yield (mg)	se.yield	mean.height (m)	se.height	mean.branches	se.branches	mean.aboveground biomass (mg)	se.abbiomass
100.00	modern	original	3431.8	69.1	0.6817	0.0021	4.76	0.09	10393	2079
100.00	modern	biomass	3402.3	98.8	0.7739	0.0048	5.12	0.07	13178	2636
100.00	modern	RF	3415.8	49.2	0.6870	0.0017	4.56	0.10	10238	2048
100.00	modern	connecting	3385.0	81.1	0.7784	0.0042	5.04	0.04	13122	2624
156.25	average	original	2161.1	41.0	1.0198	0.0018	7.00	0.00	7915	1583
156.25	average	biomass	3147.7	81.4	0.7586	0.0066	9.04	0.14	9453	1891
156.25	average	RF	2382.2	45.4	0.9134	0.0031	8.72	0.09	8794	1759
156.25	average	connecting	3244.9	122.7	0.7069	0.0041	11.36	0.30	10530	2106
156.25	modern	original	2720.4	53.9	0.6992	0.0023	4.48	0.10	8183	1637
156.25	modern	biomass	2555.0	76.2	0.8158	0.0072	5.00	0.00	9951	1990
156.25	modern	RF	2681.0	46.8	0.7045	0.0020	4.16	0.07	7951	1590
156.25	modern	connecting	2621.3	57.6	0.8177	0.0063	4.96	0.04	10033	2007
277.78	average	original	1481.7	27.6	1.0337	0.0017	7.00	0.00	5590	1118
277.78	average	biomass	2108.9	70.1	0.8112	0.0080	8.56	0.12	6403	1281
277.78	average	RF	1618.0	39.7	0.9493	0.0047	8.28	0.09	6110	1222
277.78	average	connecting	2176.0	89.0	0.7611	0.0130	9.72	0.26	6946	1389
277.78	modern	original	1884.1	54.3	0.7239	0.0020	4.12	0.07	5633	1127
277.78	modern	biomass	1752.3	69.4	0.8651	0.0051	4.68	0.10	6661	1332
277.78	modern	RF	1900.9	56.5	0.7284	0.0023	4.04	0.07	5638	1128
277.78	modern	connecting	1767.0	64.7	0.8697	0.0050	4.68	0.10	6663	1333
625.00	average	original	948.9	48.3	1.0226	0.0035	5.84	0.12	3237	647
625.00	average	biomass	1163.3	118.2	0.8286	0.0077	6.72	0.21	3419	684

density (plants/m2)	wheat.base	op.type	mean.yield (mg)	se.yield	mean.height (m)	se.height	mean.branches	se.branches	mean.aboveground biomass (mg)	se.abbiomass
625.00	average	RF	964.0	60.3	0.9941	0.0018	7.28	0.09	3445	689
625.00	average	connecting	1191.1	129.0	0.7833	0.0194	7.52	0.25	3645	729
625.00	modern	original	1034.4	98.4	0.6919	0.0120	3.64	0.11	3096	619
625.00	modern	biomass	916.0	116.4	0.7923	0.0288	3.72	0.18	3468	694
625.00	modern	RF	1055.8	80.4	0.7084	0.0093	3.80	0.08	3137	627
625.00	modern	connecting	929.4	131.9	0.7606	0.0369	3.60	0.21	3471	694
2500.00	average	original	338.2	68.3	0.6712	0.0517	4.04	0.14	1078	216
2500.00	average	biomass	404.0	112.0	0.4271	0.0651	3.72	0.31	1160	232
2500.00	average	RF	340.2	84.0	0.6792	0.0438	4.60	0.21	1148	230
2500.00	average	connecting	406.0	126.0	0.4310	0.0589	4.12	0.41	1232	246
2500.00	modern	original	322.2	89.4	0.3630	0.0464	2.24	0.14	1001	200
2500.00	modern	biomass	290.1	97.5	0.3442	0.0657	1.72	0.21	1100	220
2500.00	modern	RF	316.5	81.6	0.3913	0.0440	2.08	0.13	979	196
2500.00	modern	connecting	300.1	86.9	0.3748	0.0675	1.96	0.18	1137	227

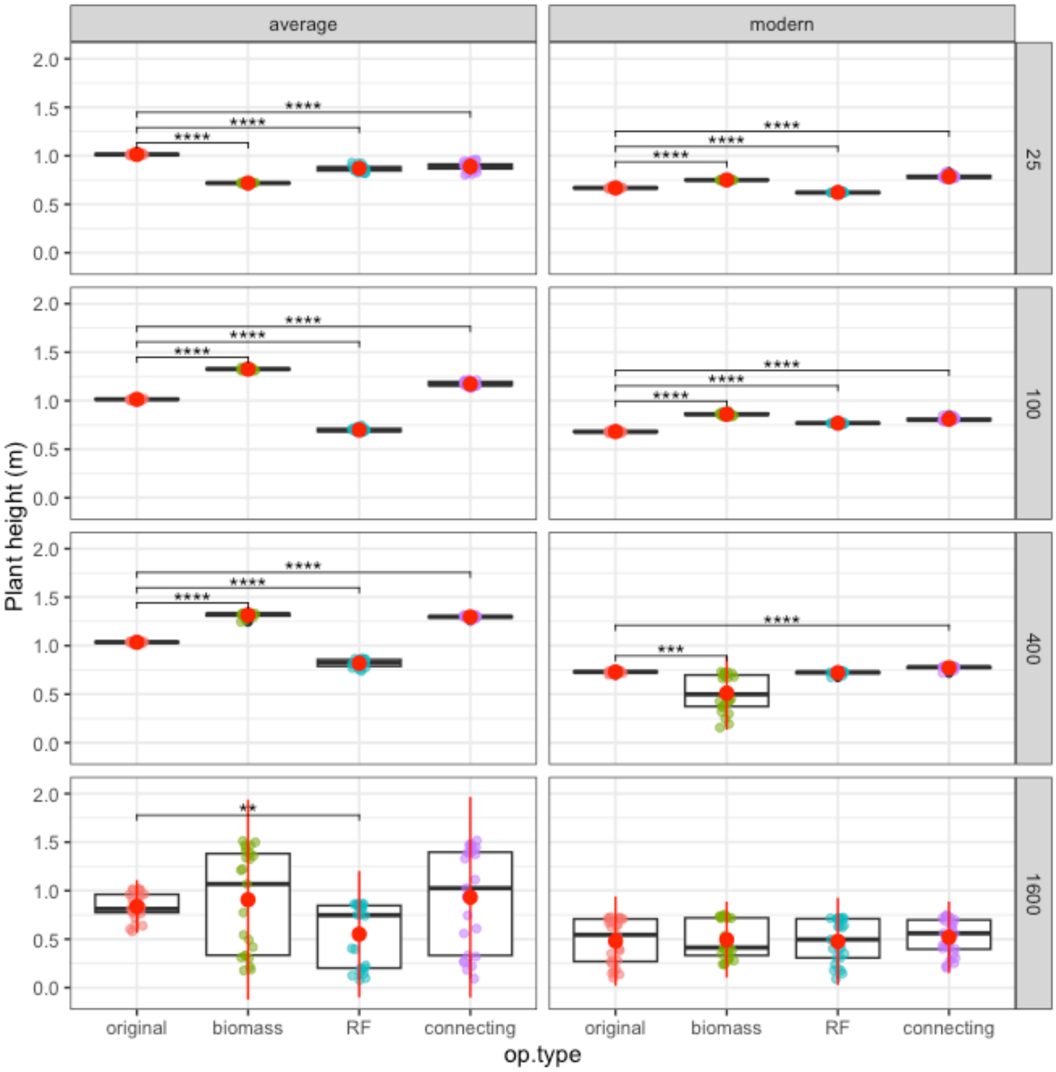


Figure S 1: The plant height of ideotypes for different planting densities.

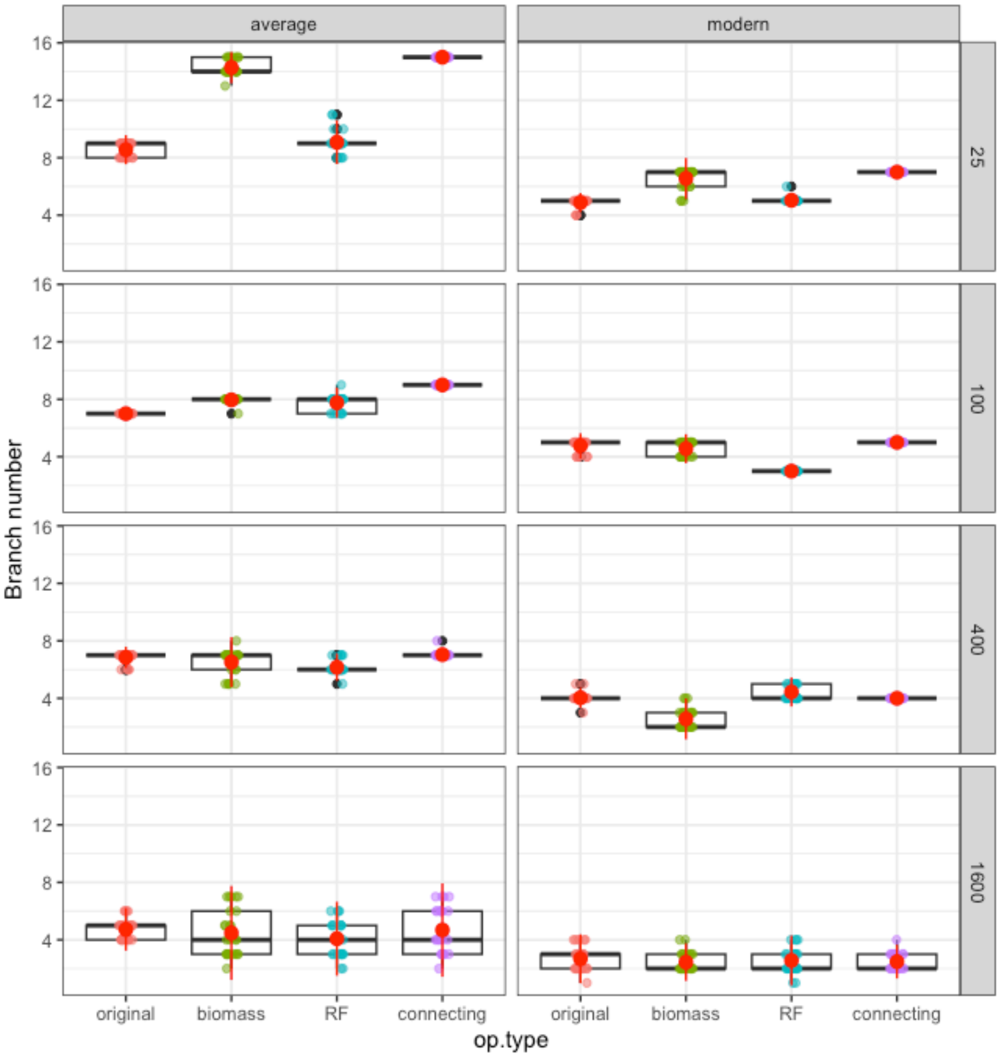


Figure S 2: The branch numbers of ideotypes for different planting densities.

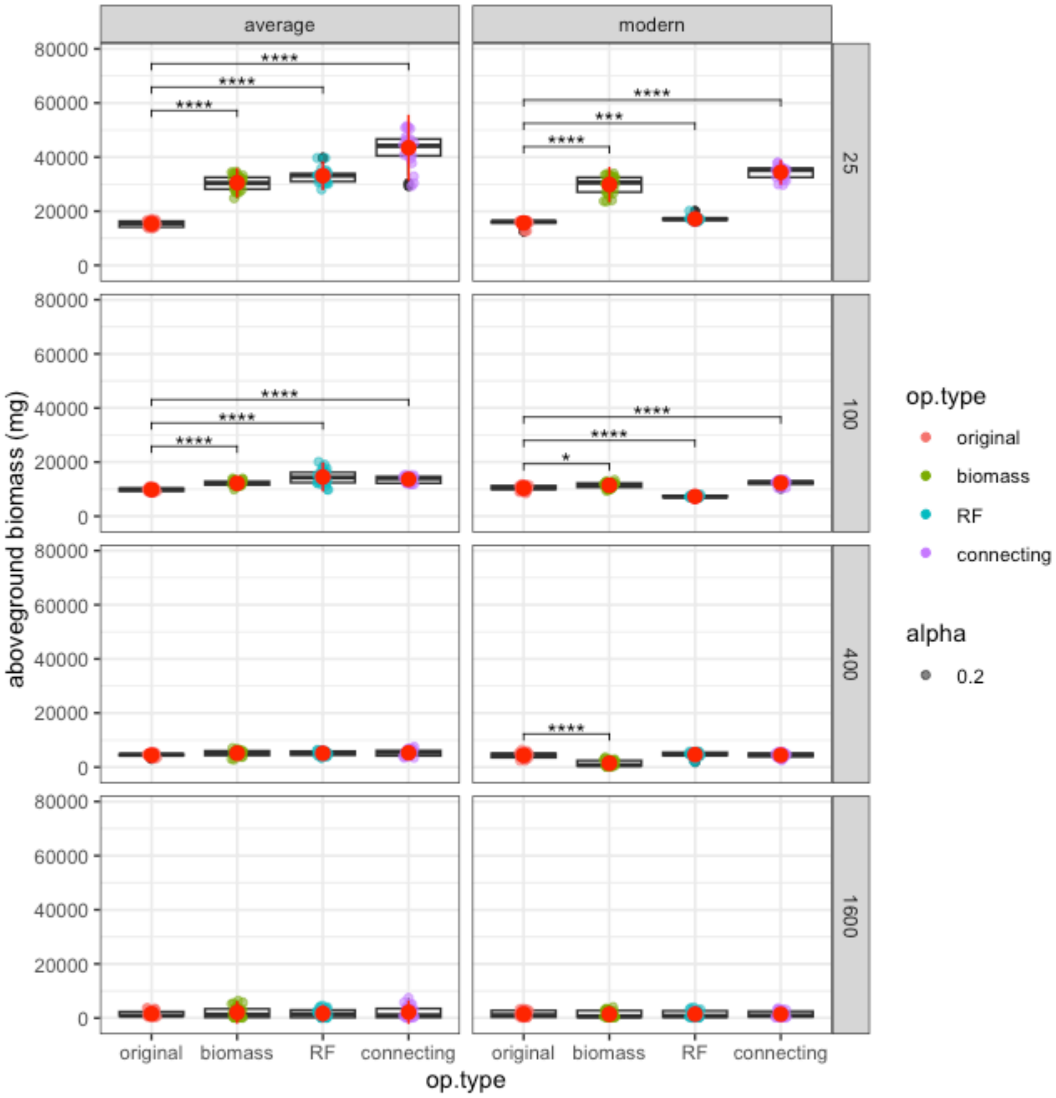


Figure S 3: The aboveground biomass of ideotypes for different planting densities.

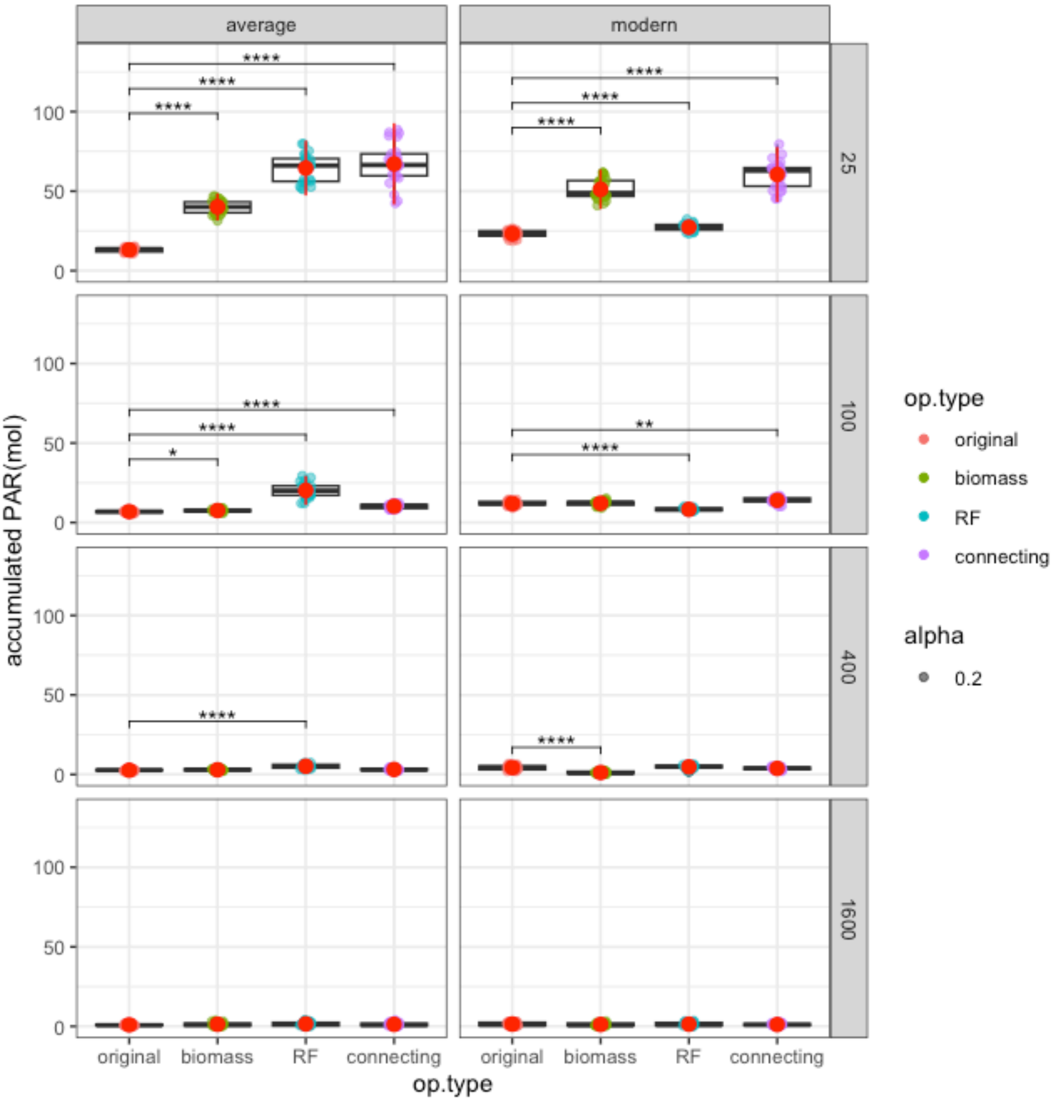


Figure S 4: The accumulated PAR of ideotypes for different planting densities.

Chapter 4: Association mapping identifies quantitative trait loci for wheat awn

Yixiang Shan & Colin Osborne

Plants, Photosynthesis and Soil, School of Biosciences, University of Sheffield,
Sheffield S10 2TN, UK;

4.1 Abstract

Bread wheat (Triticum aestivum) is one of the world's most important food crops and is crucial to human food security. After becoming a hexaploid, it has undergone a long period of selection in landrace improvement. Many wild morphological traits of bread wheat have been lost during this period, although they are valuable for improving modern wheat yield. To elucidate these lost traits, I conducted a genomic association study (GWAS) to identify genetic factors influencing wheat morphological traits. I used a wide range of wheat varieties and germplasm resources to collect data on several traits, including awn appearance, plant height and spike number. Through high-density single nucleotide polymorphism (SNP) sequencing and molecular marker analysis, we were able to identify several SNPs that were significantly associated with these traits. We identified a number of key SNPs strongly associated with awns, which promote yield potential and offer opportunities for production trait improvement. Through functional annotation and genomic analysis of the GWAS results, we gained insights into the molecular mechanisms underlying these traits. Our study not only contributes to the understanding of wheat genetic diversity, but also provides important genetic resources and candidate genes for wheat breeding.

4.2 Introduction

Wheat (*Triticum aestivum L.*) stands as a cornerstone of global sustenance, representing a preeminent food crop and securing the second-highest position in total food production (Erenstein *et al.*, 2022). Wheat, as one of the main foods in the world, provides 20% of food calories (‘FAOSTAT’). Wheat experienced long term domestication and polyploid formation, leading to today’s bread wheats (Gustafson *et al.*, 2009b). Approximately 95% of the global crop is hexaploidy bread wheat (*Triticum aestivum L. aestivum*, genomic constitution AABBDD), whereas the remainder includes tetraploid durum wheat (*Triticum turgidum L. durum*, AABB) and other wheat types of smaller economic importance (Peng *et al.*, 2011). Thereby, bread wheat improvement represents important work to increase yield to feed the world.

Ideotype breeding is based on the modification of individual traits to enhance genetic yield potential, and the traditional process uses multiple rounds of trial and error for phenotypic selection (Rasmusson, 1987). Throughout the history of wheat domestication, a range of traits have been subject to human intervention, including plant height (Zhang *et al.*, 2020), tillering (Kuraparthy *et al.*, 2007), spike length (Sharma *et al.*, 2019) and awn length (Elbaum *et al.*, 2007). These traits were all selected and contributed to yield increases. Our previous experiment in Chapter 2 shows that landrace improvement after domestication is an important stage in wheat improvement. During this period, bread wheats (*T. aestivum*) emerged and were improved by artificial selection (Curtis *et al.*, 2002) to adapt the crop to its local environment (Wingen *et al.*, 2017). This characteristic means that landrace collections in general show a much higher level of genetic diversity than elite varieties, making them valuable for exploring the use of ancient traits in breeding (Moore, 2015). Modern breeding is therefore now increasingly focused on the inclusion of novel allelic diversity from landraces to expand existing wheat diversity. For example, there are related experiments has been done in awns (Karagöz & Zencirci, 2005), plant height (Murphy *et al.*, 2008) and spikes (Denčić *et al.*, 2000). Therefore, identification and introduction of favourable genes or alleles controlling these traits are crucial for improving grain yield in bread wheat breeding.

Modern crop breeding has benefited from advances in genomics technology, providing markers that aid in breeding and using them to characterise trait performance in hybrid progeny. The International Wheat Genome Sequencing Consortium (IWGSC) has now published a high-quality assembly of the genome, with chromosome-level assembly (Consortium (IWGSC) *et al.*, 2018). Refseq V1 is an important quality standard for the hexaploidy wheat reference genome, created by the IWGSC (Alaux *et al.*, 2018). It provides detailed information on the location and sequence of 107,891 genes from 21 sequenced chromosomes and allows the discovery of more than 4 million molecular markers. Information about the association of specific genomic regions with desirable traits could facilitate the efficient use of landraces, wild relatives, and other "exotic" sources, especially if DNA polymorphism assays from these regions could be deployed in marker-assisted selection. Single nucleotide polymorphism (SNP) arrays in bread wheat have been studied many times before (Ravel *et al.*, 2006). Wheat breeders use high-density SNP profiles to identify genomic regions associated with quantitative traits in parental mapping experiments or genome-wide association studies (GWAS) (Neumann *et al.*, 2011). For example, GWAS has been used to investigate the significant associations of quantitative seed traits in wild *T. urartu* wheat (Talini *et al.*, 2020), and to identify an allele related to seed size in bread wheat (Yu *et al.*, 2022). There have also been many GWAS studies identifying the loci associated with wheat internode length and tillering (Liu *et al.*, 2023), leaf rust (Talebi *et al.*, 2023) and grain sizes (Garcia *et al.*, 2019).

Genome-wide association study (GWAS) was first proposed in 2002 (Ozaki *et al.*, 2002) to conduct association analysis on the genetic variation of complex traits at the genome-wide level. In the subsequent two decades, with the rapid development of genome technology, especially the improvement of sequencing technology, the human genome project (human genome project, HGP) and the whole genome sequencing of many animals and plants, GWAS has become a widely used research tool (Loos, 2020). Based on linkage disequilibrium (LD), GWAS detects molecular markers associated with target traits based on high-density molecular markers in the localized population (Flint-Garcia *et al.*, 2003). In recent times, the application of GWAS has gained significant traction within the domain of wheat research, featuring prominently in a multitude of investigations (Arriagada *et al.*, 2020).

This study aimed to perform a GWAS on a panel of 304 bread wheat cultivars using an SNP array based on transcriptome data. Its goals were: (1) investigating marker-trait associations for plant domestication traits; (2) assessing correlations between these traits and further highlighting SNPs shared by multiple traits; (3) detecting candidate genes responsible for the corresponding morphological features. Overall, 1581 SNP markers were used in this study to identify significant associations with seven physiological and agronomic traits. The utilization of genomic regions undergoing selection during wheat domestication and improvement is discussed and will contribute to the establishment of regulatory networks for genetic improvement of morphological traits in wheat.

4.3 Materials and Methods

4.3.1 Plant materials and trait measurements

Plant materials are from YoGI landrace panel, which constitutes 342 *T. aestivum* accessions sourced from wheat collections held at the Germplasm Resource Unit (GRU, https://www.jic.ac.uk/research-impact/germplasm-resource-unit), the International Maize and Wheat Improvement Center (Centro Internacional de Mejoramiento de Maíz y Trigo, CIMMYT, https://www.cimmyt.org) and the Crop Research Institute (Výzkumný Ústav Rostlinné Výroby, https://www.vurv.cz). Landraces were selected to maximize the diversity and representation of countries across the global wheat mega-environment (Sonder, 2016), including both spring and winter accessions.

We grew 304 accessions of the YoGI panel in the greenhouse of the University of York. Seeds were sown in Levington Advance Seed & Modular F2S compost mixed with Aggregate Industries Garside Sands 16/30 sand (80:20 ratio), treated with CaLypso insecticide (Bayer CropScience Ltd., 0.083ml mixed with 100ml water, applied to each liter of compost) and grown under long day (16/8h, 20°C/14°C) glasshouse conditions.

We measured 8 morphological traits in total (as shown in table 1).

Table 1: Traits measured in this experiment.

Trait name	**Explanation**

Plant_height_node	The max height of the tallest part of the plant from soil to the base of tallest spike (does not contain the spike length).
Peduncle_length	Length from the base of the spike to the first node on the tallest stem.
Leaf_length	Length of the flag leaf.
Spike_length	Length of the longest spike (corresponding to the main stem).
Spikelet_number	Number of spikelets on the main stem/largest stem.
Plant_height_spike	The max height of the tallest part of the plant from soil to tip of tallest spike.
Spike_number	The number of spikes on one plant.
Awns	If the wheat has awns, the value is 1; otherwise it is 0 (awns less than 0.5 cm in length are coded as absent).

These traits were measured in July 2021, when wheat ended their reproductive growth and were drying. The period corresponds to Zadoks stage 91.

4.3.2 Genotyping data

The SNPs and Q matrix (population structure) data are from University of York. The specific RNA sequence and process can be found in these references (Barratt *et al.*, 2023b) (Barratt *et al.*, 2023a).

4.3.3 Genome-wide association analyses

An association test was performed using the GAPIT package (https://zzlab.net/GAPIT/) in R (version. 4.0.2). The MLM model analyzed trait data with Q (population structure) and P (principal component) to find trait-marker associations. If the logarithmic P-value base 10 was more than -6.5, the SNPs in this case were regarded significant for GWAS results. Furthermore, Q-Q plots were drawn and used to check whether there were any deviations between the P value of our observed SNP and the null hypothesis P value, thereby confirming the accuracy of our GWAS analysis.

4.4 Results

4.4.1 Phenotype statistics

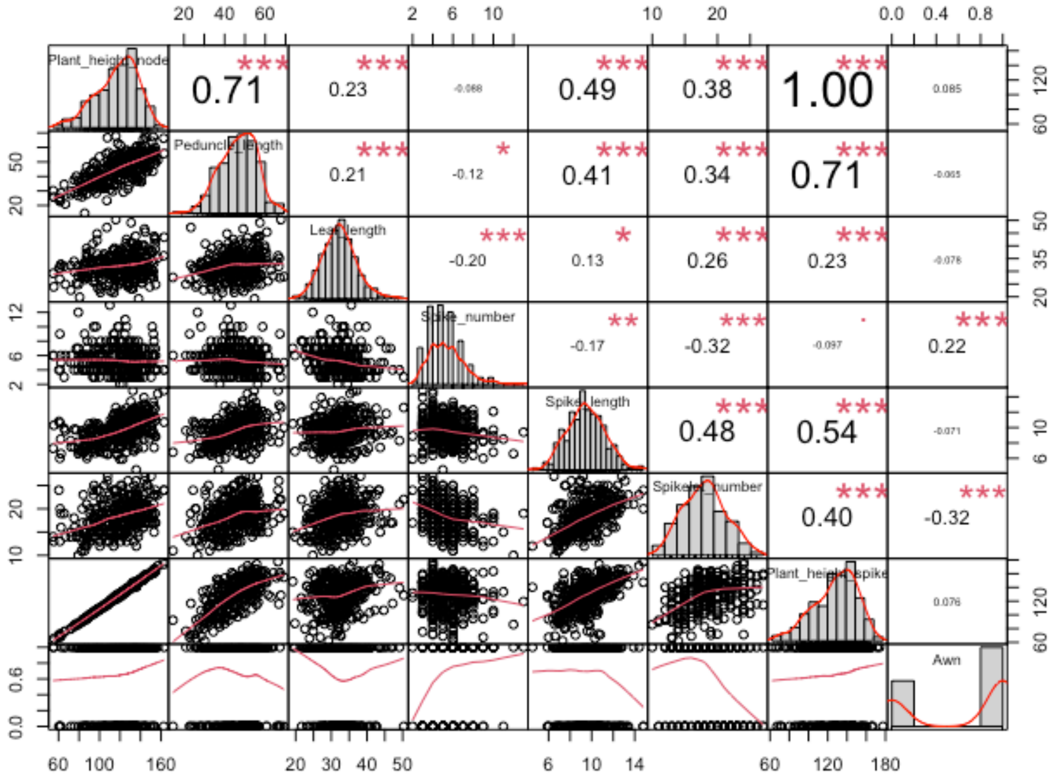


Figure 3: Distribution and correlation analysis of wheat phenotypic traits. The distribution of each variable is shown on the diagonal. Below the diagonal, the bivariate scatter plots with a fitted line are displayed. Above the diagonal, the value of the correlation were calculated by Pearson correlation coefficients, with the significance level indicated by stars (* p<0.05, ** p<0.01, *** p<0.001).

The value distribution and correlation anlaysis are detailed in Figure 1. There were eight traits studied in bread wheat. With the exception of awns, the other seven traits follow normal distributions or skewed normal distribution. There were 111 wheat accessions with no awns and 193 accessions with awns. Among all the traits, plant height with or without spikes shows a strong relationship (1). Moreover, [Peduncle_length] also shows positive relationship with [Plant_height_node] (0.71) and [Plant_height_spike] (0.71). The [Spike_length] is positive correlated with [Spikelet_number] (0.48) and [Plant_height_spike] (0.54). The strongest negative correlation is between [Spike_number] and [Spikelet_number] (-0.32).

4.4.2 Marker–trait associations

The presence of awns is one important trait lost after domestication. In our diverse panel of accessions, there are 111 domesticated wheats without awns and 193 wheats with them. In the GWAS study, we find four SNPs with a significant relationship to awn appearance as shown in Figure 2. This Manhattan plot shows the SNPs, positioned along the x-axis according to chromosomal position, and coded with different colours to mark their locations on different chromosomes. Plotted on the y-axis is the negative log of the SNP's associated P-value. The solid and dashed horizontal lines in Figure 2 indicate the genome-wide suggestive (P values $< 2.4 \times 10^{-7}$) and significant (P values $< 1.2 \times 10^{-8}$) threshold, respectively. The four significant SNPs are all located in the same region of chromosome 5A, forming a well-defined peak that belongs to the TraesCS5A01G542600 gene region. The highest peak marker was *TraesCS5A01G542600.2:171:G*, with $-\log_{10}P = 27.11377$. The q-q plot shows that observed P values and expected P values are distributed along the 1:1 line. When $-\log_{10}(P)$ is larger than 4, some observed P values are clearly more significant than expected under the null hypothesis and they move towards the y-axis (Figure 2B). Therefore genetic shift and selection stress both affect the GWAS results, which verifies that awn appearance was under some selection stress.

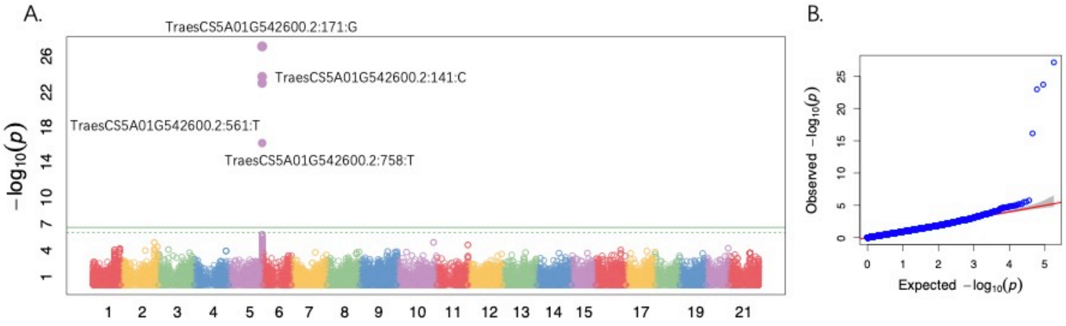


Figure 2: Manhattan and quantile–quantile (Q–Q) plots for awn traits : (A) the genome-wide association plots for statistically significant P values across 21 wheat chromosomes for SNP markers associated with the awn trait; Each dot represents a SNP. Green line indicates threshold of significance at − log10P 6.5 .(B) Q–Q plots for awn appearance.

There is only one SNP showing a significant association with plant height. It is *TraesCS4D01G040400.1:181:G*, which stands at chromosome 4D (Figure 3A). Spike number has two significant SNP markers from our analysis. They are *TraesCS6D01G226700.1:1082:T* and *TraesCS6B01G511800.3:902:A* (Figure 4A). The q-q plots of plant height support the GWAS analysis, showing that observed P value is smaller than expected P values (Figure 3B) thus deviating from the diagonal line. That means the distribution of P values was influenced by natural selection and genetic drift. However, the q-q plot of spike number shows that the relationship between P-value distributions quickly deviates from the sloping line (Fig. 4B), which might be because that of population stratification in our wheat samples.

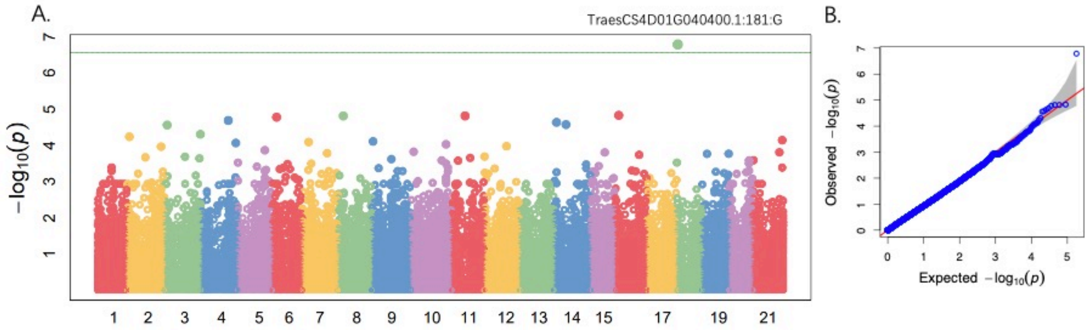


Figure 3: Manhattan and quantile–quantile (Q–Q) plots for plant height: (A) the genome-wide association plots for statistically significant P values across 21 wheat chromosomes for SNP markers associated with plant height; Each dot represents a SNP. green line indicates threshold of significance at − log10P 6.5. (B) Q–Q plots for plant height.

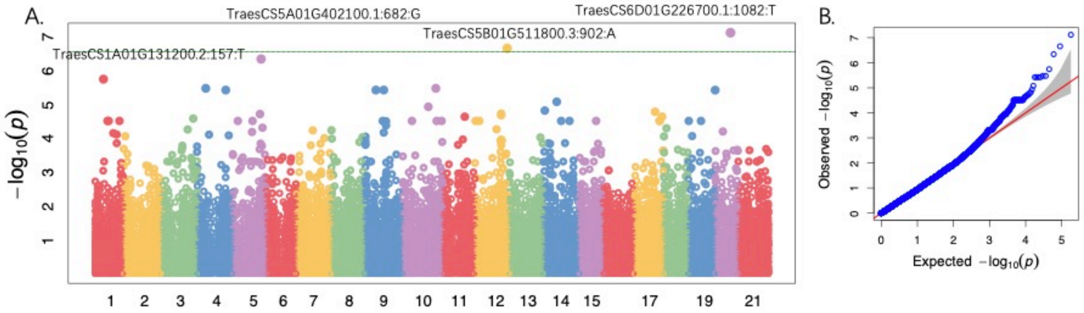


Figure 4: Manhattan and quantile–quantile (Q–Q) plots for spike number: (A) the genome-wide association plots for statistically significant P values across 21 wheat chromosomes for SNP markers associated with spikes; Each dot represents a SNP. green line indicates threshold of significance at − log10P 6.5 .(B)) Q–Q plots for spikes.

The other five traits (Spike_length, Spikelet_number, Plant_height_spike, Peduncle_length and Leaf_length) have no strong relation with current SNPs, when -log10 P was set at a threshold of 6.5.

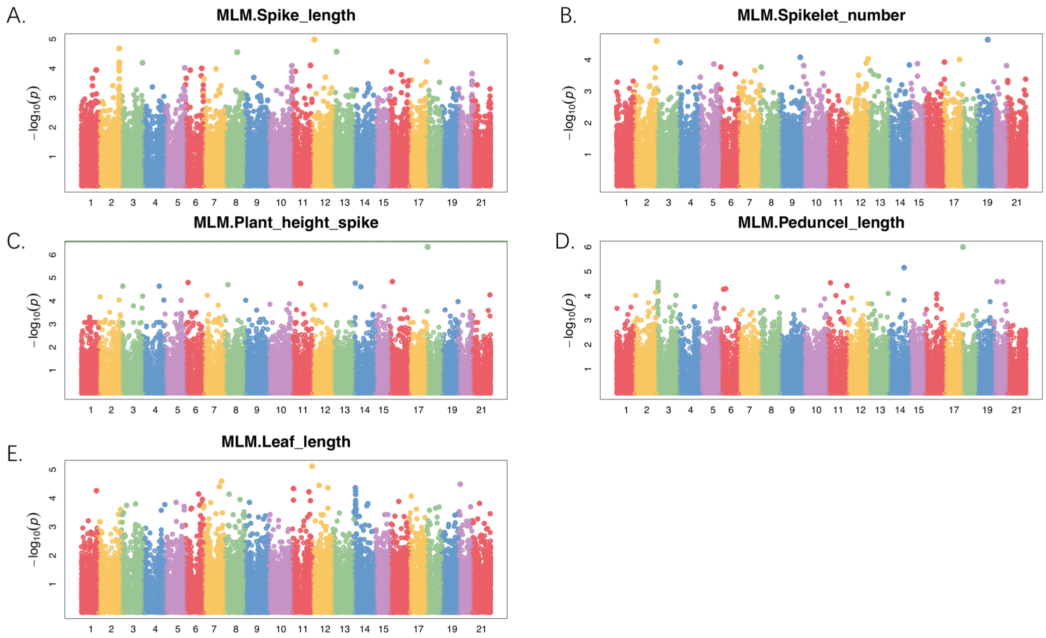


Figure 5: the five traits and their manhattan plots. A. Spike_length; B. Spikelet_number; C.Plant_height_node; Peduncle_length; Leaf_length.. There are on SNP reach the significant P-value levels.

4.5 Discussion

By connecting bread wheat phenotypic data and SNPs, we found several marker-trait associations with awns, plant height and spike number. The awn length expression was especially well identified at the chromosome level.

Awn presence is a distinctive feature observed in various grain crops, including wheat, wherein both awned and non-awned varieties exist. Awns confer advantageous attributes to wheat, such as enhanced photosynthesis and protective functions (Duwayri, 1984). Previous work has identified three major inhibitors of awn development in wheat: *Tipped 1 (B1)*, *Tipped 2 (B2)* and *Hooded (Hd)*, located on chromosomes 5A, 6B and 4A, respectively (Rakszegi *et al.*, 2010). Genetic analyses have revealed the involvement of multiple genes in awn formation and elongation. Recent elucidations have shed light on a potential candidate for *Tipped 1*, namely a *C2H2* zinc finger protein harboring an EAR domain, indicative of transcriptional repressors, proposing its role in this context (DeWitt *et al.*, 2020). Up-regulation of this gene in awnless *B1* compared to awned *b1* plants has been observed, suggesting that the misexpression of this transcriptional regulator might contribute to the reduction of awn length in *B1* plants (Huang *et al.*, 2020). There are three candidate genes: *TraesCS5A02G542600*, *TraesCS5A02G542700* and *TraesCS5A02G542800*. All of them are expressed in awns. Both TraesCS5A01G542600 and TraesCS5A01G542700 appear to be more universally expressed, while *TraesCS5A01G542800* showed a more specific expression, being restricted to tissues within spikes (Würschum *et al.*, 2020). Our study supports this finding, in the *Tipped 1* candidate genes, we also find the *TraesCS5A01G542600* loci and it shows a strong relationship in awn expression (Fig. 2). The candidate gene *TraesCS5A01G542600* are identified in hexose carrier protein HEX6-like (‘NCBI Blast:Nucleotide Sequence’).

In wheat, awns are subject to farmer selection. It is confirmed that selection for the absence of awns did not exist from the beginning of domestication (Sanchez-Bragado *et al.*, 2023). Rather, it is because emmer was domesticated as local varieties with long awns (Araus *et al.*, 2007). It is therefore assumed that farmers chose wheat with long awns at the beginning (Yoshioka *et al.*, 2017). However, bread wheat has evolved to be almost awnless. This is because the absence of awns makes it easier for farmers to harvest the wheat and store it (Mach, 2015).That might result in relaxed selection for dispersal, as plant does not need to disperse seeds in farming (Lahti *et al.*, 2009). Morevoer, the disappearance of awn may also be related to the resource reallocation of the seeds during domestication (Zohary & Hopf, 2000).

In our study, we also identified significant SNP loci associated with plant height and spike number, although their levels of significance were comparatively lower. Numerous genes have been shown to influence wheat height, with several previous investigations detecting relevant loci on chromosomes 7A and 7B (Khan *et al.*, 2022) (Abou-Elwafa & Shehzad, 2021). RNAi-mediated knock-down of TaARF12 (*TraesCS2A01G547800*) resulted in a reduction of plant height by up to 20.7% (Li *et al.*, 2022). There are also different experimental results on GWAS of bread wheat height. For example, Carmen found loci on 2B associated with Spanish bread wheat height (Ávila *et al.*, 2021). Another wheat GWAS experiment in China found significant SNPs in chromosomes 4DS, 6DL, 2DS and 1BL (Sun *et al.*, 2017). The reason may be that we selected different local groups of wheat in different geographical regions. It also suggests that there may be many genetic variants that affect height. The same phenomenon occurs in spikes. Jamil’s work shows the spike number relevant locus on chromosomes 1B, 2D and 4B (Jamil *et al.*, 2019). Liu found the 36 significant SNPs about spike number per plants, and some of them located in chromosome 6B (Liu *et al.*, 2018). Our two SNPs at TraesCS6D01G226700 and TraesCS6B01G511800 genes have partly commonalities (6B) and differences with theirs.

The size of the dataset may limit our work, although we were able to identify 4 SNPs for awns, 2 SNPs in spike number and one SNP in plant height. However, only the awn-related SNPs have received much support from previous research. Although some other yield traits such as spikelet number, leaf length, spike length and peduncle length did not show significant association with our SNPs, they were mentioned in some other studies (Neumann *et al.*, 2011) (Mwadzingeni *et al.*, 2017) (Zheng *et al.*, 2022) (Ahmed *et al.*, 2022). With more SNP data and bread wheat, we may be able to obtain more marker-trait associations and better understand bread wheat improvement. And we believe that with more GWAS research results, the mechanisms of bread wheat trait variation will become better resolved.

4.6 Reference

Abou-Elwafa SF, Shehzad T. **2021**. Genetic diversity, GWAS and prediction for drought and terminal heat stress tolerance in bread wheat (Triticum aestivum L.). *Genetic Resources and Crop Evolution* **68**: 711–728.

Ahmed HGM-D, Zeng Y, Iqbal M, Rashid MAR, Raza H, Ullah A, Ali M, Yar MM, Shah AN. **2022**. Genome-wide association mapping of bread wheat genotypes for sustainable food security and yield potential under limited water conditions. *PloS one* **17**: e0263263.

Alaux M, Rogers J, Letellier T, Flores R, Alfama F, Pommier C, Mohellibi N, Durand S, Kimmel E, Michotey C, *et al.* 2018. Linking the International Wheat Genome Sequencing Consortium bread wheat reference genome sequence to wheat genetic and phenomic data. *Genome Biology* **19**: 111.

Araus JL, Ferrio JP, Buxó R, Voltas J. **2007**. The historical perspective of dryland agriculture: lessons learned from 10 000 years of wheat cultivation. *Journal of Experimental Botany* **58**: 131–145.

Arriagada O, Marcotuli I, Gadaleta A, Schwember AR. **2020**. Molecular mapping and genomics of grain yield in durum wheat: a review. *International Journal of Molecular Sciences* **21**: 7021.

Ávila CM, Requena-Ramírez MD, Rodríguez-Suárez C, Flores F, Sillero JC, Atienza SG. **2021**. Genome-Wide Association Analysis for Stem Cross Section Properties, Height and Heading Date in a Collection of Spanish Durum Wheat Landraces. *Plants* **10**: 1123.

Barratt LJ, He Z, Fellgett A, Wang L, Mason SM, Bancroft I, Harper AL. **2023a**. Co-expression network analysis of diverse wheat landraces reveals markers of early thermotolerance and a candidate master regulator of thermotolerance genes. *The Plant Journal* **115**: 614–626.

Barratt LJ, Reynolds IJ, Franco Ortega S, Harper AL. **2023b**. Transcriptomic and co-expression network analyses on diverse wheat landraces identifies candidate master regulators of the response to early drought. *Frontiers in Plant Science* **14**.

Consortium (IWGSC) IWGS, Appels R, Eversole K, Stein N, Feuillet C, Keller B, Rogers J, Pozniak CJ, Choulet F, Distelfeld A. **2018**. Shifting the limits in wheat research and breeding using a fully annotated reference genome. *Science* **361**: eaar7191.

Curtis BC, Rajaram S, Gómez Macpherson H. **2002**. Bread wheat: improvement and production. *Bread wheat: improvement and production.*

Denčić S, Kastori R, Kobiljski B, Duggan B. **2000**. Evaluation of grain yield and its components in wheat cultivars and landraces under near optimal and drought conditions. *Euphytica* **113**: 43–52.

DeWitt N, Guedira M, Lauer E, Sarinelli M, Tyagi P, Fu D, Hao Q, Murphy JP, Marshall D, Akhunova A, *et al.* 2020. Sequence-based mapping identifies a candidate transcription repressor underlying awn suppression at the B1 locus in wheat. *New Phytologist* **225**: 326–339.

Duwayri M. **1984**. Effect of flag leaf and awn removal on grain yield and yield components of wheat grown under dryland conditions. *Field Crops Research* **8**: 307–313.

Elbaum R, Zaltzman L, Burgert I, Fratzl P. **2007**. The Role of Wheat Awns in the Seed Dispersal Unit. *Science* **316**: 884–886.

Erenstein O, Jaleta M, Mottaleb KA, Sonder K, Donovan J, Braun H-J. **2022**. Global trends in wheat production, consumption and trade. In: Wheat improvement: food security in a changing climate. Springer International Publishing Cham, 47–66.

FAOSTAT.

Flint-Garcia SA, Thornsberry JM, Buckler IV ES. **2003**. Structure of linkage disequilibrium in plants. *Annual review of plant biology* **54**: 357–374.

Garcia M, Eckermann P, Haefele S, Satija S, Sznajder B, Timmins A, Baumann U, Wolters P, Mather DE, Fleury D. **2019**. Genome-wide association mapping of grain yield in a diverse collection of spring wheat (Triticum aestivum L.) evaluated in southern Australia. *PLOS ONE* **14**: e0211730.

Gustafson P, Raskina O, Ma X, Nevo E. **2009**. Wheat evolution, domestication, and improvement. *Wheat science and trade*: 3–30.

Huang D, Zheng Q, Melchkart T, Bekkaoui Y, Konkin DJF, Kagale S, Martucci M, You FM, Clarke M, Adamski NM, *et al.* 2020. Dominant inhibition of awn development by a putative zinc-finger transcriptional repressor expressed at the B1 locus in wheat. *New Phytologist* **225**: 340–355.

Jamil M, Ali A, Gul A, Ghafoor A, Napar AA, Ibrahim AMH, Naveed NH, Yasin NA, Mujeeb-Kazi A. **2019**. Genome-wide association studies of seven agronomic traits under two sowing conditions in bread wheat. *BMC Plant Biology* **19**: 149.

Karagöz A, Zencirci N. **2005**. Variation in wheat (Triticum spp.) landraces from different altitudes of three regions of Turkey. *Genetic Resources and Crop Evolution* **52**: 775–785.

Khan H, Krishnappa G, Kumar S, Mishra CN, Krishna H, Devate NB, Rathan ND, Parkash O, Yadav SS, Srivastava P, *et al.* 2022. Genome-wide association study for grain yield and component traits in bread wheat (Triticum aestivum L.). *Frontiers in Genetics* **13**.

Kuraparthy V, Sood S, Dhaliwal HS, Chhuneja P, Gill BS. **2007**. Identification and mapping of a tiller inhibition gene (tin3) in wheat. *Theoretical and Applied Genetics* **114**: 285–294.

Lahti DC, Johnson NA, Ajie BC, Otto SP, Hendry AP, Blumstein DT, Coss RG, Donohue K, Foster SA. **2009**. Relaxed selection in the wild. *Trends in ecology & evolution* **24**: 487–496.

Li A, Hao C, Wang Z, Geng S, Jia M, Wang F, Han X, Kong X, Yin L, Tao S. **2022**. Wheat breeding history reveals synergistic selection of pleiotropic genomic sites for plant architecture and grain yield. *Molecular Plant* **15**: 504–519.

Liu Y, Shen K, Yin C, Xu X, Yu X, Ye B, Sun Z, Dong J, Bi A, Zhao X. **2023**. Genetic basis of geographical differentiation and breeding selection for wheat plant architecture traits. *Genome Biology* **24**: 1–25.

Liu J, Xu Z, Fan X, Zhou Q, Cao J, Wang F, Ji G, Yang L, Feng B, Wang T. **2018**. A Genome-Wide Association Study of Wheat Spike Related Traits in China. *Frontiers in Plant Science* **9**.

Loos RJF. **2020**. 15 years of genome-wide association studies and no signs of slowing down. *Nature Communications* **11**: 5900.

Mach J. **2015**. *Domesticated versus wild rice? Bring it awn!* American Society of Plant Biologists.

Moore G. **2015**. Strategic pre-breeding for wheat improvement. *Nature Plants* **1**: 1–3.

Murphy KM, Dawson JC, Jones SS. **2008**. Relationship among phenotypic growth traits, yield and weed suppression in spring wheat landraces and modern cultivars. *Field Crops Research* **105**: 107–115.

Mwadzingeni L, Shimelis H, Rees DJG, Tsilo TJ. **2017**. Genome-wide association analysis of agronomic traits in wheat under drought-stressed and non-stressed conditions. *PloS one* **12**: e0171692.

NCBI Blast:Nucleotide Sequence.

Neumann K, Kobiljski B, Denčić S, Varshney RK, Börner A. **2011**. Genome-wide association mapping: a case study in bread wheat (Triticum aestivum L.). *Molecular Breeding* **27**: 37–58.

Ozaki K, Ohnishi Y, Iida A, Sekine A, Yamada R, Tsunoda T, Sato H, Sato H, Hori M, Nakamura Y, *et al.* **2002**. Functional SNPs in the lymphotoxin-α gene that are associated with susceptibility to myocardial infarction. *Nature Genetics* **32**: 650–654.

Peng JH, Sun D, Nevo E. **2011**. Domestication evolution, genetics and genomics in wheat. *Molecular Breeding* **28**: 281–301.

Rakszegi M, Kisgyörgy BN, Tearall K, Shewry PR, Láng L, Phillips A, Bedő Z. **2010**. Diversity of agronomic and morphological traits in a mutant population of bread wheat studied in the Healthgrain program. *Euphytica* **174**: 409–421.

Rasmusson DC. **1987**. An Evaluation of Ideotype Breeding1. *Crop Science* **27**: cropsci1987.0011183X002700060011x.

Ravel C, Praud S, Murigneux A, Canaguier A, Sapet F, Samson D, Balfourier F, Dufour P, Chalhoub B, Brunel D. **2006**. Single-nucleotide polymorphism frequency in a set of selected lines of bread wheat (Triticum aestivum L.). *Genome* **49**: 1131–1139.

Sanchez-Bragado R, Molero G, Araus JL, Slafer GA. **2023**. Awned versus awnless wheat spikes: does it matter? *Trends in Plant Science* **28**: 330–343.

Sharma JS, Running KLD, Xu SS, Zhang Q, Peters Haugrud AR, Sharma S, McClean PE, Faris JD. **2019**. Genetic analysis of threshability and other spike traits in the evolution of cultivated emmer to fully domesticated durum wheat. *Molecular Genetics and Genomics* **294**: 757–771.

Sun C, Zhang F, Yan X, Zhang X, Dong Z, Cui D, Chen F. **2017**. Genome-wide association study for 13 agronomic traits reveals distribution of superior alleles in bread wheat from the Yellow and Huai Valley of China. *Plant Biotechnology Journal* **15**: 953–969.

Talebi R, Mahboubi M, Naji AM, Mehrabi R. **2023**. Physiological specialization of Puccinia triticina and genome-wide association mapping provide insights into the genetics of wheat leaf rust resistance in Iran. *Scientific Reports* **13**: 4398.

Talini RF, Brandolini A, Miculan M, Brunazzi A, Vaccino P, Pè ME, Dell'Acqua M. **2020**. Genome-wide association study of agronomic and quality traits in a world collection of the wild wheat relative Triticum urartu. *The Plant Journal* **102**: 555–568.

Wingen LU, West C, Leverington-Waite M, Collier S, Orford S, Goram R, Yang C-Y, King J, Allen AM, Burridge A, *et al.* **2017**. Wheat Landrace Genome Diversity. *Genetics* **205**: 1657–1676.

Würschum T, Jähne F, Phillips AL, Langer SM, Longin CFH, Tucker MR, Leiser WL. **2020**. Misexpression of a transcriptional repressor candidate provides a molecular mechanism for the suppression of awns by Tipped 1 in wheat. *Journal of Experimental Botany* **71**: 3428–3436.

Yoshioka M, Iehisa JC, Ohno R, Kimura T, Enoki H, Nishimura S, Nasuda S, Takumi S. **2017**. Three dominant awnless genes in common wheat: Fine mapping, interaction and contribution to diversity in awn shape and length. *PloS one* **12**: e0176148.

Yu H, Hao Y, Li M, Dong L, Che N, Wang L, Song S, Liu Y, Kong L, Shi S. **2022**. Genetic architecture and candidate gene identification for grain size in bread wheat by GWAS. *Frontiers in Plant Science* **13**.

Zhang L, Liu P, Wu J, Qiao L, Zhao G, Jia J, Gao L, Wang J. **2020**. Identification of a novel ERF gene, TaERF8, associated with plant height and yield in wheat. *BMC Plant Biology* **20**: 263.

Zheng X, Qiao L, Liu Y, Wei N, Zhao J, Wu B, Yang B, Wang J, Zheng J. **2022**. Genome-wide association study of grain number in common wheat from Shanxi under different water regimes. *Frontiers in Plant Science* **12**: 806295.

Zohary D, Hopf M. **2000**. *Domestication of plants in the Old World: The origin and spread of cultivated plants in West Asia, Europe and the Nile Valley.* Oxford university press.

Chapter 5: Domestication increases wheat competitiveness

Yixiang Shan & Colin Osborne

Plants, Photosynthesis and Soil, School of Biosciences, University of Sheffield,
Sheffield S10 2TN, UK

5.1 Abstract

The history of crop improvement can be attributed to domestication and selective breeding. People cultivated and improved crops, causing changes to crop morphology and yield increases. My previous work shows domesticated wheats achieve high yield per plant by becoming larger in size. However, this strategy might be detrimental for the crop as a whole. Although growing bigger may help an individual plant gain an advantage in resource competition with its neighbours, that competition could actually limit the yield of the whole population of crop plants in high density farming. We wanted to test the hypothesis that this selfish strategy evolved through natural selection in early domesticated wheats. We compared the competitive abilities of three pairs of wild and domesticated wheats. Based on previous work, we expected competitive ability to increase, but via different mechanisms across the independent wheat domestication events. By increasing the density of neighbours, we observed the reaction of growth in target plants. Results show that domesticated wheat landraces are less affected by competition than wild wheats in aboveground biomass and tiller number. In contrast, both biomass and tillering were significantly reduced in wild wheats by competition with domesticated forms. We also applied an FSP (Functional Structural Plant) model to simulate this competition experiment in *silico*. The model was parameterised for each wheat species using data from a previous experiment and supported the conclusion that domestication increased wheat competitiveness. This finding has important implications for crop breeding, showing that domestication has had unintended negative consequences for crops, that must be reversed or overcome through selective breeding. Future work should evaluate the extent to which the Green Revolution has achieved this goal, and the potential in modern varieties for further cooperation rather than competition with neighbours.

5.2 Background

Domestication has led to notable changes in crop morphology and improvements in yields. The agricultural practices employed in cultivation alter the growing environment of crops, forcing them to adapt to new farming conditions (Roucou *et al.*, 2018). Under this natural selection by the cultivation environment and artificial selection by farmers, crop phenotypes have changed in multiple ways. In the case of staple cereal crops like wheat, these include changes to seed size (Kluyver *et al.*, 2017), plant size (Preece *et al.*, 2017a), and canopy height (Milla et al., 2014), accompanied by glume reduction (Doebley et al., 2006) and loss of the natural seed dispersal mechanism (Peng *et al.*, 2003). These phenotypic changes associated with domestication have been elucidated by numerous studies, but phenotype-induced changes in plant competitiveness have been less studied.

Jones et al. (2022) recently hypothesized that increasing plant size during domestication might confer greater competitive ability, arising from the cultivation of crops at high densities, which selected for more vigorous genotypes. The larger seeds of domesticated crops (Kluyver *et al.*, 2017; Golan *et al.*, 2015) are strongly associated with seedling vigor (Lafond & Baker, 1986). This helps domesticated plants establish competitive advantages at the seedling stage, including faster growth and assimilation rates, and larger body sizes (Preece *et al.*, 2021). The asymmetry of competition with neighbouring plants makes it highly dependent on a head start on the part of the eventual winner (Weiner, 1990). Improved early vigour also confers better survival in the presence of deep shade, drought, physical damage and the presence of competing vegetation (Westoby *et al.*, 1996). Domestication also generates gigantism in establishing and mature plants, thereby increasing aboveground biomass and allocation, plant height and leaf size. This means that domesticated crops occupy more aboveground space and intercept more light, improving carbon source strength (Milla *et al.*, 2014), and shading competing plants to limit their photosynthesis.

Although natural selection might favour phenotypes with higher competitiveness, these do not necessarily contribute to overall population performance, and could be detrimental for area-based yield from the crop as a whole (Denison, 2012). Donald (1968) first proposed that a successful crop ideotype should actually be a weak competitor, since it heavily invests carbohydrates into yield. In contrast, selfish wheat individuals will invest in occupying space and intercepting light, to compete for resources with their neighbours, resulting in a tragedy of the commons (Anten & Vermeulen, 2016). It has therefore been argued that breeders should decrease individual competitiveness to achieve a high-yielding ideotype (Donald, 1981). However, the relationship of competitiveness and yield is not entirely antagonistic. In low-density or resource-rich environments, improving crop competitiveness can enhance yield (Weiner, 2019). Crop competitiveness also plays an important role in weed defence (van der Meulen & Chauhan, 2017), and consequently there have been attempts to improve weed suppression ability via breeding (Lemerle *et al.*, 2001) and management (Drews *et al.*, 2009). As a consequence, the relationship between yield and individual fitness is unimodal, such that the highest-yielding populations derive from cultivars with intermediate fitness (Weiner *et al.*, 2017).

Some scientists hypothesize that crop competitiveness has decreased as a result of domestication (e.g. Sedgley, 1991). This idea traces back to Donald's ideotype breeding theory (Blackshaw & Brandt, 2009), in which individual crop plants compete with one another at a minimum cost, so as to avoid "growth redundancy" (Zhang *et al.*, 1999). In this case, crop plants cooperate instead of becoming strong individual competitors, for example by producing fewer tillers (Peng *et al.*, 2003) and fewer, more erect leaves (Budak *et al.*, 2013). Additionally, previous research has demonstrated that domestication has led to a decrease in root biomass (Roucou *et al.*, 2018). Wild wheat progenitors typically possess thicker roots, lower specific root length and higher root mass fraction than domesticated forms (Martín-Robles *et al.*, 2019), potentially improving nitrogen and water uptake (Nakhforoosh *et al.*, 2014). This pattern extends to modern forms, with evidence for stronger roots in landraces than modern varieties (Zhu *et al.*, 2022).

Here, we compare the competitiveness of wild and domesticated wheats, to test the alternative hypotheses that domestication has either increased or reduced competitive ability**.** We compare three pairs of species that represent independent domestication events within the wheat genus: *T. dicoccoides* (wild) – *T. dicoccum* (domesticated), *T. araraticum* (wild) – *T. timopheevii* (domesticated) and *T. boeoticum* (wild) – *T. monococcum* (domesticated). Wheat *T. dicoccoides – T. dicoccum* represents the main route of wheat domestication, leading to *T. aestivum*, modern bread wheat (Weiner, 1990). Domesticated *T. dicoccum* have stronger early vigour than wild *T. dicoccoides*, which might bring competitive advantages. Conversely, *T. timopheevii* obtains an obvious height gain from domestication. Compared with its wild relative *T. araraticum* which has a height of 1.1 m, *T. timopheevii* will grow up to about 1.6 m. This height advantage might provide competitive benefits. Domesticated einkorn *T. monococcum* differs in tiller number from its wild progenitor *T. boeoticum*. Tillering strength has proven important in competing with weeds (Haefele *et al.*, 2004). However, whether it confers a competitive advantage to domesticated *T. monococcum* is yet to be determined. Consequently, our hypothesis is that domestication changes competitive ability via different mechanisms in each domestication event.

1. **Wild *T. dicoccoides* vs Domesticated *T. dicoccum* (main group)**

This is the domestication event that led to bread and pasta wheats. How does domestication change competitive ability in this case?

2. **Wild *T. araraticum* vs Domesticated *T. timopheevii* (gigantism group)**

In this domesticated event, the height of the shoot increased a lot. Will the increased height associated with domestication increase competitive ability?

3. **Wild *T. boeoticum* vs Domesticated *T. monococcum* (tillering group)**

In this domestication event, shoot branching increased. Will this tillering increase affect competitive ability?

5.3 Materials and Methods

5.3.1 Plant materials and growth

We compared three pairs of wheat species: *T. dicoccoides* (wild) – *T. dicoccum* (domesticated), *T. araraticum* (wild) – *T. timopheevii* (domesticated) and *T. boeoticum* (wild) – *T. monococcum* (domesticated). In each case, we chose a single accession based on a previous experiment that screened the phenotypic diversity within the species. Based on our last wheat growing experiment, we selected wheat accessions with values closest to the average biomass in their respective groups, ensuring that they were representative of their respective groups.

All the seeds were picked from the harvest of our last experiments in 2021. Seeds were first stored at 4°C for 24 h, and then germinated on moist filter paper in a closed petri dish ('Introduction to Wheat Growth', 2016). Germination was carried out under the following conditions in an incubator (versatile environmental test chamber, Panasonic, UK): 12 h dark, 12 h light, 20 ºC, photosynthetic photon flux density (PPFD) 300 μmol m^{-2} s^{-1} and 60% relative humidity (RH).

Germinated seeds were transplanted (one plant per pot) into pots (15*15*20cm, 3.5ltr, LBS Horticulture, UK) containing high nutrient compost (M3, Levington Horticulture Ltd., Ipswich, UK), supplemented with perlite (Sinclair Nursery Stock Propagation, Levington Horticulture Ltd., Ipswich, UK) in a 3:1 ratio. These pots were labelled and moved into a new controlled-environment growth cabinet (Conviron BDW 40, Conviron, Winnipeg, Manitoba, Canada). This controlled environment, designed for vernalizing winter wheats, was: 12 h dark, 12 h light, 4 ºC, PPFD 300 μmol m^{-2} s^{-1} and 60% RH.

After an eight-week vernalization period, wheat seedlings were moved to a controlled environment greenhouse. Here, the environmental settings were: 16 h light (PPFD at least 300 µmol m^{-2} s^{-1}) at 20 ºC, and 8 h dark at 15 ºC, with constant 70% RH. At this point, the wheat plants were 7-17 cm in height, and had 2 - 4 leaves and 1 -2 tillers. They were transplanted into pots ((15*15*20cm, 3.5ltr, LBS Horticulture, UK), applying the competition experimental design, as outlined below.

5.3.2 Competition experiment

We applied a gradient neighbour density design (Fig. 1) as described by Goldberg & Landa (1991). There are five pots in each replicate block. Each pot contains one focal plant of one species in the centre, surrounded by neighbours comprised of the other species, i.e. when the central plant is wild wheat, the neighbouring plants will be its domesticated relatives, whereas if the central plant is domesticated wheat, the neighbouring plants are its wild progenitor. The focal central plant is used to observe growth responses to competition, while the neighbouring plants provide a competitive environment. Densities of the neighbours varied from low to high (0, 1, 4, 9 and 21 individuals), which corresponded to field densities of 0, 44, 178, 400 and 933

Figure 1: Experiment design for evaluating wheat competition. The yellow term "wd" means wild wheats. The blue term "dd" means the domesticated wheats. The "wd" or "dd" at the centre of of each box represents the target plant. The "wd" or "dd" at the corners of each box mean the neighbours, which are used to provide varying levels of competition with the target plant.

plants/m^2. A sowing density of 400 plants/m^2 is typical for wheat in an intensive agricultural system.

5.3.3 Trait measurements

During plant growth, plant height and the leaf length of the central plant were measured non-destructively and weekly. We ended the experiment when most of the central wheat plants had transitioned from vegetative to reproductive growth (i.e. spikes had fully emerged on the main stem). At this time, we measured plant height, maximum leaf length, tiller number and spike number. At the same time, we measured PPFD at the top of the central plant using a spectrometer (LI-180, LI-COR

Biosciences, Lincoln, Nebraska, USA), since height and light are reported as the main drivers of competitive interactions between shoots (Gaudet & Keddy, 1988). After that, we killed and removed the aboveground parts of each central plant from the soil, dividing tissues into spikes, leaves and stems (including leaf sheaths). These samples were dried in a 45 ºC oven for one week and weighed to obtain dry mass.

5.3.4 FSP modelling

We used an FSP (functional structural plant) model to simulate the competition experiment *in silico*. Model parameters were fitted for *T. dicoccoides*, *T. dicoccum*, *T. araraticum*, *T. timopheevii*, *T. boeoticum* and *T. monococcum* using data from our previous experiment (Chapter 2). In the simulations, we replicated the experimental design, setting one plant of each species in the centre of a plot, with its corresponding wild/domesticated relatives as neighbours, simulating their densities and growth as in the experiment.

5.3.5 Statistical analysis

All the measured data were transformed into size-standardized values, by normalizing them relative to a reference value from the plants without neighbours. The transformed data were analysed by a multivariable linear regression model with interaction effects (domestication and neighbours) in R version 4.2.3 (https://www.r-project.org/). The overall variation among all the wheat groups was analysed by ANOVA, including three factors: domestication event (i.e. the species pair), domestication effect (i.e. wild vs domesticated), and neighbour density. After this, one more ANOVA analysis was applied to test the effects of domestication and neighbour density for each domestication event.

5.4 Results

5.4.1 Domesticated wheats win in aboveground competition

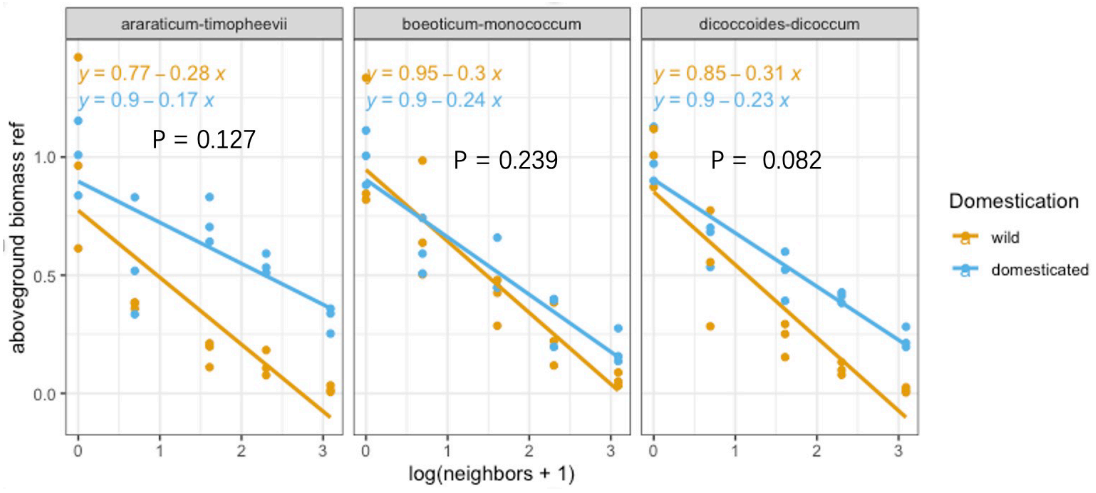


Figure 2: Size-standardized aboveground biomass in response to increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belongs to domesticated wheats. The panels (left to right) show comparisons between *T. araraticum* - *T. timopheevii, T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. The P value for each comparison is shown in plots. The overall P value across all three comparisons is 0.01106, which means there is a significant overall difference between wild and domesticated slopes.

Our results illustrate that domesticated wheats win in aboveground competition. In all three wild-domesticated comparisons of aboveground biomass, wild lines have steeper negative slopes than domesticated ones (Fig. 2), meaning that the growth of wild wheats is more impacted by competition from domesticated wheats. Conversely, domesticated wheats have stronger competitiveness when the densities of wild neighbours increase. We find that this impact of competition is seen largely in the vegetative biomass of shoots and leaves (Fig. S1). In comparison, wild wheats and domesticated wheats do not show significant differences in the loss of flower biomass during the transition to reproductive growth (Fig. S2). This implies that competitive effects happened during vegetative rather than reproductive growth.

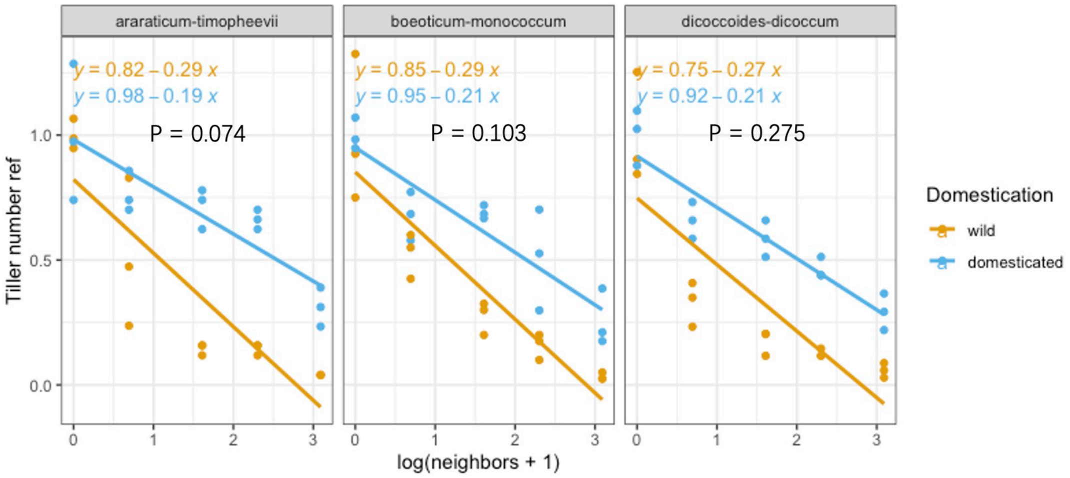


Figure 3: Size-standardized tiller number in response to increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belong to domesticated wheats. The panels show (left to right) comparisons between *T. araraticum* - *T. timopheevii*, *T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. The P value for each comparison is shown in plots. The overall P value across all three comparisons is 0.008743, which means there is significant differences between wild and domesticated slopes.

The higher competitiveness of domesticated wheats is also shown in tillering strength. The tiller numbers of domesticated wheats decreased slowly with increasing neighbour density, whereas those of wild wheats reduced more quickly (Fig. 3). In wild *T. araraticum* and *T. dicoccoides*, we even found that some of the central plants growing with 21 domesticated neighbours had only one tiller from the start until the end. None of these one-tiller plants had generated flowering spikes by the time we harvested them (Fig. S3). As the species with particularly strong tillering ability, *T.*

boeoticum and *T. monococcum* seem not to suffer fierce spike competition as the other two groups. The slopes of their spike numbers are almost similar (Fig S3). However, it is worth mentioning that *T. monococcum* with 1 or 0 neighbours generates a large number of tillers, and these tillers have not turned to spikes at the end of our experiment. It may be that this result is therefore an artefact of using a fixed harvest date for all plants.

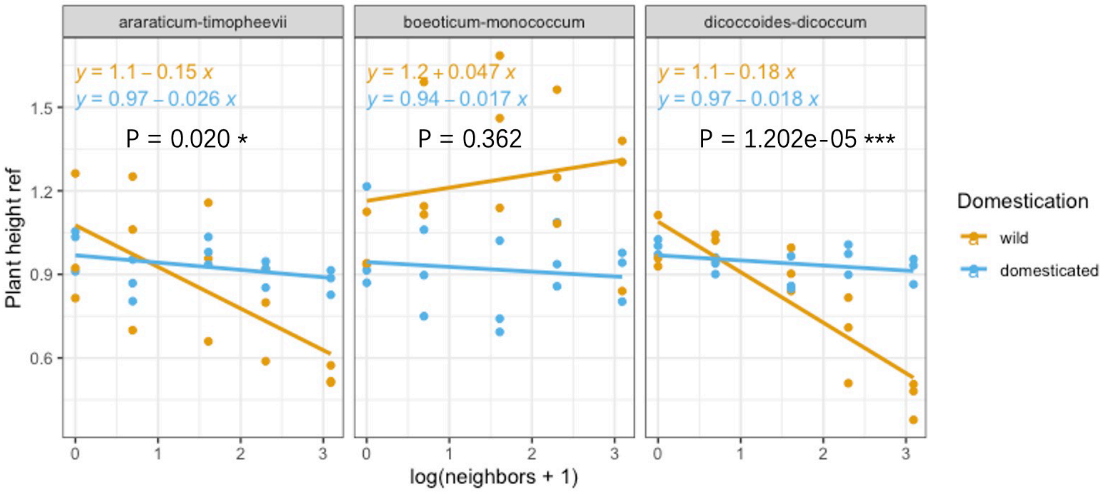


Figure 4: Size-standardized plant height in response to increased neighbour densities. Orange points and slopes represents wild wheats while blue points and slopes belongs to domesticated wheats. The panels show (left to right) comparisons between *T. araraticum* - *T. timopheevii, T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. The P value for each comparison is shown in plots. The overall P value across all three comparisons is 0.0167933, which means there is significant difference between wild and domesticated slopes.

The slopes of plant height show one way that domesticated emmer gains obvious advantages. In the *T. araraticum* – *T. timopheevii* and *T. dicoccoides* – *T. dicoccum* comparisons, we find the slopes for domesticated plants are close to zero, while the lines for the corresponding wild species drop quickly in response to competition from neighbours (Fig. 4). For the tallest species in our experiment, *T. timopheevii*, its height advantages are also shown in PPFD plots (Fig. S5 and S6). Although we do not find significant differences in wild and domesticated PPFD slopes, domesticated *T. timopheevii* shows strong light competition and shading effects that make it difficult for wild *T. araraticum* to capture light. The contrast between *T. boeoticum* – *T. monococcum* shows different patterns (Fig. 4). Here, the wild slope is greater than the domesticated slope, and even obtains a positive value (+ 0.047), meaning that final height increased in response to neighbour density. The difference may arise from shade avoidance (Wille *et al.*, 2017) or tillering, since domesticated *T. monococcum* generates so many branches that the main stem may not be able to elongate. The existence of neighbours limits the space available for tillers and forced wild *T. boeoticum* to allocate resources into the main stem to elongate upwards. However, in our PPFD measurements, this feature does not bring any significant differences in shading (Fig. S5 and S6).

5.4.2 Modelling supports experimental results

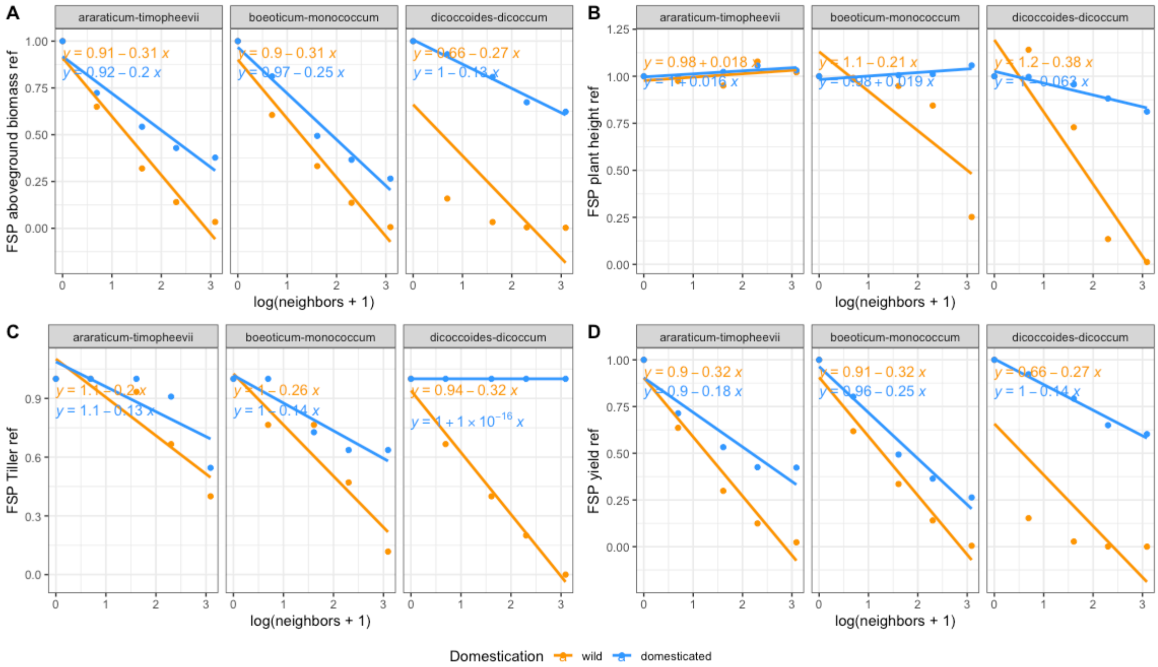


Figure 5: Size-standardized values of FSP model outputs in response to increased neighbour densities. Orange points and slopes represent wild wheats, while blue points and slopes belongs to domesticated wheats. (A). aboveground biomass, P value 0.033908; (B) plant height, P value 0.0003436; (C) tiller number, P value $5.699e^{-05}$; and (D) yield, P value 0.03246. All the four groups show significant differences in wild and domesticated slopes.

FSP modelling provides *in silico* support for our experimental findings. In Fig. 5A, the negative slopes of wild wheats are significantly steeper than those of domesticated wheats in aboveground biomass. In plant height, *T. ararticum* and *T. timopheevii* do not show significant differences in their slopes (Fig. 5B). However, domesticated *T. monococcum* and *T. dicoccum* both have obviously higher slopes than their wild relatives (Fig. 5B). In tiller number and yield performance, domesticated wheats maintained their superiority over wild species (Fig. 5C). Since seed size is fixed in FSP simulations, the yield also corresponds directly to individual plant fitness (i.e. fecundity = yield / seed mass). Although the FSP model only simulated competition between aboveground parts, its results closely match those in our real experiments, indicating that our results arose through shoot competition for space and light, and demonstrating a fitness advantage for domesticated plants under neighbour competition.

5.5 Discussion

Our empirical and *in silico* experiments support the hypothesis that domestication increased wheat competitiveness. In all three groups, domesticated *T. timopheevii*, *T. dicoccum* and *T. monococcum* show a fitness advantage under neighbour competition that increases with density and arises from shoot competition.

5.5.1 Competition Traits

A canonical conceptual model attributes the competitive ability of plants to three distinct components (Aarssen & Keogh, 2002): (1) growth, denoting the relative capacity of an individual to acquire resources ahead of competitors through resource pre-emption (Harper, 1977); (2) survival, referring to the relative capacity of an individual to endure resource deprivation induced by competitors (Aarssen, 1983); and (3) reproduction, signifying the relative ability of an individual to optimize fecundity per unit plant size over a given period despite constraints imposed by competition (Aarssen, 1989). In the context of this study, our primary focus revolves around the dimensions of growth. Although we might expect that survival should differ among our treatments, none of the wild plants competing with 21 domesticated neighbours died in our experiment. Instead, greater early vigour in growth, and enlarged sizes in plant height and aboveground biomass of domesticated wheats confer advantages in competition. However, the origin of these greater sizes is a subject of debate. One perspective is that domesticated wheats exhibit accelerated growth rates compared to their wild counterparts, resulting in earlier flowering time (Meyer & Purugganan, 2013). An alternative view is that domestication has a negligible impact on the relative growth rate, yet domesticated wheats begin growth from a heavier seed and therefore larger seedlings, resulting in a greater size at each developmental stage (Preece *et al.*, 2017) (Gómez-Fernández & Milla, 2022).

5.5.2 Cooperation versus Competition

Our experimental approach focuses on testing competition while also acknowledging the potential for cooperation among plants. The notion that plants can perceive their environment and respond, including to the presence of neighboring plants, was put forward 30 years ago (Aphalo & Ballare, 1995). Prior empirical evidence has indicated that individual plants may cooperate with kin while engaging in relatively intense competition with non-kin counterparts (Biernaskie, 2010). This is possible because of kin recognition (Hamilton, 1964) (Bais, 2018). One possibility is that kin recognition among plant roots may alleviate competitive pressures within the underground system, leaving aboveground competition largely unaffected (File *et al.*, 2011). This idea is supported by experimental findings that root allocation does not significantly differ among relatives in certain plant species (Murphy & Dudley, 2009) (Bhatt *et al.*, 2011). This hypothesis posits that cooperative effects among plants may reduce belowground competition while maintaining robust aboveground competition, a characteristic that appears to confer an advantage to domesticated wheats. Therefore, we also conjecture that instead of a competitive comparison between wild and domesticated wheat, the introduction of a third party object, such as weeds from other species, may be involved. Weeds were compared separately between wild and domesticated wheat in competition to assess their growth effects. This may avoid the kin recognition of the same species, resulting in different outcomes from our experiments. Alternatively, future investigations could investigate the effects of aboveground and underground competition, quantifying their respective impacts. Recent work that partitioned soil compartments in a pot-based setup provides a methodological basis for examining root competition in wheat experiments (Zhu *et al.*, 2023).

5.5.3 Implications for Agricultural Breeding

The concept of selecting for weak competitors in crop breeding to enhance yield has been elucidated by Weiner *et al.* (2010). Given that the primary concern of farmers is the productivity per unit area rather than individual plant performance, there has been a longstanding proposal for plant breeding to employ mechanisms that optimize population productivity in order to augment crop yields (Harper, 1977). The inclusion of wild wheats as valuable breeding resources serves to not only restore lost genetic diversity but also reintegrate weakly competitive traits, such as reduced height. This perspective finds partial validation in the Green Revolution, during which the cultivation of dwarf plants increased collective yields. In addition to plant height, reducing carbohydrate allocation into tissues important for shoot competition, such as leaves or stems, might also improve cooperation (Golan *et al.*, 2022). It may be more effective to prioritize these cooperative traits in future breeding efforts, rather than focusing solely on yield maximization (Montazeaud *et al.*, 2020). Prioritizing cooperative traits can mitigate underlying tendencies to act selfishly, refusing to fall into the yield trap of maximizing individual benefits (Fischer, 2020). In addition, it is imperative for agricultural workers to prioritize field management and pay more attention to the most competitive resource factor. This will enable wheat plants to allocate fewer resources towards addressing environmental limitations and instead allocate more resources towards maximizing yield production. (Fasoula, 1990) (Reynolds *et al.*, 1994).

5.6 Conclusion

In conclusion, we tested the fitness of wild and domesticated wheats and found that domestication increased wheat competitiveness. Model simulations indicated that this arose through shoot rather than root competition, and translated into fitness benefits. The effect was observed across three independent domestication events, but we hypothesise that it arose through distinct mechanisms in each case: i.e. increased plant height in *T. timopheevii*, increased early vigor in *T. aestivum* and increased tiller strength in *T. monococcum*. Domesticated wheats therefore exhibit stronger anti-interference ability and stability when faced with more neighbouring competitors.

5.7 Reference

Aarssen LW. **1983**. Ecological combining ability and competitive combining ability in plants: toward a general evolutionary theory of coexistence in systems of competition. *The American Naturalist* **122**: 707–731.

Aarssen LW. **1989**. Competitive ability and species coexistence: a'plant's-eye'view. *Oikos*: 386–401.

Aarssen LonnieW, Keogh T. **2002**. Conundrums of competitive ability in plants: what to measure? *Oikos* **96**: 531–542.

Anten NPR, Vermeulen PJ. **2016**. Tragedies and Crops: Understanding Natural Selection To Improve Cropping Systems. *Trends in Ecology & Evolution* **31**: 429–439.

Aphalo PJ, Ballare CL. **1995**. On the Importance of Information-Acquiring Systems in Plant-Plant Interactions. *Functional Ecology* **9**: 5–14.

Bais HP. **2018**. We are family: kin recognition in crop plants. *The New Phytologist* **220**: 357–359.

Bhatt MV, Khandelwal A, Dudley SA. **2011**. Kin recognition, not competitive interactions, predicts root allocation in young Cakile edentula seedling pairs. *New Phytologist* **189**: 1135–1142.

Biernaskie JM. **2010**. Evidence for competition and cooperation among climbing plants. *Proceedings of the Royal Society B: Biological Sciences* **278**: 1989–1996.

Blackshaw RE, Brandt RN. **2009**. Phosphorus fertilizer effects on the competition between wheat and several weed species. *Weed Biology and Management* **9**: 46–53.

Budak H, Kantar M, Yucebilgili Kurtoglu K. **2013**. Drought Tolerance in Modern and Wild Wheat. *The Scientific World Journal* **2013**: e548246.

Denison RF. **2012**. *Darwinian Agriculture: How Understanding Evolution Can Improve Agriculture*. Princeton University Press.

Doebley JF, Gaut BS, Smith BD. **2006**. The Molecular Genetics of Crop Domestication. *Cell* **127**: 1309–1321.

Donald CM. **1968**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Donald CM. **1981**. 14 COMPETITIVE PLANTS, COMMUNAL PLANTS, AND YIELD IN WHEAT CROPS. *Wheat science-today and tomorrow*: 223.

Drews S, Neuhoff D, Köpke U. **2009**. Weed suppression ability of three winter wheat varieties at different row spacing under organic farming conditions. *Weed Research* **49**: 526–533.

Fasoula DA. **1990**. Correlations between auto-, allo-and nil-competition and their implications in plant breeding. *Euphytica* **50**: 57–62.

File AL, Murphy GP, Dudley SA. **2011**. Fitness consequences of plants growing with siblings: reconciling kin selection, niche partitioning and competitive ability. *Proceedings of the Royal Society B: Biological Sciences* **279**: 209–218.

Fischer RA. **2020**. Breeding wheat for increased potential yield: Contrasting ideas from Donald and Fasoulas, and the case for early generation selection under nil competition. *Field Crops Research* **252**: 107782.

Gaudet CL, Keddy PA. **1988**. A comparative approach to predicting competitive ability from plant traits. *Nature* **334**: 242–243.

Golan G, Abbai R, Schnurbusch T. **2022**. Exploring the trade-off between individual fitness and community performance of wheat crops using simulated canopy shade. *Plant, Cell & Environment*.

Golan G, Oksenberg A, Peleg Z. **2015**. Genetic evidence for differential selection of grain and embryo weight during wheat evolution under domestication. *Journal of Experimental Botany* **66**: 5703–5711.

Goldberg DE, Landa K. **1991**. Competitive Effect and Response: Hierarchies and Correlated Traits in the Early Stages of Competition. *Journal of Ecology* **79**: 1013–1030.

Gómez-Fernández A, Milla R. **2022**. How seeds and growth dynamics influence plant size and yield: Integrating trait relationships into ontogeny. *Journal of Ecology* **110**: 2684–2700.

Haefele SM, Johnson DE, M'Bodj D, Wopereis MCS, Miezan KM. **2004**. Field screening of diverse rice genotypes for weed competitiveness in irrigated lowland ecosystems. *Field Crops Research* **88**: 39–56.

Hamilton WD. **1964**. The genetical evolution of social behaviour. II. *Journal of theoretical biology* **7**: 17–52.

Harper JL. **1977**. Population biology of plants. *Population biology of plants.*

Introduction to Wheat Growth. **2016**. *Wheat Training.*

Kluyver TA, Jones G, Pujol B, Bennett C, Mockford EJ, Charles M, Rees M, Osborne CP. **2017**. Unconscious selection drove seed enlargement in vegetable crops. *Evolution Letters* **1**: 64–72.

Lafond GP, Baker RJ. **1986**. Effects of Genotype and Seed Size on Speed of Emergence and Seedling Vigor in Nine Spring Wheat Cultivars1. *Crop Science* **26**: cropsci1986.0011183X002600020027x.

Lemerle D, Gill GS, Murphy CE, Walker SR, Cousens RD, Mokhtari S, Peltzer SJ, Coleman R, Luckett DJ. **2001**. Genetic improvement and agronomy for enhanced wheat competitiveness with weeds. *Australian Journal of Agricultural Research* **52**: 527–548.

Levy AA, Feldman M. **2022**. Evolution and origin of bread wheat. *The Plant Cell* **34**: 2549–2567.

Martín-Robles N, Morente-López J, Freschet GT, Poorter H, Roumet C, Milla R. **2019**. Root traits of herbaceous crops: Pre-adaptation to cultivation or evolution under domestication? *Functional Ecology* **33**: 273–285.

van der Meulen A, Chauhan BS. **2017**. A review of weed management in wheat using crop competition. *Crop Protection* **95**: 38–44.

Meyer RS, Purugganan MD. **2013**. Evolution of crop species: genetics of domestication and diversification. *Nature reviews genetics* **14**: 840–852.

Milla R, Morente-López J, Alonso-Rodrigo JM, Martín-Robles N, Stuart Chapin F. **2014**. Shifts and disruptions in resource-use trait syndromes during the evolution of herbaceous crops. *Proceedings of the Royal Society B: Biological Sciences* **281**: 20141429.

Montazeaud G, Rousset F, Fort F, Violle C, Fréville H, Gandon S. **2020**. Farming plant cooperation in crops. *Proceedings of the Royal Society B: Biological Sciences* **287**: 20191290.

Murphy GP, Dudley SA. **2009**. Kin recognition: Competition and cooperation in Impatiens (Balsaminaceae). *American Journal of Botany* **96**: 1990–1996.

Nakhforoosh A, Grausgruber H, Kaul H-P, Bodner G. **2014**. Wheat root diversity and root functional characterization. *Plant and Soil* **380**: 211–229.

Peng J, Ronin Y, Fahima T, Röder MS, Li Y, Nevo E, Korol A. **2003**. Domestication quantitative trait loci in Triticum dicoccoides, the progenitor of wheat. *Proceedings of the National Academy of Sciences* **100**: 2489–2494.

Preece C, Jones G, Rees M, Osborne CP. **2021**. Fertile Crescent crop progenitors gained a competitive advantage from large seedlings. *Ecology and Evolution* **11**: 3300–3312.

Preece C, Livarda A, Christin P-A, Wallace M, Martin G, Charles M, Jones G, Rees M, Osborne CP. **2017a**. How did the domestication of Fertile Crescent grain crops increase their yields? *Functional Ecology* **31**: 387–397.

Preece C, Livarda A, Christin P-A, Wallace M, Martin G, Charles M, Jones G, Rees M, Osborne CP. **2017b**. How did the domestication of Fertile Crescent grain crops increase their yields? *Functional Ecology* **31**: 387–397.

Reynolds MP, Acevedo E, Sayre KD, Fischer RA. **1994**. Yield potential in modern wheat varieties: its association with a less competitive ideotype. *Field Crops Research* **37**: 149–160.

Roucou A, Violle C, Fort F, Roumet P, Ecarnot M, Vile D. **2018**. Shifts in plant functional strategies over the course of wheat domestication. *Journal of Applied Ecology* **55**: 25–37.

Sedgley RH. **1991**. An appraisal of the Donald ideotype after 21 years. *Field Crops Research* **26**: 93–112.

Weiner J. **1990**. Asymmetric competition in plant populations. *Trends in ecology & evolution* **5**: 360–364.

Weiner J. **2019**. Looking in the Wrong Direction for Higher-Yielding Crop Genotypes. *Trends in Plant Science* **24**: 927–933.

Weiner J, Andersen SB, Wille WK-M, Griepentrog HW, Olsen JM. **2010**. Evolutionary Agroecology: the potential for cooperative, high density, weed-suppressing cereals. *Evolutionary Applications* **3**: 473–479.

Weiner J, Du Y-L, Zhang C, Qin X-L, Li F-M. **2017**. Evolutionary agroecology: individual fitness and population yield in wheat (Triticum aestivum). *Ecology* **98**: 2261–2266.

Westoby M, Leishman M, Lord J. **1996**. Comparative ecology of seed size and dispersal. *Philosophical Transactions of the Royal Society of London. Series B: Biological Sciences* **351**: 1309–1318.

Wille W, Pipper CB, Rosenqvist E, Andersen SB, Weiner J. **2017**. Reducing shade avoidance responses in a cereal crop. *AoB Plants* **9**: plx039.

Zhang D-Y, Sun G-J, Jiang X-H. **1999**. Donald’s ideotype and growth redundancy: a game theoretical analysis. *Field Crops Research* **61**: 179–187.

Zhu Y-H, Weiner J, Jin Y, Yu M-X, Li F-M. **2022**. Biomass Allocation Responses to Root Interactions in Wheat Cultivars Support Predictions of Crop Evolutionary Ecology Theory. *Frontiers in Plant Science* **13**.

Zhu L, Xiang J, Zhang D-Y, Wang W, Zhu S-G, Wang B-Z, Yang L-Y, Li M-Y, Xiong Y-C. **2023**. Does a tragedy of the commons due to individual competition arise from genetically fixed traits or plastic traits in dryland wheat? An experimental verification. *Journal of Plant Ecology* **16**: rtad004.

5.8 Supplemental Information

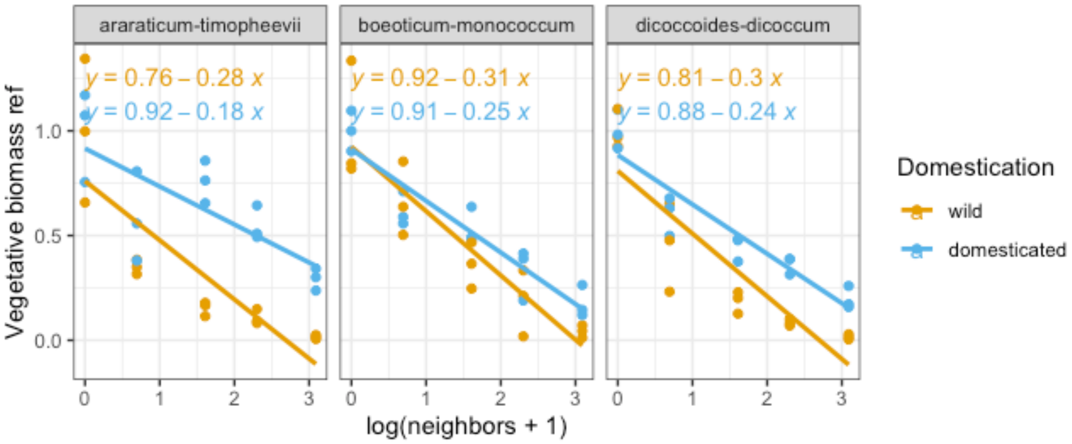


Figure S 1: Size-standardized vegetative biomass in response to increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belongs to domesticated wheats. The panels show (left to right) comparisons between *T. araraticum* - *T. timopheevii*, *T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. P values are shown for the relationships in each panel. The overall P value is 0.02204 < 0.05, which means there is significant overall difference between wild and domesticated slopes

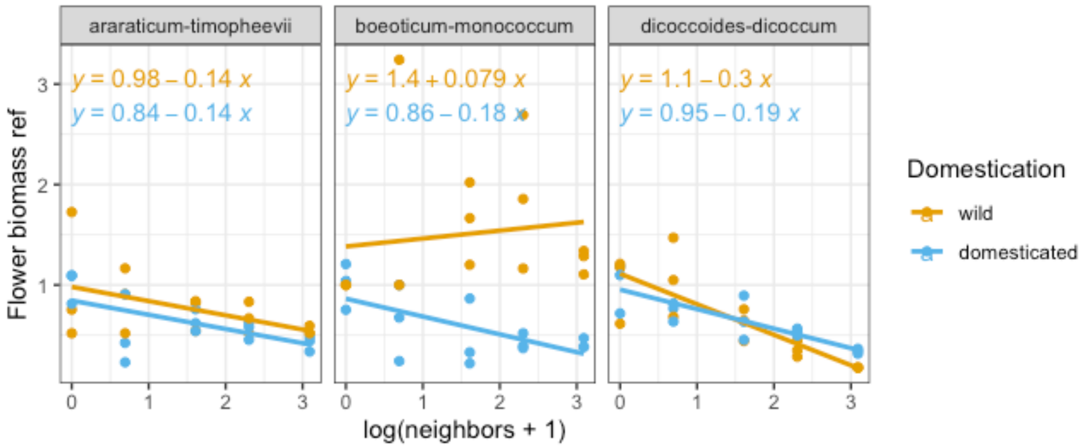


Figure S 2: Size-standardized flower biomass in response to increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belongs to domesticated wheats. The panels show (left to right) comparisons between *T. araraticum* - *T. timopheevii*, *T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. P values are shown for the relationships in each panel. The overall P value is 0.47681 > 0.05, which means there is no significant overall difference between wild and domesticated slopes

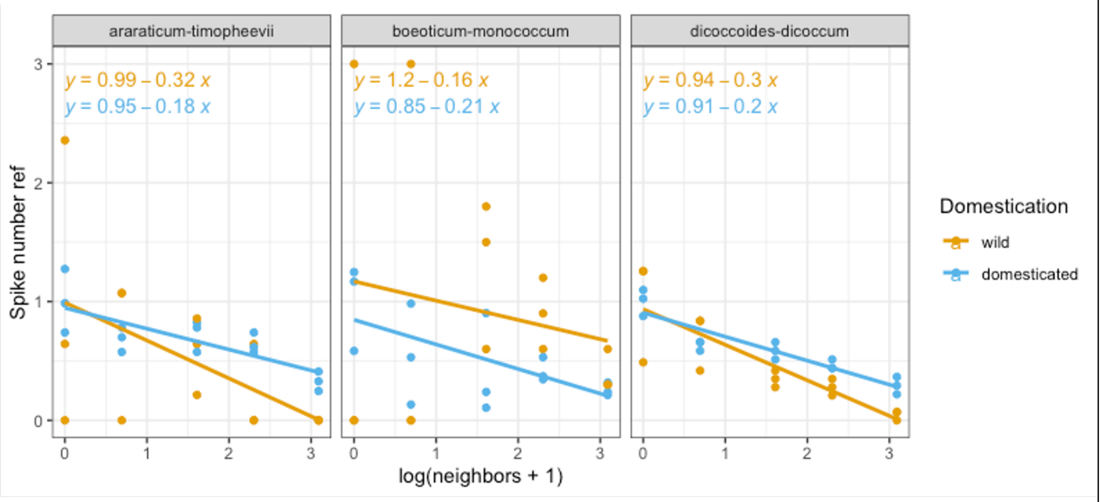


Figure S 3: Size-standardized spike number in increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belongs to domesticated wheats. The panels show *T. araraticum* - *T. timopheevii*, *T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. Because some spike numbers are zero, We add one to all spike numbers when calculating, so that the model can fit. P value of each panel were shown in their plots. The overall P value of all three patterns is 0.50456 > 0.05, which means there is no significant differences between wild and domesticated slopes.

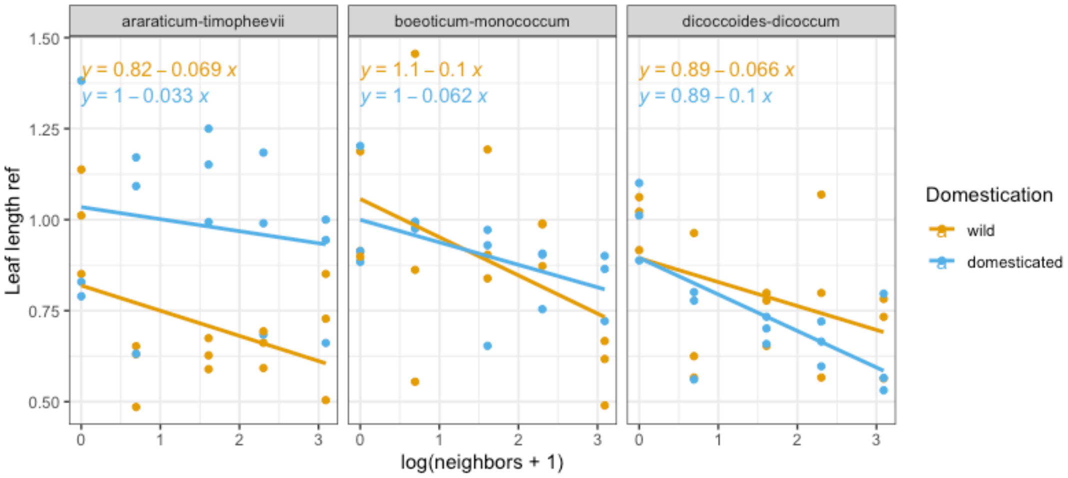


Figure S 4: Size-standardized leaf length in response to increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belongs to domesticated wheats. The panels show (left to right) comparisons between *T. araraticum* - *T. timopheevii*, *T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. P values are shown for the relationships in each panel. The overall P value is 0.666098, which means there is no significant overall difference between wild and domesticated slopes.

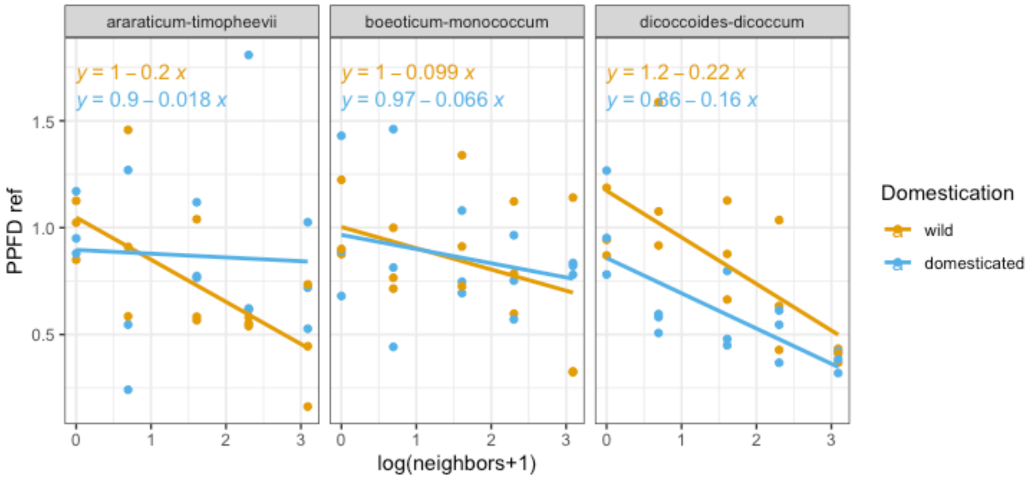


Figure S 5: Size-standardized PPFD in increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belongs to domesticated wheats. The panels show *T. araraticum* - *T. timopheevii*, *T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. Because some spike number are zero, We add one to all spike numbers when calculating, so that the model can fit. P value of each panel were shown in their plots. The overall P value of all three patterns is 0.43503 > 0.05, which means there is no significant differences between wild and domesticated slopes.

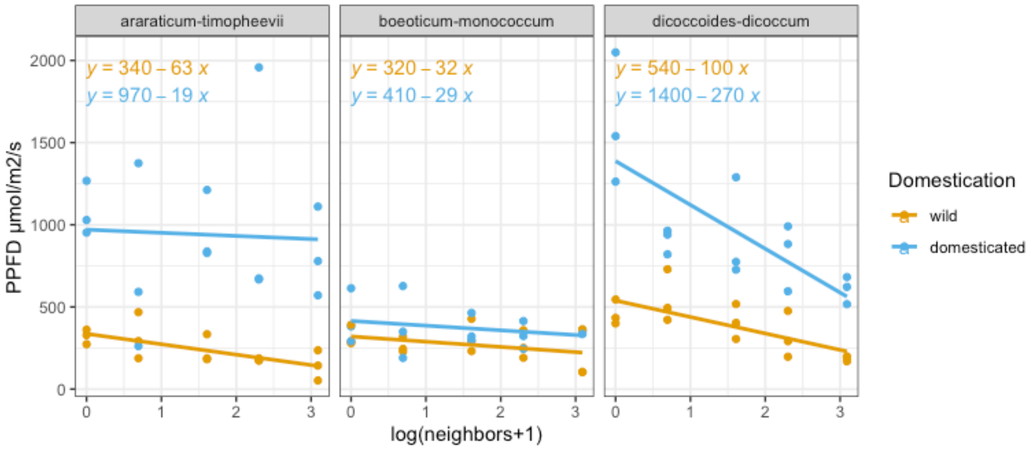


Figure S 6: PPFD in increased neighbour densities. Orange points and slopes represent wild wheats while blue points and slopes belongs to domesticated wheats. The panels show *T. araraticum* - *T. timopheevii*, *T. boeoticum* – *T. monococcum* and *T. dicoccoides* – *T. dicoccum* respectively. Because some spike number are zero, We add one to all spike numbers when calculating, so that the model can fit. P value of each panel were shown in their plots. The overall P value of all three patterns is 0.3589308 > 0.05, which means there is no significant differences between wild and domesticated slopes.

Chapter 6: General Discussion

6.1 Central findings of the thesis

My PhD thesis focused on the morphological changes in wheat domestication and how these changes can be used to increase yield. I conducted four experiments using various methods, including plant growth analysis, PCA, FSP models, GWAS and linear regression. This work has helped us to better understand wheat domestication and to provide phenotypic decision support for ongoing wheat breeding. In this chapter, I will review the results of the previous four chapters and highlight the novel contributions they have made. I will also compare my work with findings in the literature to further analyse the breadth and relevance of the work. As part of this discussion, I will also compare the research methods I used with alternative approaches used by others, to see if they might be effective for future work. In addition, I will summarise the relationships between my four chapters and draw out general conclusions. Finally, I will look forward to future breeding work and suggest some tasks that I am interested in, but was not able to complete in this thesis, hoping to address them in future research.

6.1.1 Why is this work important?

Crop production presents a persistent global challenge. With the world population expected to grow to 9 billion by 2050, alongside a global dietary transition, it is imperative to increase crop production by 70% to meet this demand (Hawkes, 2006) (Tilman & Clark, 2014) (Godfray *et al.*, 2010). Wheat, a key food crop, provides around one-fifth of the total calories and protein consumed annually by the planet's

7.9 billion inhabitants (Food and Agriculture Organization of the United Nations). The urgent need to increase food production requires attention to wheat yields. The question of how to increase wheat yields by 2050 has long been of concern to many scientists. (Ray *et al.*, 2012). My thesis seeks to address this query by analysing and defining a high yielding wheat phenotype, and understanding how wheat phenotypes have evolved through the crop's history. Utilising phenotype as the impetus for a breeding target is a significant agronomic approach (Ghanem *et al.*, 2015). It can be traced back to ancient times (10,000 years ago) when humans selected the best-performing plant individuals for domestication (Bell, 1987). Donald codified the theory of phenotypic selection, and proposed breeding for ideotypes (Donald, 1968b). I adopt his conceptualisation here.

My study provides a comprehensive overview of wheat evolution and documents the diversification of wheat morphological traits in Chapter 2. This information is of interest to archaeologists and botanists seeking to better understand the historical development of phenotypic traits. My analysis of morphospace identifies critical domestication bottlenecks (Haudry *et al.*, 2007a). For breeders, my work offers valuable insights into traits found in wild wheats that can be used to enhance germplasm resources (Harlan, 1976) (Brush, 1995). I also identified the genetic loci associated with awn appearance in bread wheats in Chapter 4. Awn appearance is a distinctive characteristic of yield that has diminished with time (Duwayri, 1984). The reason for the disappearance of awns could be relaxed selection (no need for seed dispersal mechanisms) or artificial selection (easier to harvest and store) (Sanchez-Bragado *et al.*, 2023a). This finding supports the identification of a wheat awn-associated locus, while hinting at loci associated with other spikes or harvest traits, and informs future GWAS work on larger samples. The information on genomic markers facilitates breeding work in selecting and enhancing desirable traits (Gupta *et al.*, 1999). The work conducted in Chapter 3 involves creating a virtual ideotype and predicting its growth. This can be viewed as an application of Donald's theory in the field of computer science. It aids in understanding of crucial wheat yield traits and how they interact when integrated into a wheat crop. Although the virtual wheat created by the model is not real, it simulates the morphological structure and physiological processes of wheat. When working on breeding, scientists can refer to the virtual wheat in my Chapter 3 and think about the possible effects of combining individual traits to develop an efficient experimental programme. Considering the yield of individual plants and groups, Chapter 5 presents a comparison of the fitness of wild and domesticated wheats under competition. Its findings point to the need for a more comprehensive recognition that domestication can produce traits that are detrimental to population production and that need to be reversed through modern breeding. Overall, this research is significant for multiple fields, including crop domestication, wheat breeding, phenotypic modelling, and agricultural production.

6.1.2 What is the significance of this work?

My work improves previous understanding of plant science. Previous studies had suggested that domestication had led to a loss of wheat genetic diversity due to long-term artificial selection, causing bottlenecks (Reif *et al.*, 2005). However, my findings indicate from a phenotypic perspective that, while there may be a reduction in phenotypic diversity, the morphospace of wild wheat does not entirely cover that of domesticated wheat. At the same time, the domesticated wheat trait range does not fully encompass the wild morphospace. The morphologies of modern wheat align with domesticated wheat, as expected. This indicates that wheat exhibits a range of trait values, some of which may have been lost during evolution, but domestication has also generated novel traits that exceed the range of values exhibited by its ancient ancestors. This could be a result of both genotypic and phenotypic plasticity during the process of domestication, as well as genetic recombination (Dubcovsky & Dvorak, 2007) (Tang *et al.*, 2010) (Katamadze *et al.*, 2023).

My work breaks down different periods of domestication, analysing their similarities and differences. By making multiple independent comparisons, and sampling a diversity of wheat accessions, my work shows that the pattern of variation in quantitative traits during wheat history differs by trait. Some trait values show progressive changes in the same direction (e.g. leaf size, grain weight), others change in a punctuated way at particular stages (e.g. leaf angle), while other trait values switch directions during wheat evolution (e.g. plant height, flower biomass proportion). These findings remind us that some of the morphological changes during domestication have come from natural selection, and may be deleterious, needing to be reversed in our breeding efforts. Based on the evidence outlined above, I present a clear and comprehensive map of wheat morphological evolution, which advances my understanding of crop evolution. I draw inferences about the roles of natural selection and artificial breeding, and the ways in which selection for competition may have promoted traits that are undesirable in modern crops.

Previous work on ideotypes usually requires a high cost to verify each trait experimentally (Thurling, 1991), and shows that it is difficult to handle the complex relations between multiple traits (Rasmusson, 1991). Using model-assisted phenotype design has been proposed, but has been limited by the lack of quantitative relationships between agronomic and model parameters (Martre *et al.*, 2015). My work is an innovative attempt to connect plant physiology and computer science. Wheat morphological data were input into FSP model, which helps us to identify virtual ideotypes. I first verified that using the diversities of wild and landrace traits to improve modern wheats is successful, at least in models. This supports the idea of using crop wild relatives in breeding programmes (Migicovsky & Ourles, 2017)

(Bohra *et al.*, 2022) (Kashyap *et al.*, 2022). My ideotype modelling proposed two new architectures (based on average and modern wheat backgrounds) that do not exist within the current diversity. This result may attract more botanists to verify my physiological traits, and give agronomists more to think about the direction of improving wheat traits in the future.

Wheat competitiveness is another important feature that changed during domestication. Traditional breeding strategies for high-yielding wheat emphasize low competitiveness (Zhang *et al.*, 1999). As cultivation provides a resource-sufficient environment, wheat is thought to contribute more carbohydrates into yield traits instead of competitive traits (Milla *et al.*, 2015). Therefore, domesticated wheats should lose their competitiveness. My work refutes this idea. Through comparative experiments, different lineages of domesticated wheat exhibited stronger competitive abilities when competing with their wild relatives for space, light and limited pot resources. This result advances understanding of domestication, implying that early events in domestication were the reason for the high competitiveness of domesticated wheat. Agronomists need to consider the unintended consequences of domestication more fully. In terms of yield, we need cooperative wheat, but historical processes have instead bred a highly competitive selfish wheat, which had to be reversed by later breeding work.

6.2 Integration between the data chapters

In this section, I will primarily focus on the interconnection between the chapters (Fig. 1), the scientific implications of their collective findings, and the similarities and disparities between these conclusions and prior research studies.

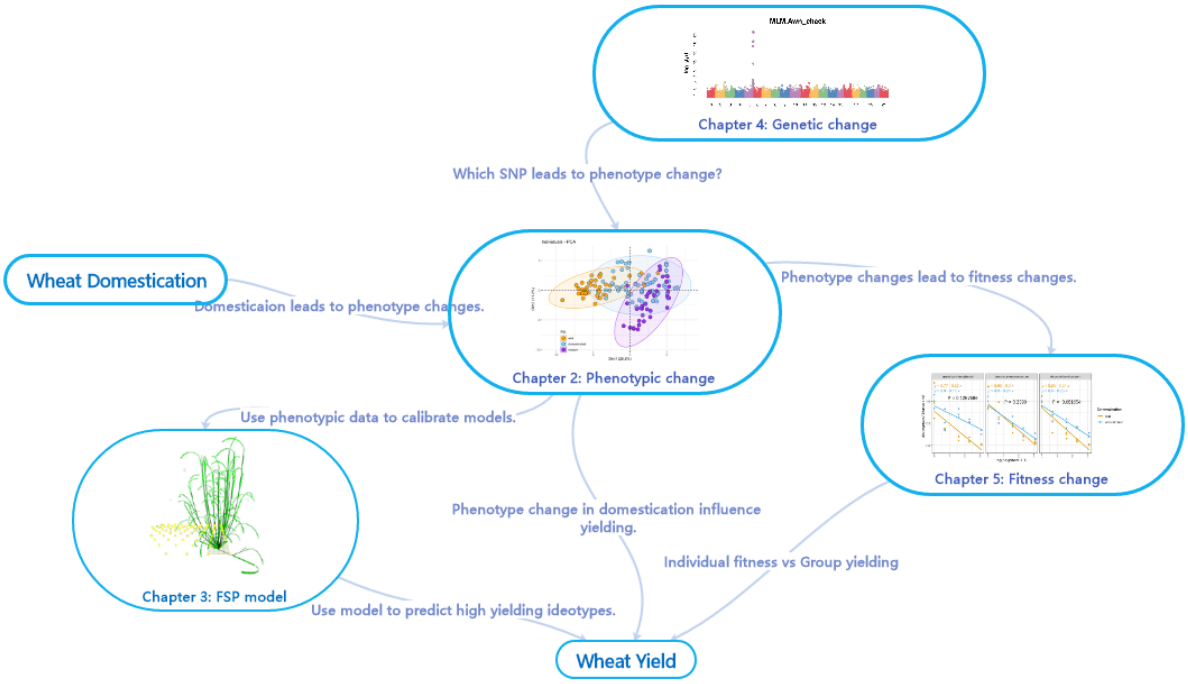


Figure 1: the relationship among wheat domestication, wheat yielding and my data chapters.

6.2.1 Phenotypic and genetic changes caused by selection during domestication (Chapter 2 + Chapter 4)

My thesis contributes to identifying the genetic markers of awns, as important traits lost in domestication (Chapter 2, Chapter 4). These losses are thought to have arisen from natural selection (the environment does not require awns to ward off birds; reduce awns to increase grain investment; relaxed selection for dispersal) and/or artificial selection (more convenient to store and move) (Sanchez-Bragado *et al.*, 2023b). There has been a lot of work on the genetic basis of domestication traits. One good example is the reduction in glumes controlled by tenacious glume genes Tg^{2A} and Tg^{2B} (Simons *et al.*, 2006). Wild wheats are therefore hulled, while modern wheats are free-threshing with reduced glumes (Dvorak *et al.*, 2012). Further study shows that the mutation of the *q* allele (wild wheats) to *Q* (domesticated wheats) causes the phenotypic traits of subcompact spikes, free-threshing grains (Debernardi *et al.*, 2017), tough rachis (Avni *et al.*, 2017) and loss of dormancy (Nave *et al.*, 2016). People's behaviour selects for crop traits under cultivation. Sometimes this selection is deliberate, for example in the case of selective breeding towards ideotypes. Alternatively, this process may be unconscious (Kilian *et al.*, 2010) (Preece *et al.*, 2017). For example, when people are harvesting wild plants with sickles, the ones with tough rachis will tend to be over-represented in the next generation, so this process selects automatically (unconsciously) for that trait (Hillman & Davies, 1990). With these "useless" trait values lost, their expressed genes are also lost from germplasm (Rahman *et al.*, 2020). Therefore, it is normally thought that the diversity of wheats has been harmfully decreased by selective breeding, as evidenced by nucleotide diversity loss in wheats (Haudry *et al.*, 2007b). However, my work in Chapter 2 affirms this selection pressure and describes different directions of selection during four historical periods.

Since people use their preferences to select plants with useful trait values, some wild wheats with the trait values that people do not need will be given up in domestication. Apart from the awn gene on chromosome 4 (Chapter 4), another example is a locus on the long arm of wheat chromosome 4B that controls within-spikelet variation in both grain size and seed dormancy (Nave *et al.*, 2016). On wild emmer spikelets, each spike produces two grains. One is larger and is not dormant. The other is smaller and dormant. Domestication has resulted in the loss of the latter's dormancy, leaving both grains on the spikelet large and undormant (Ohta, 2022). Although seed dormancy can increase the probability that at least some offspring will survive in unstable environmental conditions, domestication improved crop productivity by selecting for rapid and uniform germination (Harlan *et al.*, 1973). This trait value might be changed by farmers because smaller dormant grains were a biased later choice in the harvest and could even be unconsciously lost. Thus, the average size of wheat grain also increased in domestication. With the loss of seed dormancy, resistance to preharvest sprouting (PHS), controlled by *TaPHS1* genes (Lin *et al.*, 2018), also decreased in domesticated wheats. Hence, PHS in wheat, the germination of kernels in a spike prior to harvest when prolonged rainfall occurs, brings about significant losses in both yield and quality (Liu *et al.*, 2015). Moreover, *TaAGP-L-1B* genes for enzymes in starch synthesis in the developing endosperm have also been lost in the process of tetraploid wheats becoming hexaploid (Hou *et al.*, 2017). This loss leads to a reduction of grain weight during human breeding. Despite people's desire to filter phenotypes that they want, there are therefore multiple examples showing that wild trait values with their expressed genes are still useful. A recent work shows that there has been ongoing gene flow from wild plants into domesticated crops (Iob & Botigué, 2023). My work on Chapter 2 support this opinion and I propose that wild trait values occupy a different morphospace to domesticated wheat. Hence, it is expected that trait values exist in wild wheats that have disappeared in modern wheats.

6.2.2 Breeding improved by genetic and phenotypic data (Chapter 2 + Chapter 3 + Chapter 4)

Plant breeding focuses on developing superior genotypes using available genetic and non-genetic resources and improving plant breeding methods to maximize genetic gain and cost-effectiveness (Tao *et al.*, 2017). Although my Chapter 2 and Chapter 4 emphasize using the phenotype to drive breeding, the application of genetic data is also important. Nowadays, crop breeding has a high requirement for phenotypic and genotypic data processing (Marsh *et al.*, 2021). My Chapter 2 provides a prediction of the effects of combining multiple phenotypic traits. Through this modelling, I defined the key traits that I wanted to change. Then I applied GWAS in Chapter 2 to find the alleles for wild traits. The next step beyond this work is to insert the newly discovered gene sequences to achieve breeding of new wheat varieties. The traditional method is introgression breeding. It requires a cross between the modern genotype and a wild relative. Subsequently, unwanted alleles in the wild genotype while retaining the desired wild allele are removed from the offspring by repeated backcrosses with the modern genotype (Warschefsky *et al.*, 2014). With gene engineering improvements, breeders are increasingly using precision mutagenesis by designing sequence-specific nucleases to modify target DNA sequences (Lozano-Juste & Cutler, 2014). One of the most representative breeding techniques is CRISPR-Cas9 (Chen *et al.*, 2019).

Another breeding advancement is to enhance modelling efforts in order to improve gene-to-phenotype predictions. Phenotypes, as traditionally understood, are determined by a combination of genes and environment (P = G * E) (Kang, 1997). My crop growth prediction modelling is based on crop physiological processes, primarily in photosynthesis, carbon allocation and morphogenesis (development of branches and organs). However, for gene-to-phenotype prediction, I rely mainly on linear statistical models. Connecting these two methods, to simulate the genotypes and phenotypes via modelling, is becoming increasingly vital (Martre *et al.*, 2017). Up to now, most of the work has relied on the quantitative trait loci (QTL), the mechanism of which is similar to GWAS that I used in Chapter 4 (Kearsey & Farquhar, 1998). For example, Technow applied Bayesian algorithms to incorporate biological concepts in the form of crop growth models into genome-wide predictions (Technow *et al.*, 2015). Uptmoor applied a combination of genome-wide prediction and phenological modelling to predict maize tassel dates for a large number of independent plant individuals, in crosses used for model parameterisation (Uptmoor *et al.*, 2017). Based on these examples, I believe that my Chapter 3 modelling work, and the Chapter 4 GWAS work, have methodological possibilities to collaborate and may yield better predictions for genotype-phenotype of wheat growth.

6.2.3 External environment changes ideotype targets (Chapter 2 + Chapter 3 + Chapter 5)

Ideotype targets are typically established based on the environment (Austin, 1988). This is partly similar to early domestication and natural selection. The early wheat can be viewed as the best phenotype that meets the requirements of the external environment at the time (Purugganan & Fuller, 2009). In this case, the notion of the external environment could be more extensive, encompassing factors such as weather, space, soil, density, and field management. Past domestication was examined in Chapter 2, and four strategies were proposed across different time periods for the selection of wheat crops. Donald's view was that the ideotype should be group friendly but competitively disadvantaged at the individual level (Donald, 1968a). However, my experiment highlighted in Chapter 5 demonstrates that domestication appears to have produced more competitive domesticated wheat varieties and higher population yields. The reason may be that wild wheats are not able to adapt themselves to improved environments. Domestication has transferred these wild varieties from hostile environments to arable environments that have relatively better resources, such as adequate moisture, soil, and defence from natural enemies (Abbo *et al.*, 2012). My guess is that there are small trait differences within wild wheat populations (possibly due to genetic mutations). When domestication occurs, wild wheat is moved by farmers from infertile wild soils to improved arable fields. It is easier to acquire nutrients from soil and therefore roots are not key factor. Some of these individuals (possibly because of certain traits such as stronger shoot systems and larger grain sizes) are better able to grow faster, take up more space and compete with their neighbours for sunlight. These plants produce more seeds, are more readily selected by farmers and the environment, and are favoured and retained over successive generations. The result is that these domesticated species are more competitive (more able to exploit resources). The relationship between group production and individual fitness is often inverse after both have reached a certain size (Weiner *et al.*, 2017). In the presence of abundant external resources, high-yielding varieties are likely to correspond with high individual competitiveness. Conversely, when external resources are scarce, high-yielding varieties correspond to population-friendly varieties as opposed to the most individually competitive varieties.

This point is also demonstrated in Chapter 3. According to my findings, the modelling of ideotypes exhibits distinct strategies with increasing density. Notably, as density reaches its maximum point, wheat models allocate an increasing amount of biomass towards the development of flowers. This comes at the expense of intense competition, causing many individual plants to die, and leaving only a select few to be harvested for their yield. In the simulation, stochastic resource constraints still resulted in some individuals dying so that to allow others to survive in order to achieve maximum population efficiency on the given area. This implies that in times of scarce resources (such as light and space), it is difficult for plants to co-exist in a friendly manner where resources are shared equally. That is, despite the fact that these plants are even more group friendly (egalitarian), there is still competition, even to the point of death, when resources are scarce. The ideotype proposed by Donald and other ecologists that is beneficial for populations simply prioritises allocating as much resource as possible to the production organs, without guaranteeing that resource competition won't occur in the end.

Therefore, ideotypes should additionally consider the limited factors in the environment. Liebig tells us that crop yields are determined by the lack of a single key resource (limiting factor) (Kho, 2000). I suggest that the ideotype should be group-friendly for this factor and as resource-accessible (competitive) as possible on other well-resourced factors.

6.3 Future directions.

Based on the studies presented in this thesis, the following recommendations can be made for further research that will enhance my understanding of crop domestication and the relationships between phenotype and yield.

- This thesis focuses on morphological variation during the domestication of wheat. However, when it comes to measuring physiological traits such as photosynthesis and metabolic rate, there is a lack of efficient equipment to support phenotypic measurements. Much previous research shows that physiological traits are closely related to changes in morphology (Gartner, 1995) (Freschet *et al.*, 2018) (Loss & Siddique, 1994) (Reynolds *et al.*, 1997) (Wang *et al.*, 2016). I therefore encourage further research to investigate the changes in physiological traits during wheat domestication and their correlation with morphological variation.
- There is still considerable scope for improvement in the use of crop models to support phenotyping. For example, I can add more descriptive traits to more accurately simulate plant physiological growth. Alternatively, I can use more accurate algorithms to optimise the combination of phenotypic traits. These tasks require an interdisciplinary background in computer science and agronomy to work together. I believe that optimising the model can improve my ability to predict phenotypic selection.
- Regarding the morphological changes in wheat domestication and the impact on individual competitiveness, I believe that there is a need to improve the monitoring of underground parts. Follow-up research could focus on investigating changes in underground root systems as a result of wheat domestication. This could be done by analysing morphological characteristics

such as mass, thickness, length and number, as well as chemical components such as nitrogen assimilation. In addition, it would be valuable to investigate differences in competition for underground resources.

6.4 Conclusions

My work focused on the phenotypic changes during wheat domestication and their corresponding genetic basis and competitiveness changes. I applied empirical wheat phenotypic data in virtual plant modelling and explored what the ideal wheat phenotype should look like. The key conclusions of this work are:

Chapter 2.1: Wild, domesticated and modern wheat morphospaces overlap and also have their own distinct areas.

Chapter 2.2: Traits arose during different stages of wheat history. There are three patterns of trait variation: gradual directional change, punctuated change at one period, and reversal in direction. Differences between wild and modern wheats are the product of multiple phases of historical change.

Chapter 3.1: Wheat ideotypes could be optimized by modifying potential biomass allocation, leaf insertion angle, stem diameter and seed weight.

Chapter 3.2: As density rises, optimization makes the ideotype more population-friendly but reduces individual competitiveness.

Chapter 4: The gene associated with awn loss during landrace improvement is at chromosome 4B.

Chapter 5: Domestication increases wheat competitiveness.

Overall, my thesis summarizes wheat morphological traits that have appeared or disappeared since domestication and discusses the contribution of these phenotypic traits to yield, combining genetic, modelling and ecological perspectives.

6.5 Reference

Abbo S, Lev-Yadun S, Gopher A. **2012**. Plant domestication and crop evolution in the Near East: on events and processes. *Critical Reviews in Plant Sciences* **31**: 241–257.

Austin RB. **1988**. A different ideotype for each environment. In: Cereal Breeding Related to Integrated Cereal Production. Proceedings of the EUCARPIA conference. Pudoc Wageningen, the Netherlands, 47–60.

Avni R, Nave M, Barad O, Baruch K, Twardziok SO, Gundlach H, Hale I, Mascher M, Spannagl M, Wiebe K, *et al.* 2017. Wild emmer genome architecture and diversity elucidate wheat evolution and domestication. *Science* **357**: 93–97.

Bell GDH. **1987**. The history of wheat cultivation. In: Lupton FGH, ed. Wheat Breeding. Wheat Breeding: Its scientific basis. Dordrecht: Springer Netherlands, 31–49.

Bohra A, Kilian B, Sivasankar S, Caccamo M, Mba C, McCouch SR, Varshney RK. **2022**. Reap the crop wild relatives for breeding future crops. *Trends in Biotechnology* **40**: 412–431.

Brush SB. **1995**. In Situ Conservation of Landraces in Centers of Crop Diversity. *Crop Science* **35**: cropsci1995.0011183X003500020009x.

Chen K, Wang Y, Zhang R, Zhang H, Gao C. **2019**. CRISPR/Cas genome editing and precision plant breeding in agriculture. *Annual review of plant biology* **70**: 667–697.

Debernardi JM, Lin H, Chuck G, Faris JD, Dubcovsky J. **2017**. microRNA172 plays a crucial role in wheat spike morphogenesis and grain threshability. *Development* **144**: 1966–1975.

Donald C t. **1968a**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Donald CM. **1968b**. The breeding of crop ideotypes. *Euphytica* **17**: 385–403.

Dubcovsky J, Dvorak J. **2007**. Genome plasticity a key factor in the success of polyploid wheat under domestication. *Science* **316**: 1862–1866.

Duwayri M. **1984**. Effect of flag leaf and awn removal on grain yield and yield components of wheat grown under dryland conditions. *Field Crops Research* **8**: 307–313.

Dvorak J, Deal KR, Luo M-C, You FM, von Borstel K, Dehghani H. **2012**. The Origin of Spelt and Free-Threshing Hexaploid Wheat. *Journal of Heredity* **103**: 426–441.

Food and Agriculture Organization of the United Nations. FAOSTAT statistical database.

Freschet GT, Violle C, Bourget MY, Scherer-Lorenzen M, Fort F. **2018**. Allocation, morphology, physiology, architecture: The multiple facets of plant above- and below-ground responses to resource stress. *New Phytologist* **219**: 1338–1352.

Gartner BL. **1995**. *Plant stems: physiology and functional morphology*. Elsevier.

Ghanem ME, Marrou H, Sinclair TR. **2015**. Physiological phenotyping of plants for crop improvement. *Trends in Plant Science* **20**: 139–144.

Godfray HCJ, Beddington JR, Crute IR, Haddad L, Lawrence D, Muir JF, Pretty J, Robinson S, Thomas SM, Toulmin C. **2010**. Food security: the challenge of feeding 9 billion people. *science* **327**: 812–818.

Gupta PK, Varshney RK, Sharma PC, Ramesh B. **1999**. Molecular markers and their applications in wheat breeding. *Plant Breeding* **118**: 369–390.

Harlan JR. **1976**. Genetic resources in wild relatives of crops 1. *Crop science* **16**: 329–333.

Harlan JR, de Wet JM, Price EG. **1973**. Comparative evolution of cereals. *Evolution* **27**: 311–325.

Haudry A, Cenci A, Ravel C, Bataillon T, Brunel D, Poncet C, Hochu I, Poirier S, Santoni S, Glémin S, *et al.* 2007a. Grinding up Wheat: A Massive Loss of Nucleotide Diversity Since Domestication. *Molecular Biology and Evolution* **24**: 1506–1517.

Haudry A, Cenci A, Ravel C, Bataillon T, Brunel D, Poncet C, Hochu I, Poirier S, Santoni S, Glémin S, *et al.* 2007b. Grinding up Wheat: A Massive Loss of Nucleotide Diversity Since Domestication. *Molecular Biology and Evolution* **24**: 1506–1517.

Hawkes C. **2006**. Uneven dietary development: linking the policies and processes of globalization with the nutrition transition, obesity and diet-related chronic diseases. *Globalization and Health* **2**: 4.

Hillman GC, Davies MS. **1990**. Measured Domestication Rates in Wild Wheats and Barley Under Primitive Cultivation, and Their Archaeological Implications. *Journal of World Prehistory* **4**: 157–222.

Hou J, Li T, Wang Y, Hao C, Liu H, Zhang X. **2017**. ADP-glucose pyrophosphorylase genes, associated with kernel weight, underwent selection during wheat domestication and breeding. *Plant Biotechnology Journal* **15**: 1533–1543.

Iob A, Botigué L. **2023**. Genomic analysis of emmer wheat shows a complex history with two distinct domestic groups and evidence of differential hybridization with wild emmer from the western Fertile Crescent. *Vegetation History and Archaeobotany* **32**: 545–558.

Kang MS. **1997**. Using genotype-by-environment interaction for crop cultivar development. *Advances in agronomy* **62**: 199–252.

Kashyap A, Garg P, Tanwar K, Sharma J, Gupta NC, Ha PTT, Bhattacharya RC, Mason AS, Rao M. **2022**. Strategies for utilization of crop wild relatives in plant breeding programs. *Theoretical and Applied Genetics* **135**: 4151–4167.

Katamadze A, Vergara-Díaz O, Uberegui E, Yoldi-Achalandabaso A, Araus JL, Vicente R. **2023**. Evolution of wheat architecture, physiology, and metabolism during domestication and further cultivation: Lessons for crop improvement. *The Crop Journal*.

Kearsey MJ, Farquhar AGL. **1998**. QTL analysis in plants; where are we now? *Heredity* **80**: 137–142.

Kho RM. **2000**. On crop production and the balance of available resources. *Agriculture, ecosystems & environment* **80**: 71–85.

Kilian B, Martin W, Salamini F. **2010**. Genetic Diversity, Evolution and Domestication of Wheat and Barley in the Fertile Crescent. In: Glaubrecht M, ed.

Evolution in Action: Case studies in Adaptive Radiation, Speciation and the Origin of Biodiversity. Berlin, Heidelberg: Springer, 137–166.

Lin M, Liu S, Zhang G, Bai G. **2018**. Effects of TaPHS1 and TaMKK3-A genes on wheat pre-harvest sprouting resistance. *Agronomy* **8**: 210.

Liu S, Sehgal SK, Lin M, Li J, Trick HN, Gill BS, Bai G. **2015**. Independent mis-splicing mutations in TaPHS1 causing loss of preharvest sprouting (PHS) resistance during wheat domestication. *New Phytologist* **208**: 928–935.

Loss SP, Siddique KHM. **1994**. Morphological and physiological traits associated with wheat yield increases in Mediterranean environments. *Advances in agronomy* **52**: 229–276.

Lozano-Juste J, Cutler SR. **2014**. Plant genome engineering in full bloom. *Trends in plant science* **19**: 284–287.

Marsh JI, Hu H, Gill M, Batley J, Edwards D. **2021**. Crop breeding for a changing climate: integrating phenomics and genomics with bioinformatics. *Theoretical and Applied Genetics* **134**: 1677–1690.

Martre P, Quilot-Turion B, Luquet D, Memmah M-MO-S, Chenu K, Debaeke P. **2015**. Chapter 14 - Model-assisted phenotyping and ideotype design. In: Sadras VO, Calderini DF, eds. Crop Physiology (Second Edition). San Diego: Academic Press, 349–373.

Martre P, Yin XY, Ewert F. **2017**. Modeling crops from genotype to phenotype in a changing climate. *Field Crops Research* **202**: 1–157.

Migicovsky Z, Myles S. **2017**. Exploiting wild relatives for genomics-assisted breeding of perennial crops. *Frontiers in Plant Science* **8**: 460.

Milla R, Osborne CP, Turcotte MM, Violle C. **2015**. Plant domestication through an ecological lens. *Trends in Ecology & Evolution* **30**: 463–469.

Nave M, Avni R, Ben-Zvi B, Hale I, Distelfeld A. **2016**. QTLs for uniform grain dimensions and germination selected during wheat domestication are co-located on chromosome 4B. *Theoretical and Applied Genetics* **129**: 1303–1315.

Ohta S. **2022**. Genetic variation and genetic control of intraspikelet differences in grain weight and seed dormancy in wild and domesticated emmer wheats. *Breeding Science* **72**: 198–212.

Preece C, Livarda A, Christin P-A, Wallace M, Martin G, Charles M, Jones G, Rees M, Osborne CP. **2017**. How did the domestication of Fertile Crescent grain crops increase their yields? (A Brody, Ed.). *Functional Ecology* **31**: 387–397.

Purugganan MD, Fuller DQ. **2009**. The nature of selection during plant domestication. *Nature* **457**: 843–848.

Rahman S, Islam S, Yu Z, She M, Nevo E, Ma W. **2020**. Current progress in understanding and recovering the wheat genes lost in evolution and domestication. *International journal of molecular sciences* **21**: 5836.

Rasmusson DC. **1991**. A plant breeder’s experience with ideotype breeding. *Field Crops Research* **26**: 191–200.

Ray DK, Ramankutty N, Mueller ND, West PC, Foley JA. **2012**. Recent patterns of crop yield growth and stagnation. *Nature Communications* **3**: 1293.

Reif JC, Zhang P, Dreisigacker S, Warburton ML, van Ginkel M, Hoisington D, Bohn M, Melchinger AE. **2005**. Wheat genetic diversity trends during domestication and breeding. *Theoretical and Applied Genetics* **110**: 859–864.

Reynolds MP, Singh RP, Ibrahim A, Ageeb OAA, Larque-Saavedra A, Quick JS. **1997**. Evaluating physiological traits to complement empirical selection for wheat in warm environments. In: Wheat: Prospects for Global Improvement: Proceedings of the 5th International Wheat Conference, 10–14 June, 1996, Ankara, Turkey. Springer, 143–152.

Sanchez-Bragado R, Molero G, Araus JL, Slafer GA. **2023a**. Awned versus awnless wheat spikes: does it matter? *Trends in Plant Science* **28**: 330–343.

Sanchez-Bragado R, Molero G, Araus JL, Slafer GA. **2023b**. Awned versus awnless wheat spikes: does it matter? *Trends in Plant Science* **28**: 330–343.

Simons KJ, Fellers JP, Trick HN, Zhang Z, Tai Y-S, Gill BS, Faris JD. **2006**. Molecular Characterization of the Major Wheat Domestication Gene Q. *Genetics* **172**: 547–555.

Tang H, Sezen U, Paterson AH. **2010**. Domestication and plant genomes. *Current Opinion in Plant Biology* **13**: 160–166.

Tao F, Rötter RP, Palosuo T, Díaz-Ambrona CGH, Mínguez MI, Semenov MA, Kersebaum KC, Nendel C, Cammarano D, Hoffmann H, *et al.* 2017. Designing future barley ideotypes using a crop model ensemble. *European Journal of Agronomy* **82**: 144–162.

Technow F, Messina CD, Totir LR, Cooper M. **2015**. Integrating Crop Growth Models with Whole Genome Prediction through Approximate Bayesian Computation. *PLOS ONE* **10**: e0130855.

Thurling N. **1991**. Application of the ideotype concept in breeding for higher yield in the oilseed brassicas. *Field Crops Research* **26**: 201–219.

Tilman D, Clark M. **2014**. Global diets link environmental sustainability and human health. *Nature* **515**: 518–522.

Uptmoor R, Pillen K, Matschegewski C. **2017**. Combining genome-wide prediction and a phenology model to simulate heading date in spring barley. *Field Crops Research* **202**: 84–93.

Wang JY, Turner NC, Liu YX, Siddique KH, Xiong YC. **2016**. Effects of drought stress on morphological, physiological and biochemical characteristics of wheat species differing in ploidy level. *Functional Plant Biology* **44**: 219–234.

Warschefsky E, Penmetsa RV, Cook DR, Von Wettberg EJ. **2014**. Back to the wilds: tapping evolutionary adaptations for resilient crops through systematic hybridization with crop wild relatives. *American journal of botany* **101**: 1791–1800.

Weiner J, Du Y-L, Zhang C, Qin X-L, Li F-M. **2017**. Evolutionary agroecology: individual fitness and population yield in wheat (Triticum aestivum). *Ecology* **98**: 2261–2266.

Zhang D-Y, Sun G-J, Jiang X-H. **1999**. Donald’s ideotype and growth redundancy: a game theoretical analysis. *Field Crops Research* **61**: 179–187.