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Unlocking Wheat Drought Tolerance: The Synergy of Omics Data and Computational Intelligence

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ABSTRACT

Currently, approximately 4.5 billion people in developing countries consider bread wheat (*Triticum aestivum* L.) as a staple food crop, as it is a key source of daily calories. Wheat is, therefore, ranked the second most important grain crop in the developing world. Climate change associated with severe drought conditions and rising global mean temperatures has resulted in sporadic soil water shortage causing severe yield loss in wheat. While drought responses in wheat crosscut all omics levels, our understanding of water-deficit response mechanisms, particularly in the context of wheat, remains incomplete. This understanding can be significantly advanced with the aid of computational intelligence, more often referred to as artificial intelligence (AI) models, especially those leveraging machine learning and deep learning tools. However, there is an imminent and continuous need for omics and AI integration. Yet, a foundational step to this integration is the clear contextualization of drought—a task that has long posed challenges for the scientific community, including plant breeders. Nonetheless, literature indicates significant progress in all omics fields, with large amounts of potentially informative omics data being produced daily. Despite this, it remains questionable whether the reported big datasets have met food security expectations, as translating omics data into pre-breeding initiatives remains a challenge, which is likely due to data accessibility or reproducibility issues, as interpreting omics data poses big challenges to plant breeders. This review, therefore, focuses on these omics perspectives and explores how AI might act as an interface to make this data more insightful. We examine this in the context of drought stress, with a focus on wheat.

1 | Introduction

The exponential increase in the world population is placing significant pressure on agriculture production and crop yield. Estimates predict that the global population will reach 8.6 billion by the year 2030, with a further growth past 9.7 billion in 2064 (Vollset et al. 2020). As one in nine persons worldwide is currently facing food insecurity, the ultimate concern remains the available food supply (FAO 2020). These fears are further exacerbated by events like the 2022 regional conflict between Russia and the Ukraine—both major exporters of wheat, the slow economic recovery post the COVID-19 pandemic, which is expected to impact negatively on food costs and food supply and the number of food insecure nations, especially in sub-Saharan Africa (Grote et al. 2021; https://www.fao.org/worldfoodsituation/csdb). As cereal crops are regarded as a staple in most countries, production thereof must increase by more than 60% annually to keep up with demand (Godfray et al. 2010). The decrease in global arable farmland is a further concern with forecast declines from 656 million (M) farms in 2020 to just 624 M farms by 2030. In the case of bread wheat, there are currently an estimated of 135 M wheat farms globally which is also predicted to decrease by 4% to 130 M by 2030 (Erenstein, Chamberlin, and Sonder 2021). To meet this demand, alternative methods, such as artificial intelligence (AI), should be considered to assist in processing large omics datasets into accessible formats for researchers who may not specialize in omics.

AI, though not novel, emulates human intelligence. However, it is important to note that notable distinctions exist within the domains of AI (Figure 1) (Helm et al. 2020). Machine learning, a subcategory of AI, refers to conditions where algorithms allow computers to learn from and make decisions based on input data. An essential component of machine learning is the neural network, a system of algorithms structured to recognize patterns. Deep learning, a subfield of machine learning, explores data processing in more depth through the utilization of intricate neural networks consisting of numerous layers, often known as deep neural networks. These machine learning models can be trained using "supervised" methods with labelled data, or "unsupervised" methods without explicit labels. Other approaches include "semi-supervised" learning, using a mix of data, and "reinforcement learning," based on feedback-driven actions.

At present, a variety of strategies, independent of AI technologies, are being utilized to maintain wheat production. These include manually optimizing irrigation schedules and practicing of traditional no-till farming (Horowitz, Ebel, and Ueda 2010). While these traditional approaches have, to some extent, ensured sustained wheat production, they do not offer the predictive and adaptive advantages that AI technologies bring. This gap becomes increasingly evident with searches in literature about the advances and release of climate resilient wheat varieties. Drought is one of the leading reasons for the decline in annual grain production (Keating et al. 2014; Gerten et al. 2020). However, contextualizing drought has remained a challenge within the scientific community. This gripping narrative generally starts with plant breeding. However, breeders are finding the transfer of omics data into their pre-breeding programs challenging, perhaps due to accessibility or reproducibility, and disparate definitions of drought across studies. As demonstrated

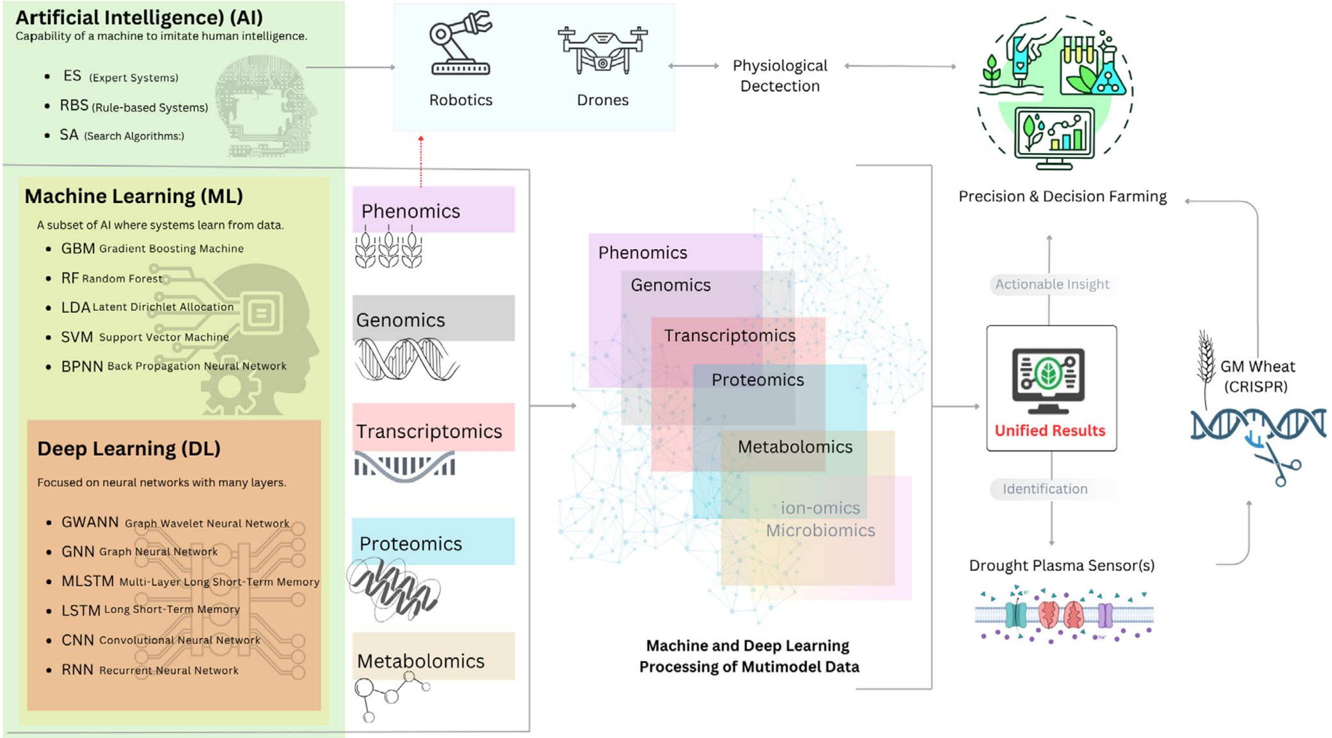

FIGURE 1 | The convergence of artificial intelligence, omics, and precision agriculture in the context of drought response. At present, the fields of artificial intelligence (AI), machine learning (ML), and deep learning (DL) are at the forefront of advancing our understanding of how cereal crops like wheat respond to drought conditions. AI, ML, and DL each possess unique features that synergistically complement one another, particularly in the intricate analysis of omics data. Modern farming practices already incorporate AI in the domains of robotics and drones systems which mostly rely on predefined algorithms (AI only), limiting their use of ML and DL capabilities. While omics outputs are typically produced as isolated results by different research teams, the integration of ML and DL with these outputs thus sometimes falling short of an holistic drought-crop response narrative. Nevertheless, combining diverse omics (multimodal) findings, followed by ML and DL strategies for simultaneous processing will lead to a unified result that may contribute to future advancements. Such integration (multimodal) will yield two pivotal outcomes: First, it will enable actionable insights in the crop field, leading to precision farming and subsequently enabling autonomously decision-making for optimizing yields. Second, it will aid in identifying specific drought-responsive plasma membrane sensors, which are proteins embedded in the cell membrane that detect external signals, such as water stress or changes in osmotic pressure. These sensors initiate signaling pathways that activate intracellular responses to mitigate the effects of drought. These sensors can be traced back to the genomic level by identifying the specific genes that encode for these receptor proteins. This understanding will enable the effective use of cutting-edge technologies, such as CRISPR, in order to develop wheat lines tailored to drought conditions. Through the integration of genetically modified wheat lines into precision farming frameworks, there is the potential to initiate a paradigm shift toward the adoption of sustainable and resilient agriculture practices.

in a recent study on potato (*Solanum tuberosum*, cv. Désirée), the integration of multi-omics data with phenotypic information offers novel insights, but the complexity of managing and interpreting these datasets remains a significant challenge for effective application in breeding programs (Zagorščak et al. 2024).

While integrating omics data into pre-breeding programs is crucial, for effective application, omics data should be both easily interpretable and directly relevant to agricultural scenarios, especially in the context of drought. While AI equipment in agriculture continually evolves, as demonstrated by Talaviya et al. (2020), a notable lag of integration of genomics, transcriptomics, proteomics, and metabolomics into AI-enhanced farming equipment for further advancement of farming practices. This gap highlights the need for more intuitive software solutions that can facilitate access to multi-omics insights and enable farmers to make data-driven decisions. We aim to review the importance of omics data for breeding drought-tolerant wheat and emphasize the emerging role of AI in enhancing these studies. We will discuss the advantages and limitations of these methods for understanding drought response to primarily benefit wheat breeding programs. While this review is aimed at biological researchers, particularly those for whom computational science is not the primary area of expertise, this review is not designed to be comprehensive but rather to initiate further research and fruitful discussions on the intersection of omics and AI.

2 | Defining Drought Within Research

Drought has been a significant factor in ecological and agricultural development, which directly correlates with trends in human urbanization (Slette et al. 2019), leading to more research detailing the wheat drought response over the last few decades. Information based on climate model predictions indicates more frequent, extreme, and spatially extensive drought periods (Stocker et al. 2013). Hence water-deficit stress in plants, because of drought will continue to be a determining factor in agricultural development. Therefore, defining and characterizing this phenomenon is essential for advancing our understanding of plant–drought interactions. The relationship between drought resistance, water-use efficiency, and yield potential is complex and often misunderstood, as highlighted by one of the renowned experts in the field of drought resistance—Abraham Blum (2005, 2009, 2017). He emphasizes that "the association among yield potential, drought resistance, and water-use efficiency is often misunderstood, which in turn can lead to conceptual oversight and wrong decisions in implementing breeding programs for drought-prone environments." This highlights the need for clarity in understanding these interactions to improve crop resilience under drought conditions. Blum's work emphasizes that breeding strategies must account for the complex interplay of these traits to improve crop resilience and yield under drought conditions, but the question remains what is drought?

Climatologists have grappled with defining drought for decades, both conceptually and operationally, and have identified many types of drought conditions, including meteorological, agricultural, hydrological, and socioeconomic drought (Wilhite and Glantz 1985; Redmond 2002; Şen 2015; Buitink, Van Hateren, and Teuling 2021; Kišš, Tárník, and Čimo 2021; Hobeichi et al. 2022). However, this creates inconsistency across the different research fields that study the influence of drought on different systems as the fundamental definition of drought is still being struggled, as with and consequently, the reproducibility of drought-driven studies poses difficulties. AI can address these inconsistencies by using of deep learning techniques, such as time series analysis employing recurrent neural networks (RNNs), particularly long short-term memory networks (LSTMs), for the examination of this metrological drought datasets (Cirstea et al. 2018; Ouma, Cheruyot, and Wachera 2021). The approach may ensure a uniform understanding of drought throughout different time periods providing a definition that can be broadly applied. Incorporating convolutional neural networks (CNNs) and remote sensing, particularly through the use of satellite and drone technologies, offers a means to obtain unbiased and up-to-date imagery that accurately assesses the severity of drought conditions (Su et al. 2020; Kattenborn et al. 2021), Moreover, there is an increasing trend toward leveraging ensemble machine learning methods, based on remote sensing data, to monitor agricultural drought, as evidenced by Wang et al. (2023). AI models can analyze these diverse data sources to provide predictions and assessments of drought conditions, but it is essential to recognize the complexity of such analyses, which are both predictive in their forecasts and suggestive in highlighting potential outcomes based on available data. These models often rely on public databases, which may contain inherent discrepancies and partialities. Therefore, AI offers great promise in enhancing our understanding of drought. The relative nature of these predictive models must, however, be considered, particularly when attempting to replicate specific climatic circumstances in studies related to drought.

Therefore, research studies must conceptualize how they define "drought" in the context of their research. One particular AI tool for this task is latent Dirichlet allocation (LDA), a machine learning algorithm for topic modelling (Blei, Ng, and Jordan 2003; Griffiths and Steyvers 2004) For example, Montes-Escobar et al. (2023) applied LDA to analyze agroforestry research spanning nearly three decades ago (1999–2022), uncovering dominant themes within the field. The study focused on categorizing topics like soil organic carbon, biodiversity, agroforestry adoption, and climate change policies from a total of 9794 research articles. By doing so, the authors were able to track trends and highlighted emerging areas of interest in agroforestry research. This approach is relevant to defining drought, as LDA can similarly be employed to identify and analyze diverse conceptualizations of "drought" across scientific literature, leading to a more standardized and refined understanding. Moreover, Vargas and Ponce (2023) introduced the Recurrent Embedded Topic Model, a modification of LDA, demonstrating that while LDA serves as a foundational tool, evolving methodologies in topic modelling can offer enhanced capabilities for such analyses.

3 | Wheat Breeding in the 20th Century

Like many other crops, common bread wheat (*Triticum aestivum* L., $2n = 6x = 42$, AABBDD), an allopolyploid serves as a staple food crop in many countries irrespective of their economic status. Bread wheat has a large genome when compared to other crop species with an estimated size at 17 G base pairs, which consists of three homeologous genomes (AA, BB, and DD). As most breeding programs are aimed at improving several traits of interest simultaneously, they are complex due to genetic correlations between traits, pleiotropic effects, and physical linkage between genes (Mathew et al. 2019; Liu, Able, and Able 2020; Ren et al. 2021; Sallam et al. 2022). Breeding programs further continue to select crops to ensure a better yield which can reduce genetic diversity known as genetic bottlenecks (Voss-Fels, Stahl, and Hickey 2019). With a low genetic diversity, the ability to select for plants that can tolerate drought stress due to soil water-deficit decreases which adds more strain on producing adaptable crops that fit the current climate and food security needs.

Plant breeders have been actively seeking ways to enhance the efficiency of crop breeding processes to keep up with the demand for improved crop varieties for food security. One significant advancement in this field is the application of speed breeding techniques, which have proven to be instrumental in accelerating the breeding cycle (Watson et al. 2018). It essentially involves manipulating environmental factors like light, temperature, and humidity to increase the rate of plant growth and development, allowing for multiple generations of crops to be produced within a single year (Ghosh et al. 2018). For example, by extending the photoperiod to 22 h of light per day, wheat plants can undergo up to six generations annually, a substantial increase compared to traditional breeding methods (Potts et al. 2023).

To further optimize the speed breeding process, several AI systems have been integrated into existing programs. These systems utilize machine learning and deep learning techniques to analyse and interpret large datasets from various sources, including sensor data on environmental conditions and plant growth parameters. This enables real-time adjustments to ensure optimal plant development (Khan et al. 2022). A key aspect of this optimization is the incorporation of enviromics, which combines environmental data with phenotypic data to model and predict plant responses to different conditions. Resende et al. (2021) highlighted the significance of enviromics by using machine learning algorithms, specifically Random Forest regression, to create a robust AI framework for predicting genotype performance across diverse environmental conditions. This approach demonstrated the significance of AI to further enhance breeding programs especially for speed breeding techniques.

To further increase genetic diversity, plant breeders have also induced heritable mutations in crop genomes to increase genetic diversity using chemical (e.g., ethyl methane sulfonate, EMS) or physical (e.g., x-rays, UV light, neutrons-alpha-beta particles, fast and thermal neutrons, especially gamma rays) mutagenesis (Hussain et al. 2021) leading to a new variety classification (https://nucleus.iaea.org/sites/mvd/SitePages/Home.aspx). Over 80% of the registered "new-mutant" crop varieties reported in the IAEA database (https://mvd.iaea.org/) was induced by exposure of the whole plant, or propagules, to either physical or chemical agents. Despite the effectiveness of these techniques, they cannot just target a specific location in the genome of the crop plant, as such, robust techniques are required to fully characterize these mutant plants since mutagenesis are synonymous with nucleotide alterations, including base substitutions, the deletion, duplication, or rearrangement of large genomic fragments (Rafi et al. 2016; Leland et al. 2017).

In an attempt to fully characterize the mutants, breeders conduct phenotypic and seed quality assessment, which is often laborious and may introduce human error during selection. AI can enhance these processes by utilizing computer vision and deep learning techniques, specifically CNNs, to analyze the phenotypic characteristics of grain crops (Patrício and Rieder 2018 and reference therein; Chen et al. 2023). In the field of plant phenotype prediction, there has been a shift toward utilizing deep learning techniques, specifically CNNs, as opposed to traditional machine learning algorithms like the support vector machine (SVM) and the back-propagation neural network (BPNN). This recent emphasis on deep learning is due to its ability to effectively capture complex patterns within plant phenotypic data (Wang and Su 2022).

However, using mutagens to develop new wheat lines required a holistic understanding of the end results. Indeed, a phenotypic evaluation during growth is the starting point of characterization of these mutants, this should be carried out in conjunction with an additional evaluation of the genome, transcriptome, proteome, and metabolome. Though there are other omics levels to consider such ions-omics and microbiomics (Mao et al. 2023 and reference therein). As these evaluations are inherently complex and multidimensional, they pose big challenges to traditional statistical analyses. Hence, there is an emergent need for specialized AI analytical tools, with machine learning and deep learning being at the forefront without relying on traditional statistical assumptions. Although these AI analytical tools may seem challenging to implement, given the necessary transfer of skills and coding pipelines, they should not decelerate the ongoing momentum in improving wheat, particularly with the rise of CRISPR-based genetic modifications.

New breeding techniques, such as the application of RNA-guided Cas9 nucleases from CRISPR and epibreeding that offer alternative approaches to improve drought tolerance in wheat, have recently surfaced in the literature (Botha 2023). However, CRISPR/Cas9 is still highly dependent on in vitro plant regeneration (Kausch et al. 2019) and unfortunately, many elite commercial varieties of wheat are recalcitrant to regeneration during the process of genetic engineering. While the issue of regeneration is a key bottleneck, several AI tools, including DeepBind, DESKGEN, and CCTop, are being employed. These AI tools, although not directly resolving the regeneration challenge can heighten the precision and efficiency of the CRISPR/Cas9 system, predicting the most effective target sites with greater accuracy especially in crops. For instance, while DeepBind utilize deep learning techniques to detect patterns in genomic sequences and predict both on-target and off-target CRISPR/Cas9 activities (Alipanahi et al. 2015; Hasani 2023), tools like DESKGEN, and CCTop focus on single-guide RNA design, guide RNA optimization, and potential off-target site prediction (Stemmer et al. 2015; Hough et al. 2016; Abadi et al. 2017). However, the relevance of these AI models often depends on specific research questions. As a result, some researchers still gravitate toward more foundational software tools, such as Benchling (https://www.benchling.com/), CHOPCHOP (https://chopchop.cbu.uib.no/), CRISPOR (https://crispor.tefor.net/), and VectorBuilder (https://en.vectorbuilder.com/). These tools, though perhaps less advanced in terms of machine learning capabilities, are valued for their direct approach and established reliability in the field.

4 | Is Wheat Prepared for the Drought Battle?

In order to improve the current understanding of the factors underpinning mechanisms involved in the drought response in hexaploidy bread wheat, Deng and co-workers are advocating an all-encompassing approach that includes the complete range of omics technologies (Deng et al. 2018, 2019). Even though such an approach will allow for a multidimensional view of the complex genomic architecture (Hussain et al. 2023), it remains still to be determined how much of the wheat genome is designated to facilitate the drought response. This knowledge gap is also due to the enormous number of wheat cultivars already available, with each cultivar possessing a unique genome quality.

Figure 2 provides an overview of the physiological response of wheat to drought conditions, which involves reduced growth rates, reduced photosynthesis, and stomatal closure, leading to changes in biomass (Shanker et al. 2014 and references within). The primary response occurs at the molecular level, involving the transcriptome, proteome, and metabolome which mediates the unique physiological and morphological responses. These responses feed into the so-called non-hierarchical drought resistance categories which are divided into four mechanisms: drought avoidance, drought tolerance, drought escape, and drought recovery (Fang and Xiong 2015 and references within). As soil water-deficit caused by drought is an unpredictable phenomenon, wheat possibly combines all four mechanisms to overcome the drought stress (Shavrukov et al. 2017). Further research studies are still needed to prove this possibility with a single drought exposure time frame. However, from a breeder's perspective, drought tolerance is the preferred trait within crops, although avoidance is likely the dominant mechanism for achieving drought tolerance (Chaichi et al. 2019; Li, Ma et al. 2021). This response is, however, dependent on the environment and frequency of drought and at which development stage the plant is subjected to drought (Lawlor 2012; Zhou et al. 2016; Basu et al. 2016 and references within). It is evident that an enormous amount of information as shown in Figure 2 must be considered to efficiently use AI-assisting tools to result in a high degree of predicting accuracy. Furthermore, every wheat line, cultivar, mutant, and transgenic variant holds genomic significance, influencing all subsequent omics levels and, consequently, the plant's response to drought. While no universal omics response exists for wheat, this complexity can be systematically harnessed using existing or newly designed AI tools, starting with phenomics.

5 | Phenomics and Drought

The central dogma states the flow of information from gene to mRNA to protein, collectively leading to an adaptable phenotype. This feeds into the idea of reverse genetics, where plant breeders select elite varieties based on the phenotypic response within a given environmental stress (Figure 2). Therefore, phenotyping provides insight into how the plant manages its resources in

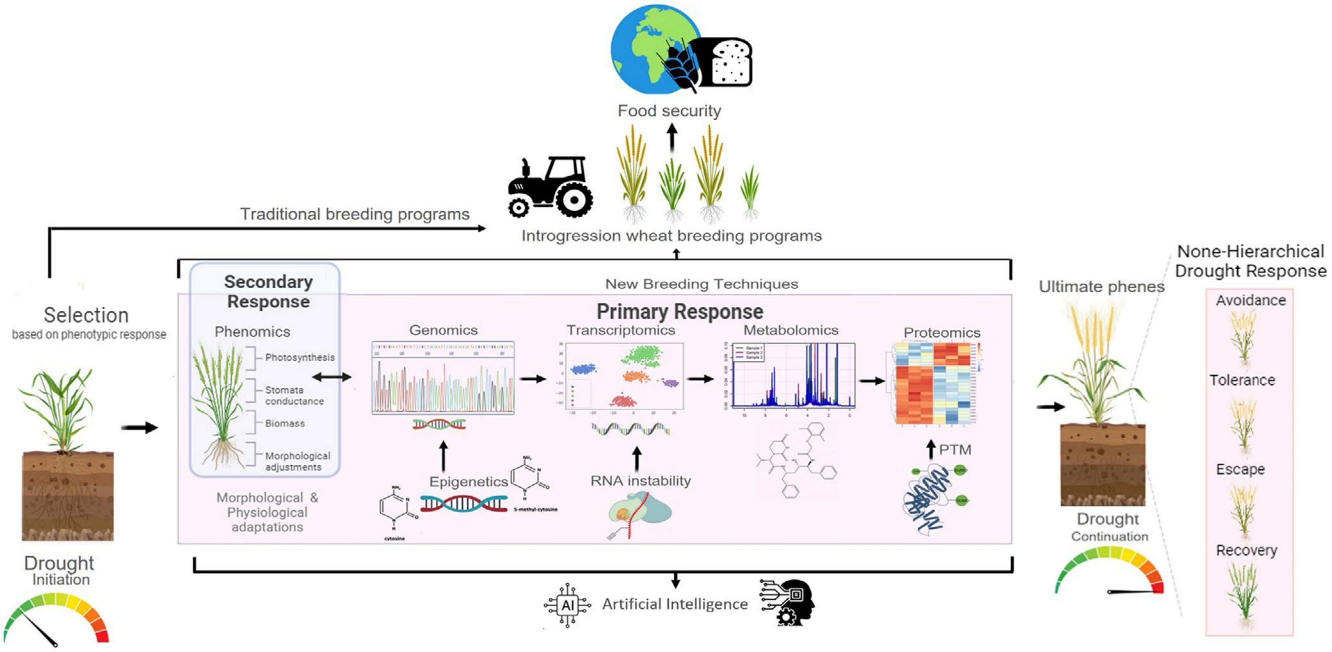

FIGURE 2 | Water-deficit deficit stress is a consequence of drought conditions; naturally, wheat can respond to these conditions by adapting its phenotype (phenomics). This feeds into the idea of reverse genetics, where traditional plant breeders select elite varieties based on the phenotypic response for drought stress. To add value to these introgression programs, breeders should keep in mind that wheat has a primary response to drought conditions that occurs at a molecular level, involving the genome (also influenced by epigenetics), transcriptome, metabolome, and proteome, all mediating the unique secondary responses affecting all physiological and morphological attributes leading to reduced growth rates, reduced photosynthesis, and stomatal closure, leading to changes in biomass. Collectively, these responses can feed into the so-called non-hierarchical drought resistance categories, where drought avoidance and tolerance are the most preferred mechanisms within crops. Understandably, breeding programs find it perhaps challenging to integrate high-throughput omics data into their programs. As omics data from gene to protein may not be a linear process, therefore leading to many contradicting publications, as gene expression patterns do not fully correlate to protein and transcript levels due to RNA stability and protein post-translational modification; therefore, there is no one-to-one association between the omics.

relation to the environment and its genetics into the presented phenotype. Therefore, information on phenotypic responses in a set environment is crucial to understand which plants are suitable for a specific environment, which is a prerequisite for breeding programs. Interestingly, even though some may not regard phenotypic data part of "omics," it is the transition of genes that showcases the expressed phenotype (i.e., "phenes"). Drought-phenomics data are, unfortunately, often synonymous with greenhouse container-grown plants, where drought is introduced abruptly by switching off the irrigation system. This results in a rapid onset of water-deficit stress, depriving the plant of a gradual drought response that would naturally occur under field conditions (Marchin et al. 2020). Studies have shown that plants and soils behave differently in greenhouses compared to field environments, often producing exaggerated responses due to the controlled conditions that lack natural stressors such as competition, temperature fluctuations, and herbivory (Forero et al. 2019). Westbrook et al. (2021) further pointed out that discrepancies between greenhouse and field results are common, thus substantiating the need for multiple experimental methods to fully understand the impacts of drought on crop growth under real-world agricultural conditions. Nonetheless, the acquired greenhouse data still serve as a fundamental progression point to initiate a large-scale field trail.

However, releasing drought-tolerant cultivars still requires intensive phenotyping assessment, especially in large-scale field trails, this is often labour intensive, time-consuming, and subjective, which causes a delay in releasing these cultivars often referred to as a breeding bottleneck. AI can mitigate these challenges by utilizing high-throughput phenotyping technology that has become more common in wheat phenomics. For instance, the utilization of aerial platforms, specifically unmanned aerial vehicles (UAVs) or drones (Figure 1), with sensors such as RGB cameras, fluorescence, near-infrared, and hyperspectral imaging have demonstrated potential in mitigating these bottlenecks (Talaviya et al. 2020; Herr et al. 2023), The imagery captured by drones is of considerable importance when applied to both machine learning and deep learning. Specifically, machine learning techniques have proven efficient in predicting wheat yield as evidenced by Pantazi et al. (2018) and Yang et al. (2019). Meanwhile, deep learning methodologies have been crucial for the detection of stress, as demonstrated by Singh, Ganapathysubramanian et al. (2016) and Ubbens and Stavness (2017). Thoroughly investigating the intricacies of wheat response to drought using AI necessitates collecting extensive phenotypic data across a variety of drought stress environments (Gill et al. 2022). The complexity arises from the inherent capability of wheat to adapt both morphologically and physiologically to abiotic (and biotic) stressors.

6 | Morphological and Physiological Response to Water-Deficit Stress

The way crops respond to drought is primarily influenced by leaf structure, root system architecture, and shoot attributes. Together the crop can extract maximum water from the local environment and minimize water loss through the same attributes (Jaleel et al. 2009). With the onset of any stress, internal leaf restructuring would occur, prompting leaf changes that influence the leaf's size and the basal angle (Xu, Zhou, and Shimizu 2009). During drought stress, leaf morphology changes drastically to maximize the effect of gaseous exchange characteristics such as stomatal conductance and transpiration. Wheat genotypes with smaller leaves are considered more able to roll their leaves to limit water loss in response to drought stress than genotypes with large leaves, thereby resulting in higher yields.

Quantitative trait loci (QTL) pyramiding has been explored for flag leaf morphology by plant breeders and has proven useful for the genetic improvement of drought tolerance in wheat (Bhutta and Ibrahim 2006; Khan et al. 2012; Hassan et al. 2016; Khanna-Chopra et al. 2020). However, as the rapid advancements in computational biology come to the fore, software like TASSEL is frequently employed to make predictions about drought-resistant phenotypes by analyzing QTLs (Bradbury et al. 2007; Sallam et al. 2022). While some might not view these tools as embodying AI in the traditional sense, where machine learning or deep learning models "learn" from data, they do automate intricate data processing tasks using preset algorithms.

Furthermore, plant breeders have also aimed to improve water-use efficiency by considering several root characters by mining for genes and QTLs controlling root traits, such as root tip diameter, gravitropism, and morphological plasticity (Li, Li et al. 2021, and references within). In recent years, several studies identified QTL controlling root characteristics, however, these markers were found in wheat lines from different genetic backgrounds, mapping populations, and/or environmental conditions which may create an influx of redundant QTLs. AI can improve this identification process using deep learning tools such as DeepVariant. This program applies deep CNN for the purpose of identifying genetic variations. It achieves this by analyzing next-generation sequence data that have been aligned to a reference genome. This is accomplished by identifying statistical correlations within visual representations of gathered data surrounding possible variations in certain regions. Such capabilities allow DeepVariant to offer precise variant calls, making them invaluable inputs for subsequent QTL analysis (Poplin et al. 2018). While the tool's efficacy for QTL analysis has been demonstrated in sorghum (Ruperao et al. 2022, 2023), its application remains highly relevant to wheat. Breeders can increase the accuracy and consistency of QTL discoveries by using deep learning and ensuring that the genetic variants they identify are reliable. This in turn contributes to a deeper understanding of how plants, such as wheat, respond at a physiological level, adjusting shoot–root ratio during drought stress.

The root system has a synchronized relationship with the shoots, which rely on the exchange of water, nutrient, and hormones. This dynamic is especially crucial during drought conditions, where the ability plants to cope is heavily influenced by its root architecture (reviewed by Ober et al. 2021). As expected, with a deficiency in water supply, this relationship would be placed under severe stress, causing a displacement in shoot–root mass. The role of AI in root system architecture phenotyping has gained significant attention in recent years, with numerous studies showcasing its potential to enhance both the efficiency and accuracy of phenotyping processes. Langridge et al. (2022) emphasize the critical role of root system architecture (RSA) in wheat performance, particularly under drought conditions, noting that traits, such as root depth and distribution, are crucial for water uptake and nutrient acquisition. Thus, they emphasize the importance of improved RSA phenotyping techniques, the incorporation of AI technologies, such as machine learning and computer vision, could provide a valuable solution. These tools have already been shown to automate SRA measurement and analysis with great precision. Falk et al. (2020), for instance, successfully employed machine learning and computer vision to automate RSA phenotyping in soybean, reducing labor intensity and variability in data collection. This integration allows for more precise extraction and quantification of RSA traits, providing reliable data on root traits that correlate with plant performance across diverse environmental conditions. Weihs et al. (2024) further support these advancements with their review on AI-driven analysis across various crops, including maize, wheat, rapeseed, pea, cotton, alfalfa, and Arabidopsis in RSA image analysis and highlighting the transformative role AI has in their root phenotyping. As AI improves our ability to accurately characterize root systems, the impact on above-ground processes becomes more evident, particularly under drought conditions. For instance, as root biomass increases in search of water, plants often compensate by adjusting above-ground structures, reducing transpiration through stomatal rhythms, which in turn affects CO2 assimilation. In C3 plants (such as wheat), this creates a shift in ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO) activity, and photosynthesis becomes compromised due to the internal lack of CO_2, which can be indirectly monitored by the RuBisCO preference of CO_2, a mechanism known as C discrimination (Busch 2020). Stomatal conductance is a major determinant of photosynthesis and can influence the performance and yield of the plant. The efficacy of deep learning, particularly the Multivariate Long Short-Term Memory (MLSTM) model designed for multivariate time series data, has been proved in the prediction and understanding of stomatal conductance and photosynthesis. Accurate predictions regarding photosynthesis in Chinese Brassica were made by Gao et al. (2021) through the use of environmental metrics such as air temperature, relative humidity, canopy temperature, transpiration rate, and photosynthetically available radiation (PAR). However, in order to further enhance the predictive capacities of these AI tools, it is imperative to integrate additional data, such as shoot–root mass ratio, root biomass, CO_2 assimilation.

The ability of wheat to adapt to a range of stresses is directly, or indirectly, related to their ability to adjust at a photosynthetic level. Additionally, a typical symptom of drought stress is pigment photo-oxidation and chlorophyll degradation. The monitoring of photosynthetic pigments for detecting changes in powdery mold diseases progression has been demonstrated by Abdulridha et al. (2020) utilizing AI-powered drones equipped with specialized sensors and cameras. The assessment of drought stress continues to rely on the measurement of total chlorophyll content as a fundamental indicator. As it is well documented that photo-oxidation and chlorophyll degradation is attributed to the disruption of equilibrium states in both chlorophyll *a* and *b*, which occurs as a result of drought-induced stress (Ahmad et al. 2018; Li et al. 2022 and references cited therein). Historically, researchers commonly used manual techniques for chlorophyll extraction, which are unfortunately destructive. Some have used handheld chlorophyll detectors to gauge the extent of drought stress experienced by crops. Nevertheless, these techniques may exhibit subjectivity due to their substantial reliance on human operators. Machine learning-based robotic systems, such as the RIPPA system (Bogue 2016) and EcoRobotix's precision weed detection system (Gandorfer et al. 2022), offer potential solutions that are more objective and non-destructive. The incorporation of chlorophyll-specific sensors into these platforms, which already possess sophisticated computer vision and precise interaction capabilities, has the potential to enhance the accuracy and consistency of chlorophyll readings. Furthermore, it should be noted that the application of these robotic systems will serve as a complementary measure to the data gathered by drones powered by AI, leading to a more comprehensive approach to crop and drought monitoring (Figure 1).

7 | Genomics and Drought

With the onset of advance technologies such as next-generation sequencing, studies that elucidate the molecular response of drought have become more credible and informative (Harfouche et al. 2019) and this can largely be attributed to QTL mapping and genome wide association studies (GWAS). Even though GWAS are useful for nominating candidate genes, the data typically are unable to establish causality or differentiate between the effects of variants in linkage disequilibrium (Flister et al. 2013). Interpreting the extensive datasets generated through next-generation sequencing in the context of the intricate genome of wheat, which consists of three distinct subgenomes (A, B, and D), is a formidable task. Although the existing algorithms applied in GWAS have demonstrated reliability, the integration of AI into GWAS has the potential to yield more adaptable solutions, especially for unique datasets or conditions (Bhat et al. 2023 and references therein). A study by Ashkenazy et al. (2022) used the graph wavelet neural network (GWANN), a deep learning algorithm specifically developed for graph-based data, to perform GWAS. The authors demonstrated the superior performance of GWANN compared to widely used GWAS tools across both simulated and real datasets. This approach facilitated the detection of association signals with enhanced sensitivity and efficiency. Thus, deep learning has the potential to facilitate the detection of patterns within the subgenomes of wheat and their interactions, hence providing a deeper understanding of drought responses.

Following a genomics approach to elucidate drought response seem to be analogous to that of a QTLs approach which is aimed at answering the questions related to whether phenotypic differences hold a relationship with specific loci. Meta-QTL analysis has further refined this process by consolidating QTLs from multiple studies, allowing breeders to focus on the most stable and consistent QTLs for traits like drought tolerance (as reviewed by Sharma et al. 2023). For instance, Acuña-Galindo et al. (2015) conducted a meta-analysis of QTLs related to drought and heat stress in wheat, consolidating data from 30 independent studies and identifying 66 meta-QTLs across all 21 wheat chromosomes. Similarly, Selamat and Nadarajah (2021) conducted a meta-QTL analysis in rice, identifying 70 meta-QTLs related to drought tolerance from 20 independent studies, identifying several important drought-responsive genes, including *ABI5*, *GBF4* and *PID*, making these regions prime targets for molecular breeding and genetic engineering efforts. These studies emphasize the power of meta-QTL analysis in identifying critical genomic regions that influence drought tolerance across diverse species, However, a recent review by Kaur et al. (2023) on meta-QTL analysis illustrates the challenges of integrating data from multiple studies, which often differ in terms of marker density, data volume, and statistical methods used. This highlights the limitations of traditional meta-analysis approaches, where the variability in study designs can complicate the process of identifying truly stable and consistent QTLs. Thus, with the increasing amount of data generated from such analyses, the integration of AI-assisted tools becomes crucial for further streamlining the process and maximizing its efficiency (Sharma et al. 2023). TensorQTL, for example, incorporates traditional statistical methods such as linear regression for the purpose of QTL mapping. It leverages TensorFlow, a library for AI and deep learning, to optimize and accelerate the QTL mapping process. In wheat more than 1200 QTLs for drought response have been reported, which is also associated with grain yield, root system, plant hight, coleoptile length and, water-soluble carbohydrates (Gupta et al. 2020). AI can further assist by integrating large datasets from meta-QTL analyses, improving the precision with which breeders identify genetic targets for marker-assisted selection (MAS). However, despite the discovery of these QTLs, it remains elusive how closely related these QTLs are too specific markers. Naturally, this creates some dissociation between molecular and traditional breeders. Therefore, reported QTLs should endow a comprehensive characterization using AI tools, with parameters extending within GWAS and phenomics. As QTL is based on DNA sequence (genome), we should not lose sight of the fact that this information only provides some context to a governing trait, as it may also be a product of epigenomic influence, which can provide information on changes of a gene function that does not entail a change on the genomic sequence itself, but can still be completely heritable (Dalakouras and Vlachostergios 2021).

Epigenetic modifications such as DNA methylations, histone modifications, and histone variants, and some non-coding RNA (ncRNA) changes are achieved by three alterations: post-translational histone modification, DNA methylation, and the action nc RNA molecules (Zhang, Lang, and Zhu 2018 and references within; Chachar et al. 2022 and references within) result in the regulation of access to and expression of DNA due to its influence on chromatin structure (Zhang, Lang, and Zhu 2018 and references within; Millán-Zambrano et al. 2022). Using either one or a combination of these alterations provides the plant with a unique ability to endure drought conditions. For example, Castelletti et al. (2014) demonstrated how a miniature transposon (MITE) insertion in maize was associated with differential DNA methylation at the *Vgt1* locus, which in turn regulated flowering time by altering the expression of the nearby gene ZmRap2.7. This example illustrates how DNA methylation plays a pivotal role in regulating gene expression under environmental stresses like drought.

An interesting integrative model posed by Begcy and Dresselhaus (2018) shows the effects of abiotic stress, including drought, on the epigenetic status of cereals during reproductive development. In most cases, there seems to be a positive correlation between epigenetic modification and drought response. However, epigenetic breeding remains a challenging narrative, even though we observed clear differential gene expression patterns during drought stress in wheat (Dalal et al. 2018; Dugasa et al. 2021; Liu et al. 2020; Nergui et al. 2022). This is attributed to the fact that transcriptomic regulations do not necessarily lead to direct changes in the epigenome; therefore, we cannot definitively argue a succinct relationship between the epigenome and drought. However, incorporating AI in this domain, especially for the intricate wheat genome, can help decipher the vast epigenetic modifications and their interactions. In a recent investigation, N'Diaye et al. (2020) applied a comprehensive set of machine learning algorithms and deep neural networks to analyze methylation profiles in wheat, achieving an impressive accuracy rate of 0.81. This study highlighted the potential of AI and deep learning in identifying differentially expressed genes (DEGs) based on tissue-specific methylation patterns, in greenhouse-grown wheat. While the results were obtained under controlled conditions, further validation in field-grown plants, where stress develops more gradually, could provide additional insights into the broader applicability of these findings. The importance of stress dynamics is illustrated by Talamè et al. (2007), who found that slowly developing drought stress in barley, typical in field conditions, induces a different set of transcript profiles compared to rapid dehydration treatments. This suggests that both greenhouse and field studies contribute unique perspectives to understanding the interplay between methylation and gene expression under drought condition. Additionally, deep learning tools such as DeepMethyl (Wang et al. 2016) can be repurposed from human to plant genomes to predict DNA methylation states, offering insights into gene regulation in wheat during drought. Similarly, DeepChrome (Singh, Lanchantin et al. 2016) uses deep learning to analyze histone modifications, potentially elucidating their influence on drought-related gene expression in wheat.

However, the remarkable plasticity of the epigenome, as demonstrated by its potential to trigger changes in phenotype, presents a novel avenue for enhancing plant breeding initiatives. This issue becomes especially relevant when examining the influence of drought-induced phytohormones, including abscisic acid, on the epigenome (Begcy and Dresselhaus 2018 and references therein). Deep learning algorithms have the capability to effectively simulate the influence of phytohormones on the epigenome, hence enabling the prediction of subsequent phenotypic outcomes. Furthermore, the phenomenon of stress priming, wherein the genome undergoes forced epigenetic modifications due to repeated drought exposures, leads to what is termed "epi-priming," manifesting as transgenerational traits. AI can be used to decipher the extent to which drought conditions must be imposed to achieve favourable outcomes through forced epigenetic modifications. By reducing the likelihood of overexposing plants to drought conditions, these simulations can prevent irreparable damage and plant mortality.

In recent years, more advanced technology has been applied to alter the epigenome, such as chemical treatments using 5-azacytidine (Boyko et al. 2010; Kim, Kim, and Cho 2022; Kumar et al. 2020) and the CRISPR/Cas system (Hilton et al. 2015; Manghwar et al. 2019). Though these techniques have been explored with success, it should be emphasized that epigenetic modification may be deleted during the meiosis; thus, stable inheritance of markers produced by epigenetics may not be achieved within breeding programs, thus vigorous genetic assessment is required post editing (Danchin et al. 2019). Importantly, an epigenetic response during drought is vastly different among crops, for example, drought stress induces DNA hypermethylation in barley (Surdonja et al. 2017) and DNA hypomethylation in rice (Gayacharan and Joel 2013). Though in wheat, the level and status of methylation during drought stress is still unclear, we do know that methylation patterns change during drought condition. Duan et al. (2020) could demonstrate that 5mC content and methylation level of wheat seedlings exhibited tissue specificity and increased significantly in leaves along with the increase of water deficit. This essentially provides a reference to reveal the molecular mechanism of wheat adapting to water deficit from the perspective of epigenetics. However, as of yet, there are no clear association between DNA methylation and drought associated genes during water-deficit stress. The advancement of sophisticated AI tools has great importance to this field, since by using existing epigenomes and AI models, including those originally developed for other species, researchers may effectively investigate and predict outcomes within the complex epigenetic landscapes.

8 | Transcriptomics and Drought

The multifaceted nature of how plants react to drought is a non-linear response. It involves multiple pathways located in various cellular compartments allowing for regulation of relative abundance of stress-responsive protein often involved in complex cross-regulation of different stress signalling pathways. Therefore, researchers often choose to investigate only gene expression levels during an anticipated stress condition and ignore the expression patterns that do not fully correlate to protein and transcript levels due to RNA stability and protein post-translational modification. The application of AI-driven models, such as DeepLGP (Fang, Pan, and Shen 2022), leverages multimodal data to improve gene prediction. This approach provides valuable insights into previously undetected expression patterns that are controlled by long non-coding RNAs (lncRNAs). This approach and has the potential to successfully address the difficulties associated with RNA stability and protein post-translational modification. However, to obtain accurate predictions, additional optimization driven AI is required due to the intricate nature of the wheat genome.

Transcriptomics investigations tell us that water-deficit stress is seen as an environmental signal that the plant cell interprets. It is further known that secondary metabolites and abscisic acid imbalance modulate the stress perception of such cells during drought stress (Zenda et al. 2019). Unlike in the case of salinity, where the plant senses changes in ion levels by a specific plasma membrane sensor known as Na^+ sensor (SOS1/SOS2/SOS3 protein complex) (Zhu 2002), no specific drought sensor has been confirmed yet. What is known is the fact that with the onset of water-deficit stress, a host of sensors is triggered, activating cytoplasmic Ca^{2+} and protein signals pathways, leading to gene expression (Xu, Zhou, and Shimizu 2010). While AI, especially machine learning and deep learning, offers promising tools for the detection and classification of plasma membrane sensors, its application for drought sensor detection is not straightforward. Challenges occur because of the potential interaction of several sensors and the dynamic nature of their activation. In this scenario, the effective application of AI will necessitate the implementation of integrative approaches that exploit multimodal data (Figure 1), encompassing cellular imaging, biosensor readings, and omics data. Fortunately, the existing research in each of these areas, though it may not be computational in nature, provides data that can undoubtedly be used by AI to initiate the search for drought sensors.

To understand the drought response, various crop species have been exposed to a range of drought intensities followed by transcriptome profiling in the past. As expected, data reveal a large number of genes involved in drought stress, which includes genes involved in photosynthesis regulation (Saibo, Lourenço, and Oliveira 2008; Burgess et al. 2019), ROS expression (Dalal et al. 2018; Dugasa et al. 2021), osmolyte synthesis (Kosová et al. 2016; Wang et al. 2019; Wang, Chen et al. 2021; Wang, Peng et al. 2021), genes coding for late embryogenesis abundant proteins (Kamarudin et al. 2019), aquaporins (Kurowska et al. 2019), as well as various transcription factors (TFs) (Joshi et al. 2016) and signal transduction elements (Hu et al. 2018; Rasool et al. 2022). The TFs are of particular interest since many of them, such as *DREB* (dehydration-responsive element-binding protein), *WKRY, PLATZ* (plant AT-rich protein and zinc-binding protein), *MYB* (Myb myeloblastosis viral oncogene homolog), *NAC* (N-acetyl cysteine), and *PFP alpha-1*, can be regarded as master switches, which trigger the simultaneous expression of a large number of stress-response genes (Bartels and Sunkar 2005; Zenda et al. 2019).

Even though transcriptomics data remain an important element in the quest of drought elucidation, the contextualization of findings is even more so. It remains highly unlikely that a single gene can be the "silver bullet" of key element to unlocking the extreme drought tolerance trait, even if a particular gene was identified in many different literature reports. Nonetheless, there is congruency in the literature regarding which gene clusters many be important in the drought response, and this is primarily due to the identification of osmotic stress-responsive genes, for example *RD29A/COR78/LTI78* (responsive to dehydration/cold-regulated/low-temperature-induced) (Seki et al. 2003 and references within). However, the activation of the signalling pathways related to these genes is largely unknown. To date, two kinds of stress-inducible genes were identified; (i) includes genes involved in water transport (aquaporins), cellular membrane protection, and integrity under stress conditions (e.g., calnexins, ABC-transporter, and xylanases-1); and (ii) genes that encodes regulatory proteins, for example, transcription factors, protein kinases, SUMO (small ubiquitin modifier) proteases, calmodulin-binding proteins, and serpins (serine protease inhibitors). AI models should be centered around the comprehensive list of genes implicated in drought stress, particularly those that underpins key regulating pathways. These genes may be regarded as high-priority features in the training of machine or deep learning models, thereby ensuring that the models pay special attention to these genes when making predictions or analyses.

Despite the fact that transcriptomics contributed immensely to our current understanding of the drought stress response in the context of wheat, the developmental stage should be considered before conducting such analysis. As each developmental stage will anticipate drought differently, for example, an RNA-Seq analysis revealed that drought stress during early reproductive periods had a more severe impact on wheat development, gene expression, and yield than drought stress during flowering. Hence, the life cycle of wheat has a significant influence on its drought response (Ma et al. 2017). Also, the water-deficit stress adaptive mechanisms differed considerably between wheat genotypes as was recently demonstrated (Mia et al. 2020). Given these intricacies, it is essential to incorporate such insights into the development and refinement of AI tools, ensuring their predictions are both detailed and accurate.

9 | Proteomics and Drought

Transcripts are translated into protein, which undergoes post-translational modification (PTM), leading to several different protein isoforms. In addition to this, protein stoichiometry is influenced by environmental factors and protein interactions, which could result in degradation, and since stoichiometry determines the function of any given protein, this creates complexity when needing to measure such proteins (Struk et al. 2019 and reference within). The advent of AI tools, such as AlphaFold(2), has significantly transformed the field of proteomics through the application of deep learning methods, specifically in the domain of protein structure prediction (Jumper et al. 2021). This advancement was recognized with the 2024 Nobel Prize in Chemistry (https://www.nobelprize.org/prizes/chemistry/2024/press-release/), awarded to the creators of AlphaFold for their contributions to resolving protein structures. Originally, AlphaFold (AF) was designed with the purpose of predicting the structures of individual proteins. However, it has been shown that AF has also expanded its prediction powers to include protein complexes. After the effective utilization of AF in the context of protein complexes, a specialized iteration called AlphaFold Multimer (AFM) was established with the specific aim of predicting the structures of protein complexes (Gao et al. 2021). The latest iteration, AlphaFold 3, introduced a diffusion-based architecture that reduces reliance on multiple sequence alignments (MSAs), enabling flexible modeling of diverse biomolecular complexes, including proteins, nucleic acids, and small molecules. While advancements continue, challenges such as occasional stereochemical issues and static structure predictions remain (reviewed by Bryant 2023; Abramson et al. 2024; Desai et al. 2024).

It is well documented that the proteome is uniquely regulated as a consequence of environmental conditions such as stress (Singh et al. 2022). This entails an adjustment to protein turnover; a leading response orchestrated through metabolic adjustments to activate necessary enzymatic pathways (Zhao et al. 2015). These pathways assure an equilibrium state of protein synthesis and degradation; controlled by highly sophisticated protein degradation machinery, of which some are shared by mammalian systems, such as ubiquitylation, autophagy, and target of rapamycin (TOR), (Urade 2007; Tajima, Iwata, and Koizumi 2008; Vitale and Boston 2008).

Ubiquitylation emphasizes the targeting of proteins for proteasomal degradation and has been implicated in a vast array of plant functions, including regulation of growth and development during both non-stress and stress conditions (Mirsanaye, Typas, and Mailand 2021 and references within). While autophagy is the process whereby cells reallocate nutrients from the metabolic non-important/non-active part of the plant to areas that are highly metabolic active during a particular stressed period. Therefore, it is vital in all senescence activities, by which tissue and cells are sacrificed to ensure the survival of the plant in totality (Wang and Schippers 2019), and hence, autophagy represents a strategy to advance crop resiliency during drought stress as recently demonstrated (Bao et al. 2020; Hickey et al. 2022). The well-characterized TOR pathway from mammalian and microbial systems is shared by plants and is contributing to the regulation of metabolism and overall growth (Fu, Wang, and Xiong 2020). Emerging data on the TOR pathway reveal that the TOR coordinate responses to various stress conditions, including energy deficiency, which is often a consequence of prolonged water-deficit stress (Schmelzle and Hall 2000; Wullschleger, Loewith, and Hall 2006; Caldana et al. 2019), the positive regulation of the plant's response to drought and osmotic stresses (Fu, Wang, and Xiong 2020). Collectively, these three pathways are integrated, thus ensuring an equilibrium state between protein synthesis, degradation, and recycling. Due to the complicated interconnections within these pathways, the utilization of modern deep learning techniques, particularly graph neural networks (GNN), holds significant potential in accurately representing proteins and their intricate interactions. While the adoption of these networks specifically for wheat proteomic pathways is emerging, there are challenges like ensuring comprehensive training data, versatility, and potential are evident. Yao et al. (2023) have presented a GNN model that effectively incorporates plant electrical signal characteristics to identify proteins associated with electrical signalling. This study effectively showcases the integration of AI models in the context of salt stress. This is particularly noteworthy as salt and drought stress considerably overlap in their proteomic response.

Protein synthesis and protein turnover is an absolute necessity for crops to cope with water-deficit stress. Various proteomic studies indicate that an estimated 16% of drought-responsive proteins are actively involved in balancing protein synthesis and protein turnover. The synthesis of proteins involves several other proteins such as ribosome recycling factor, elongation factor, translation initiation factor, tRNA synthase, and ribosomal proteins, which have been shown to increase during water-deficit conditions and aid with protein synthesis. The involvement of these proteins in protein folding and processing, however, is species and cultivar specific. Protein miss-folding is a common molecular trait of drought-sensitive plants (Kaur and Asthir 2017). This process can be controlled through the active involvement of other proteins, such as protein disulfide-isomerases, ER luminal-binding protein, trigger factor-like protein, most heat shock proteins (HSPs), and other molecular chaperones (i.e., calnexin and endoplasmin) (Wu et al. 2019; Timperio, Egidi, and Zolla 2008; Tichá et al. 2020). The comprehensive characterization of proteins and their propensity for misfolding, particularly those that play a crucial role in drought stress, highlights their importance in comprehending the reaction to drought condition. These proteins, such as ribosome recycling factor, elongation factor, and others, should be central to AI-driven analyses keeping in mind the potential of misfolding. For example, Upadhyaya et al. (2022)

suggest that feature importance methods, such as SHAP (Shapley Additive exPlanations) or Permutation Importance, can be employed in machine learning to prioritize proteins. By doing so, AI models, such as Random Forest or Gradient Boosted models, such Trees, can be effectively aligned with the significance of these proteins. Deep learning models can further refine the analysis by capturing intricate patterns associated with these proteins. This focused approach ensures that predictions or insights gained from such models are based on the most influential features of drought response.

10 | Metabolomics and Drought

The duration and intensity of stress can substantially affect the complexity of the stress response. It is well documented that water-deficit stress compromises turgor pressure, circumventing the plant's needs to accumulate active osmolytes such as sugars (polyols), quaternary ammonium compounds, and certain amino acids usually nontoxic at high cellular concentrations (Hare, Cress, and Van Staden 1998; reviewed by Mukarram et al. 2021). Recently, a significant difference (i.e., 56 metabolites) in the metabolome of drought-tolerant (HX10) and drought-sensitive (YN211) genotypes of wheat was documented during a comparative analysis (Guo et al. 2020), where the authors suggested that such data may be useful in QTL or GWAS studies to identify the locus (loci) or gene(s) associated with such traits for the improvement of the crop. Harnessing the capabilities of AI, particularly deep learning, allows for the extraction of intricate patterns from vast metabolomic datasets which has recently been reviewed by Kisiel et al. (2023). The integration of methods based on deep learning, such as TensorFlow and PyTorch, enables the development of predictive models predicting wheat responses to varying drought scenarios. These models may be trained using metabolic profiles obtained from diverse wheat genotypes exposed to varied drought situations. Researchers can explore the intricate metabolic variations across different wheat genotypes through the use of advanced deep learning methods, including CNNs and RNNs (Sampaio, Rocha, and Dias 2022). CNNs, for example, have the capability to detect distinct metabolic profile patterns that serve as indicators of drought resistance. On the other hand, RNNs can monitor the sequential alterations in metabolite concentrations as drought conditions escalate.

A change in the metabolome of plants under drought stress is often a secondary effect underpinned by changes in turgor pressure during drought stress. Destabilization of turgor pressure result in cellular damage due to the accumulation of reactive oxygen species (ROS) and consequently the activation of programme cell death initiated through an oxidative burst (Kosová et al. 2016; Dumont and Rivoal 2019). The oxidative bust is characterized by a dramatic increase in the production of superoxide radicals (O^{2-}), hydrogen peroxide (H_2O_2), and hydroxyl radicals (^{-}OH), which are all highly reactive and can cause severe impairment of the plant function, affecting protein degradation, DNA fragmentations, and lipid peroxidation, leading to cell death (Cruz De Carvalho 2008). The efficient reduction or elimination of O^{2-} and H_2O_2 in plant cells requires the action of antioxidants that are present in the peroxisome, cytoplasm, mitochondrion, and chloroplast, where superoxide dismutase can change O^{2-} to H_2O_2. Subsequently, peroxidase scavenges the H_2O_2 that was produced by superoxide dismutase, while catalase is central to eliminate H_2O_2 in the mitochondrion and microbody (Shigeoka et al. 2002), thereby overcoming the detrimental effects of oxidative stress.

Oxidative bursts, however, is an integrated part of plant growth and development, and not an exclusive drought stress response. Hence, understanding ROS accumulation under drought stress conditions provides another angle to the elucidation of water-deficit response in wheat since ROS influences the plant's adaptability during anticipated stress. Moreover, ROS can also be useful as a metabolic marker for selecting crops within breeding programs. Currently, the accurate regulation of the abundance of redox metabolism-related proteins has been found in proteomic studies dealing with drought stress, as demonstrated in wheat and barley (Hajheidari et al. 2007; Ford, Cassin, and Bacic 2011; Wendelboe-Nelson and Morris 2012; Faghani et al. 2015; Le Roux et al. 2020, 2021). However, it is evident that the antioxidant enzymes that are expressed during drought stress vary among plant species (Rao and Chaitanya 2016), and the sensitivity of the enzymatic response depends on the intrinsic genetic traits in crops (Chai et al. 2016).

Metabolomics can be a powerful analytical tool to increase our current understanding of the drought stress response in wheat. Ideally, metabolomic data should always be superimposed on other omics generated datasets (such as proteomics, genomics, or transcriptomics) to further substantiate the observed change in the metabolome. AI models can assist in this superimposition by finding patterns and correlations among these datasets, which can be a challenging task for traditional analyses with preset algorithms given the vast amount of data. This would in turn provide information on integrative biochemical networks, aid in classifying metabolic profiles, and predict metabolite behavior during wheat drought response. This is particularly true in understanding how environmental factors, like climate change, impact plant metabolism. Surprisingly, Pomyen et al. (2020), highlighted that despite the potential synergy between metabolomics and AI, the number of deep learning-associated publications in this domain remains fewer compared to other omics disciplines.

11 | Artificial Intelligence and Omics Data

In the era of the fourth industrial revolution, the integration of cutting-edge biotechnology and AI holds great promise for advancing our understanding of the drought stress response in wheat. Leveraging AI technologies, such as the learning-based computational tools and omics technologies, such data, can significantly enhance our knowledge in this area. AI, which includes machine learning and deep learning, provides a range of tools specifically developed to manage the extensive and complex datasets commonly encountered in omics research. One key application of AI in handling these multi-omics datasets is the improved estimation of heritability for complex traits like drought tolerance. Heritability, the proportion of phenotypic variance attributable to genetic factors, can be challenging to estimate using traditional methods due to the complexity of genotype-by-environment (GxE) interactions and nonlinear environmental influences (as reviewed by Zakir 2018; Teressa, Semahegn, and Bejiga 2021). AI tools can overcome these limitations by integrating multi-omics data with high-resolution environmental variables, enabling deeper insights into the genetic architecture of traits (Xu et al. 2022). This allows for more accurate heritability estimates, which are crucial for identifying genetic loci that contribute to drought resilience and ultimately the selection of these lines within breeding programs.

A study on maize (*Zea mays* L.) by Fernandes et al. (2024), evaluated 1179 hybrids across multiple environments to enhance the estimation of heritability, a critical factor in the response to selection. By integrating genetic and environmental data, the researchers aimed to improve the prediction of genotype-by-environment interactions, which directly influence heritability. Machine learning models, including Random Forests, XGBoost, and LightGBM, were applied to capture these interactions. By incorporating environmental covariates alongside genomic information, the models increased predictive accuracy by 7%–11% compared to the traditional Factor Analytic Multiplicative Mixed Model. This finding aligns with a broader trend in crop breeding, where AI models, such as Artificial Neural Networks (Leichtweis et al. 2024), Deep Kernels (Crossa et al. 2022), and CNN (Larue et al. 2024), consistently outperform traditional statistical methods (i.e., BLUP and GBLUP, LASSO and Bayes C). This has been further supported by a comprehensive survey by Jubair and Domaratzki (2023), which highlights the consistent advantages of deep learning-based models by integrating genomic and environmental data and in increasing prediction accuracy for genomic selection across various crops, including maize, wheat, barley and soybean in multi-environment trials, which may leading to improved selection in breeding programs. AI, thus, is not merely software but a tool that generate insights, make predictions, and aid decision-making. This becomes particularly invaluable when probing omics data. While research on AI in the context of drought and cereal crops is limited, several reports exploring the use of AI in conjunction with crop yield predictions (Van Klompenburg et al. 2020), soil salinity (Pereira et al. 2018; Wang, Chen et al. 2021; Wang, Peng et al. 2021), and nutritional value (Ghosh, Koley, and Professor 2014) are available in literature. The application of AI extends beyond data analytics and encompasses various practical agricultural applications. Within the domain of AI-driven machinery, specifically farming tractors which are often equipped with cameras and sensors, they have the capability to not only optimize sowing patterns, but also actively monitor the health of crops. This monitoring process serves to ensure that ideal growth conditions are maintained, and possible risks are promptly identified and addressed in real-time. Moreover, the implementation of AI-powered robots, which possess advanced capabilities in activities, such as fruit harvesting and weed eradication, serves as a tangible demonstration of the effective incorporation of AI within routine agricultural practices.

While AI's value in omics research is undeniable, it can indirectly act as a socioeconomic barrier in certain research environments with challenges that arise primarily from research funding limitations, computational power constraints, and the demand for high-performance computing infrastructure. Furthermore, Kisiel et al. (2023) emphasize some important concerns that need to be taken into account while utilizing AI tools. These include the quality of data, the complexity of learning models, the risk of overfitting, the requirement for both technical and domain experience, and the computing requirements. Therefore, there is a tangible need for initiatives that mitigate these challenges and promote the convergence of biological sciences and AI.

12 | Conclusions

Climate change is progressively worsening, as many countries already suffer from drought conditions. While researchers have produced valuable results in an attempt to understand crop–drought interactions, this is often a slow process partially because the transition of laboratory results to the field remains a challenge. This is entirely reasonable since plant–drought interaction is multidimensional (Figure 2). Therefore, research studies must conceptualize how they define drought, thus synchronizing their results with reproducibility and ensuring accessibility. The response of wheat to drought encompasses various levels of omics. This complexity is further compounded by factors such as the intensity of drought and the developmental stage of the crop. Even though, the notable increase in omics studies, such as phenomics, genomics, transcriptomics, metabolomics, and proteomics, is praiseworthy, the advances they offered today is still limited. In theory, with the availability of big datasets (both qualitative and quantitative in nature) available data should have unlocked our understanding of wheat response to drought but did not due to the lack to fully comprehend the intricacies associated with the stress response in plants. However, AI emerges as a crucial tool in effectively organizing and understanding these extensive and complex datasets (Figure 1).

From the literature, it is evident that there are enormous amounts of information (omics) that require consideration for the efficient design and use of AI. Every wheat line, cultivar, mutant, and transgenic variant carries genomic significance, impacting all subsequent omics levels, and in turn, these plants respond uniquely to each specific drought stress condition. As such, no universal omics response exists for wheat, but this complexity can be harnessed in this arms race to combatting drought stress in wheat. The integration of several omics disciplines into a unified user-friendly platform is a significant challenge, yet its potential impact is revolutionary (Figure 1). However, the development of a comprehensive, multimodal database need to seamlessly integrates with AI, machine learning, and deep learning tools. Such an interface has the potential to generate actionable outcomes, essential for the advancements in precision farming. These outcomes not only empower autonomous decision-making for optimizing yield but may also unlock the elusive identification of drought-specific plasma membrane sensors. With the detection of these sensors, cutting-edge breeding techniques, such as CRISPR can be harnessed to craft wheat variants tailored for specific geographical and meteorological conditions. The incorporation of genetically modified wheat varieties into precision farming systems has the potential to significantly transform crop productivity, leading to enhanced sustainability of food. However, to successfully achieve this objective we need to realize that AI are designed with the intrinsic capability to unravel complicated problems, Therefore, AI should be seen as an essential partner, positioned to provide an in-depth understanding of drought responses in wheat, ultimately unlocking wheat drought tolerance through the synergy of omics data and computational intelligence.

Author Contributions

M.-S.L.R. and A.-M.B. conceptualized the idea. M.-S.L.R. wrote the draft. A.-M.B., K.J.K., and C.A.C. edited the final manuscript.

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Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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