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Optimizing nitrogen application in global wheat production by an integrated Bayesian and machine learning approach

Ziyang Liu, Xiaojun Liu, Yongchao Tian, Yan Zhu, Weixing Cao, Qiang Cao

National Engineering and Technology Center for Information Agriculture, MOE Engineering and Research Center for Smart Agriculture, MARA Key Laboratory for Crop System Analysis and Decision Making, Jiangsu Key Laboratory for Information Agriculture, Collaborative Innovation Centre for Modern Crop Production Co-sponsored by Province and Ministry, Nanjing Agricultural University, Nanjing 210095, China

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Abstract.

Wheat production plays a pivotal role in global food security, with nitrogen fertilizer application serving as a critical factor. The precise application of nitrogen fertilizer is imperative to maximize wheat yield while avoiding environmental degradation and economic losses resulting from excess or inadequate usage. The integration of Bayesian and machine learning methodologies has gained prominence in the realm of agricultural research. Bayesian and machine learning based methods have great promise for crop nitrogen management, we present a novel approach that leverages Bayesian and machine learning techniques to optimize wheat nitrogen application across diverse combinations of varieties, management practices, and environmental conditions in major wheat production regions worldwide. Our dataset comprises 93 research papers on wheat yield response to nitrogen fertilizer, spanning six key geographic regions (Africa, Asia, Europe, North America, Oceania, South America) sourced from the Web of Science (2000 - 2024). The Bayesian framework is employed to define the baseline wheat yield and the response value of wheat yield to nitrogen application in each region, providing insights into the economic optimization of wheat yield and nitrogen application rates. XGBoost is applied to assess the relative importance of G×E×M factors in shaping the wheat yield-nitrogen fertilizer responses across diverse regions. Through this innovative Bayesian-based framework, we derive r understanding of wheat yield and yield-nitrogen response characteristics in different regions of the world, harmonizing them with local wheat cultivation practices. Moreover, our analysis identifies the principal G×E×M factors that exert the most significant influence on nitrogen fertilizer application all over the world, facilitating the formulation of tailored improvement strategies. This research, underpinned by a combination of Bayesian and machine learning techniques, holds the potential to optimize nitrogen fertilizer management in global wheat cultivation systems, offering benefits to agricultural sustainability and productivity.

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Keywords.
wheat, nitrogen management, Bayesian, nitrogen response

Introduction

Wheat is one of the major food crops in the world and has important economic and nutritional value (Shiferaw et al., 2013). Wheat is widely grown on all continents (Reynolds and Borlaug, 2006), and the stability and growth of global wheat production is crucial to ensuring global food security. Currently, the use of synthetic nitrogen fertilizers accounts for approximately 45-50% of current global grain production (Yu et al., 2019). Nitrogen is also important for increasing wheat yields. However, there is a complicated response connection between the amount of nitrogen fertilizer used and wheat yield.

Due to soil acidification and other reasons (Schroder et al., 2011), nitrogen fertilizer rates cannot be raised forever to boost wheat yields. Crop yield increases become insignificant over a particular point in the nitrogen fertilizer rate range, and yields may even start to drop beyond this point (Zhang et al., 2018). During the production of wheat, nitrogen fertilizers are frequently used excessively, which results in nutritional imbalances, ineffective fertilizer usage, and environmental contamination (Chuan et al., 2013). Wheat production in different regions has different requirements for nitrogen fertilizers, which is mainly due to differences in genotype, climate, soil, and management practices (Mueller et al., 2012). These differences have resulted in differences in basic wheat yields in different regions around the world, and have also led to differences in nitrogen fertilizer management practices. Developing areas, such as Africa, show soil nitrogen depletion, industrialized areas, such as the United States and Europe, have higher nitrogen fertilizer use efficiency, and China and India show excessive use of nitrogen fertilizers (Lassaletta et al., 2016; Mueller et al., 2014). Estimating the basic yield of wheat without nitrogen fertilizer in various locations is vital to more effectively regulate nitrogen management of wheat globally. In addition, even with a targeted wheat yield, it is challenging to ascertain how much nitrogen fertilizer farmers really use since crop yield response to nitrogen fertilizer is unpredictable (Lobell, 2007). Exploring the response value of wheat yield to nitrogen fertilizer dosage can help precise nitrogen fertilizer management in different regions around the world. Long-term field experiments (LTE) can quantify nitrogen responses (Sandén et al., 2018; Wei et al., 2016), but these experiments require significant investment and time, and are scarce in Africa and South America (van Grinsven et al., 2022). In addition, the extent to which wheat genotype, environment and management practices influence the response of wheat yield to nitrogen fertilizer is unclear.

The frequentist method, which treats unknown factors of interest as fixed variables and merely considers the data to be random, has been mostly used to study the Nitrogen response. The Bayesian method, on the other hand, views the calculated values and unknown model parameters as random variables (Correndo et al., 2021). The best model parameters may be estimated using a Bayesian framework that takes into account two primary factors: observational data that is readily available and past knowledge about the process of interest (Wakefield, 2013). The Bayesian model is used to define the prior distribution of model parameters through existing literature research results or data, and obtain inferences based on probability distributions (posterior). The use of Bayesian approaches in agricultural research is widespread (Ma et al., 2021; Wang et al., 2021). Large data sets may be used to find complicated correlation patterns using machine learning methods (Horvitz and Mulligan, 2015), which has been widely used in research in the agricultural area (Chlingaryan et al., 2018). Among them, the extreme gradient boosting (XGBoost) approach makes it possible to estimate the relevance of permutation-based features (Chen and Guestrin, 2016), which may be a helpful interpretive tool for determining how much G × E × M parameters impact wheat yield response to nitrogen fertilizer and wheat basal yield.

The main purpose of this study is to estimate the nitrogen-free basal yield of wheat (A) and the response value of wheat yield to nitrogen application (B) in major regions of the world, and to evaluate the importance of the impact of each G×E×M feature on these two values.

Materials and Methods

Data Collection

The data for this study was from peer-reviewed published papers. Use the keywords "wheat" and "nitrogen" to search on the Web of Science, and filter the searched papers according to the following criteria: Research must be conducted under field conditions; Clear experiment location information was provided; Unambiguous wheat yield and nitrogen rate data were provided for each experiment (not average yields); Papers provide information on the type of wheat grown (winter or spring) or provide planting and harvesting times; Papers provides specific management information (whether to irrigate and split nitrogen fertilizer). After retrieval and screening, a total of 93 papers met the criteria, and 2,200 datasets of wheat yield response data to nitrogen fertilizer were compiled from these articles. The experiment sites are classified into six regions: Asia, Europe, Africa, North America, South America, and Oceania (Fig. 1).

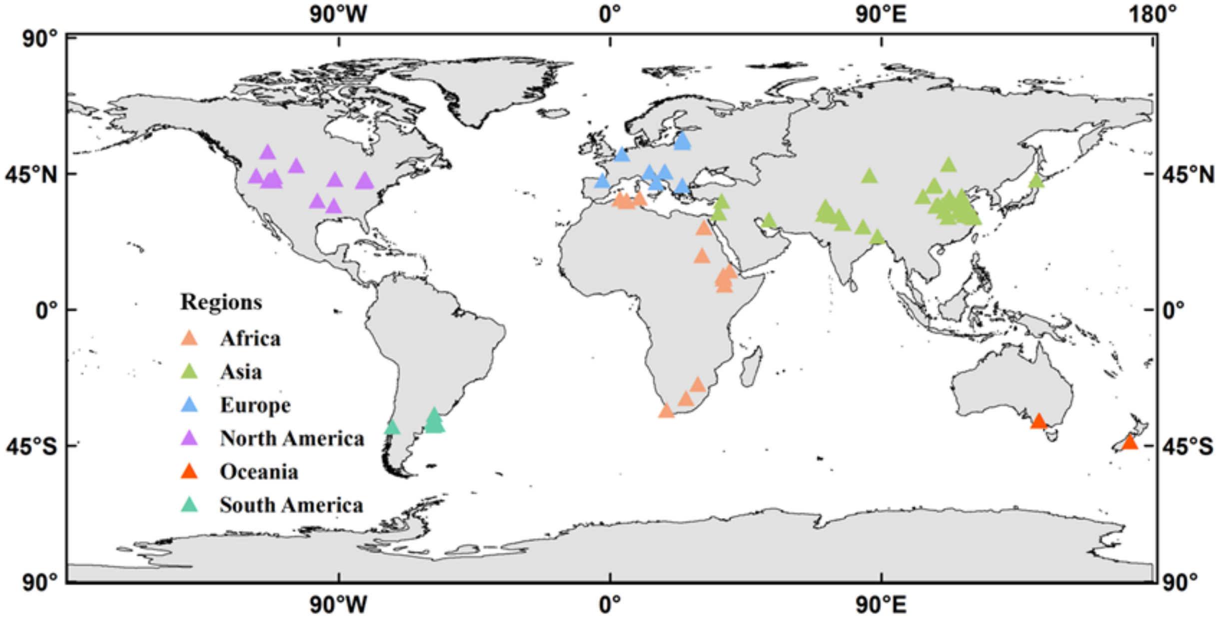

Fig 1. Distribution of data source trials across six global regions.

For each wheat yield and nitrogen fertilizer response data, G × E × M factors were integrated. The G factor is the type of wheat, and the M factor includes whether irrigation and nitrogen fertilizer are applied separately. E factors include soil and climate factors. The soil data comes from Harmonized World Soil Database v2.0 (https://www.fao.org/soils-portal/data-hub/soil-maps-and-databases/harmonized-world-soil-database-v20/en/), which is interpolated using the coordinates of the test site to extract the percentage of sand, silt, clay, soil organic carbon content and soil pH of each test site in the database. Climate attribute classification was performed based on the World Agricultural Climate Resource Data from the Food and Agriculture Organization of the United Nations (FAO) and the International Institute for Applied Systems Analysis (IIASA) Agro-Ecological Zone (AEZ) modeling framework and GAEZ v4 spatial data (https://gaez.fao.org/). This data framework divides climate into three attributes: climate zone, precipitation type, and temperature type. The collected test sites are classified according to the categories under these three attributes. All G×E×M features are shown in Table 1.

Table 1 G × E × M features and their abbreviations used in this study.

Genotype		Environment		Management	
Wheat Type	Winter Wheat	Temperate zone	Tropics (TTr)	Fertilizer Division (FD)	Y/N
	Spring Wheat		Subtropics (TS)	Irrigation (Ir)	Y/N
			Temperate (TT)		
		Precipitation type	Continental (PrC)		
			Highland (PrH)		
			Oceanic (PrO)		
			Lowland (PrL)		
			sub-continental (PrsC)		
			summer rainfall (PrS)		
			winter rainfall (PrW)		
		Thermal type	Cool (ThC)		
			Highland (ThH)		
			Lowland (ThL)		
			Moderately cool/cool (ThmC)		
			Warm/Moderately cool (ThW)		
		Soil composition	Slit (%)		
			Sand (%)		
			Clay (%)		
		Soil organic carbon (%)			
		pH			

Bayesian N response models

The use of Bayesian methods to deal with the response relationship between crop yield and nitrogen has been widely used (Asai et al., 2021; Liang et al., 2022; Ouedraogo and Brorsen, 2018). Used wheat yield as the response variable and N rate as the explanatory variable. It is a common assumption that crop yields have a quadratic-plateau response relationship with nitrogen fertilizer (Correndo et al., 2021; Dhakal and Lange, 2021). Therefore, a quadratic-plateau regression model of wheat yield and nitrogen fertilizer was fitted under a hierarchical Bayesian framework by using the following prior:

$$y_i \sim Gaussian\left(\mu_i, \sigma_i^2\right) \tag{1}$$

$$u_{i-QP} = A + Bx - Cx^2, if\ x_i < AONR, \tag{2}$$

$$A + B \cdot AONR - C \cdot AONR, if\ x_i \geq AONR \tag{3}$$

$$A \sim U(a, b); \tag{4}$$

$$B \sim U(c, d); \tag{5}$$

$$C \sim gamma(1, 10); \tag{6}$$

$$\sigma_i^2 \sim gamma(2,2); \tag{7}$$

For each dataset, y_i represents the yield of the i^{th} N rate, u_i represents the process of the quadratic plateau, σ_i^2 is the variance of the process, and Gaussian, U and gamma represent the priors for normal, uniform and gamma distributions. The prior values of A, B come from a study of the long-term nitrogen response of global cereals (Correndo et al., 2021). The study used experimental data from Asia, Europe, and North America for curve fitting and verified its applicability on a global scale. Different priors were set for six regions around the world. Asia, Europe, and North America used the experimental data in this study to set the prior, and other regions used the crop yield nitrogen fertilizer response curve applicable to the global scale to set the prior (Table 2). The prior values of C and σ_i^2 refer to previous research (Correndo et al., 2021).

Table 1 G × E × M features and their abbreviations used in this study.

Region	Parameter *a*	Parameter *b*	Parameter *c*	Parameter *d*
Asia	0.027	0.087	0	8.90
Europe	0.031	0.091	0	7.58
North America	0.032	0.092	0	6.97
Others	0.029	0.089	0	8.04

From every model, the median (50th percentile) of the posterior distribution is the predicted estimate of the descriptor. The degree of uncertainty associated with every descriptor is contingent upon the duration of the posterior distribution's 95% confidence interval, which spans from 2.5th to 97.5th percentile.

The construction of the Bayesian hierarchical model was carried out using the rstan package of R software. The NUTS algorithm is used for sampling, and the Markov Monte Carlo (MCMC) algorithm is used to generate a series of samples that approximate the posterior probability function of the parameters. Four parallel chains were used, the number of iterations was 30,000, of which 5,000 were burn-in, and a thinning interval was 10. Finally, the model was run to estimate the posterior distribution values of B_0 and B_1 for global six regions.

Importance estimation of different G×E×M features

In order to explore the impact of different G×E×M features on the response process of wheat yield and nitrogen, the XGBoost algorithm was used to evaluate the importance of the G×E ×M characteristics of 55 wheat yield-nitrogen fertilizer response curves in the data set, and explore the impact of each G × E × M feature on target variable B0 and B1. The wheat-nitrogen response curve is fitted using a quadratic function in a form similar to that applied to the global cereal-nitrogen response curve (van Grinsven et al., 2022). Since XGBoost can only handle numerical variables, one-hot encoding is used for conversion of categorical variables such as wheat type, climate attributes and management methods. For the XGBoost model, the 10-fold cross-validation method was used to perform cross-validation and extract the importance of features.

Sandy soil usually has larger particle size and lower viscosity, better drainage performance, and stronger water permeability. This helps remove excess moisture from the soil and avoids the negative effects of waterlogging on wheat.

Results and Discussion

Estimation of basic wheat yield

Bayesian hierarchical model estimates (median) show that the basic yield of wheat in the six major global regions without nitrogen fertilizer is 1.81-4.38 Mg ha^{-1} (Fig. 2). Wheat base yields are lower in Africa (1.81 Mg ha^{-1}) and Oceania (2.36 Mg ha^{-1}), while higher in Europe (3.89 Mg ha^{-1}) and South America (4.38 Mg ha^{-1}). Basic yield in Asia (3.00 Mg ha^{-1}) and North America (3.01 Mg ha^{-1}) is moderate.

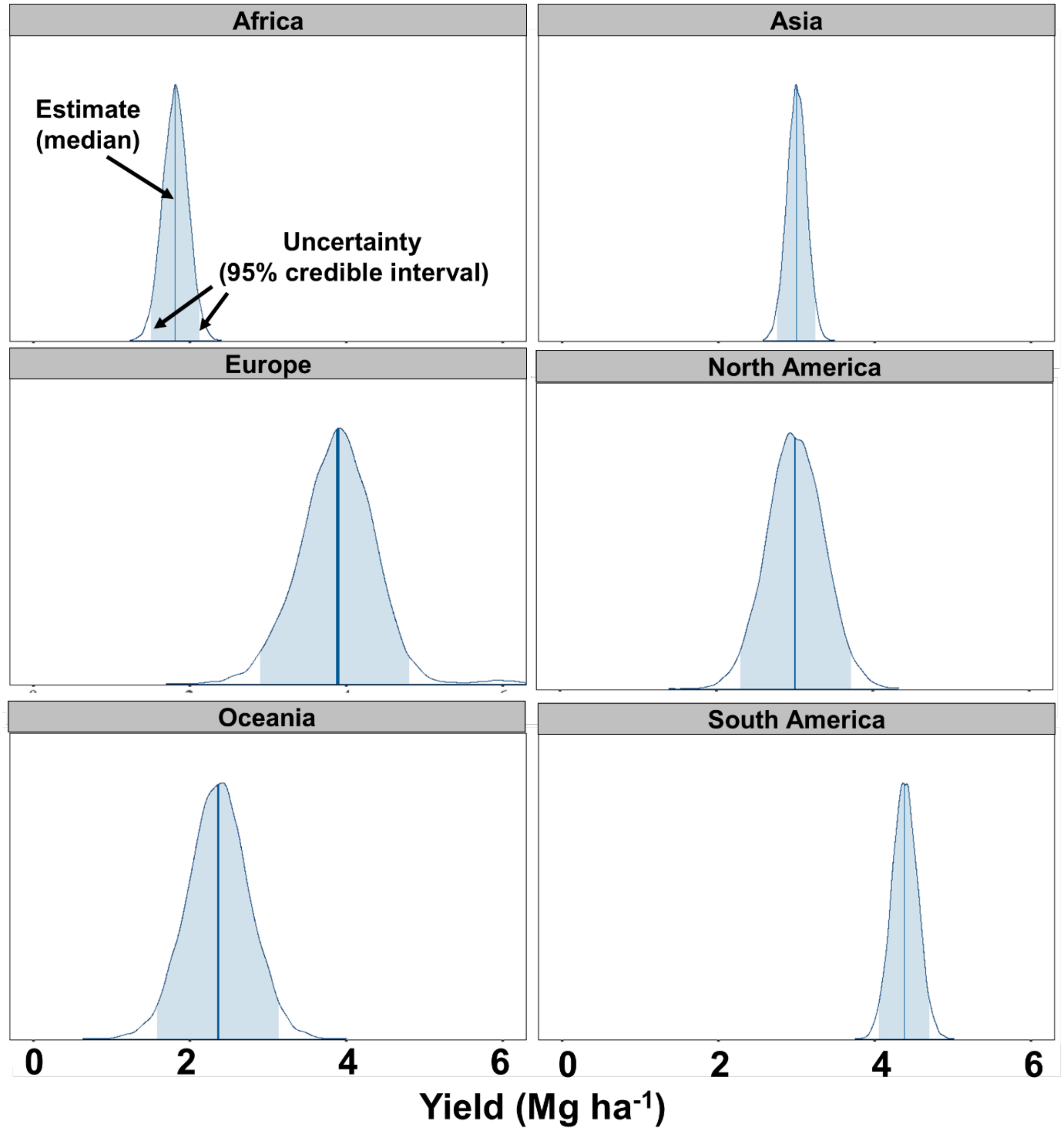

Fig 2. Basic wheat yield (yield without nitrogen application) estimates and uncertainties for six global regions based on posterior values of Bayesian hierarchical models.

Differences in basic wheat yields in different regions may be related to historical wheat cultivation and management practices. Historically, crop cultivation in Africa lacked sufficient nitrogen fertilizer inputs, while crop cultivation in Europe historically had sufficient nitrogen fertilizer inputs, which resulted in differences in soil fertility in different regions (van Grinsven et al., 2022), so the basic yield without the application of nitrogen fertilizers big different. In addition, climate differences in different regions are also an important reason for differences in basic wheat yields. High temperatures and intense sunshine in Africa may cause wheat yield losses(Lobell and Field, 2007).

Estimates of wheat yield response to nitrogen

Bayesian hierarchical model estimates (median) show that wheat yield responses to nitrogen in six major global regions range from 0.015 to 0.035 Mg kg^{-1}N (Fig. 3). The response value in North America is higher (0.035), while the response values in other regions range from 0.015 to 0.025 Mg kg^{-1}N. South America has the lowest response value at 0.015 Mg kg^{-1}N, but is not much different from the response values in Asia (0.019 Mg kg^{-1}N) and Africa (0.017 Mg kg^{-1}N).

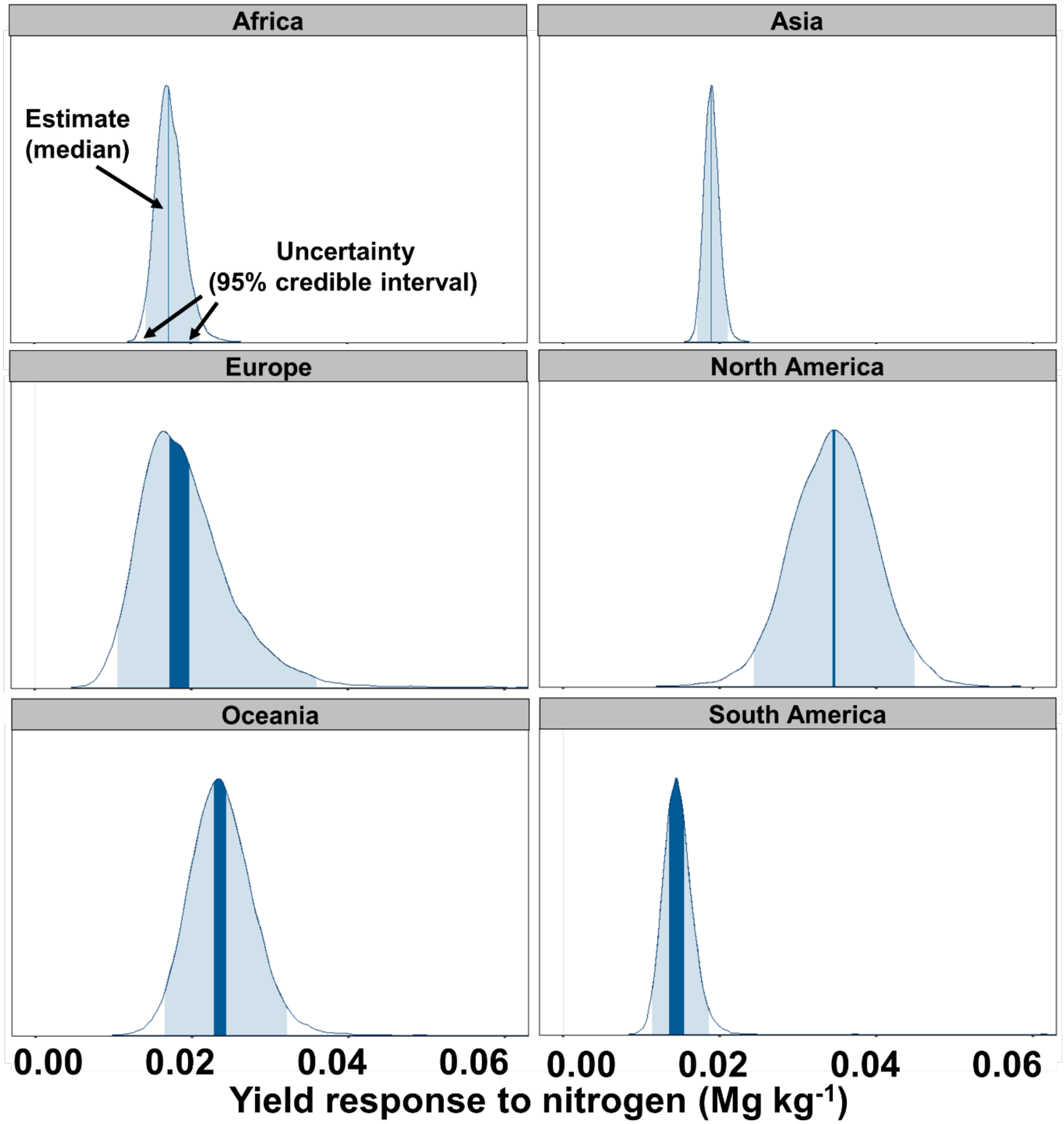

Fig 3. Estimates and uncertainties of wheat yield response to nitrogen in six global regions based on posterior values of Bayesian hierarchical models.

Factors such as soil texture and fertility, climatic conditions, crop varieties, and agricultural management levels will all affect the response of crop yields to nitrogen fertilizer (Majrashi et al., 2022). The higher response value of crops to nitrogen fertilizer in North America may be due to the combined effect of high-quality soil and climate conditions, and high-quality crop varieties (Swaney et al., 2018).

The results show that the estimation (median) of the response value of wheat yield to nitrogen in Europe, Oceania, and South America based on the Bayesian hierarchical model has a large error. This may be due to the small number of data available for these three regions, with 179 datasets for Europe, 68 datasets for Oceania, and 172 datasets for South America. Compared with Asia, which has 1,031 sets of data, Africa's 324 datasets, and North America's 426 datasets, the amount of data is much larger than the three regions with large estimation errors. It may be necessary to collect more data for these three regions in subsequent studies to improve the accuracy of the model estimates. In terms of precise nitrogen fertilizer management, farmers in different regions can optimize the amount of nitrogen fertilizer application through estimates of wheat yield response to nitrogen and target yields.

The importance of each G×E×M feature

The Xgboost method was used to explore the importance of the three G×E×M factors in the basic yield of wheat and the response value of wheat yield to nitrogen fertilizer (Fig. 4). G×E×M factors are of similar importance in influencing basic wheat yield and yield response to nitrogen fertilizer. The importance of environmental factors in both is about 90%, G and M factors together account for about 10%, and M factor is more important than G factor. The importance of each G × E × M feature is also shown in the bar chart (Fig. 4). The results show that soil type is the most important characteristic type, and sandy soil is the most important characteristic that affects the basic yield of wheat and the response value of yield to nitrogen fertilizer. In addition, the characteristics of silt, clay, and soil organic carbon content are also of great importance. In terms of climate, the subcontinental precipitation pattern is the most important feature affecting the basic yield of wheat, while the oceanic precipitation pattern is the most important feature affecting the response value of wheat yield to nitrogen. In addition, the temperate zone is also an important characteristic that affects the basic yield of wheat. Genotype and management factors are relatively less important.

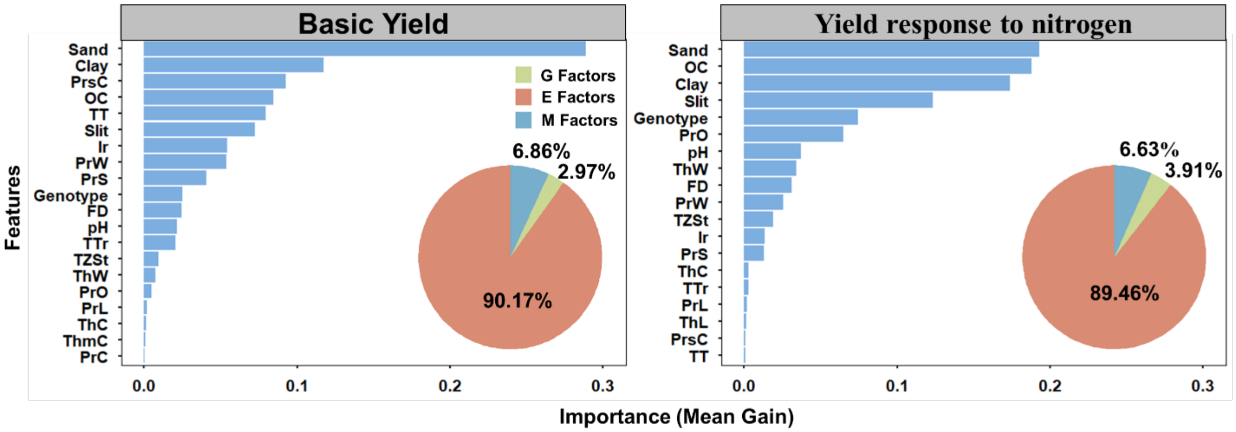

Fig 4. The importance of each G × E × M feature to wheat basic yield and yield to nitrogen response value (mean Gain value) evaluated based on the XGBoost method, and the importance proportion of G × E × M is shown.

Sandy soil usually has larger particle size and lower viscosity, better drainage performance, and stronger water permeability (Detar, 2008). This helps remove excess moisture from the soil and avoids the negative effects of waterlogging on wheat. However, sandy soil usually has low fertility and poor water-holding capacity, which can easily lead to the loss of water and nutrients (Aimanský et al., 2019). These characteristics of sandy soil may make it the most important G × E × M factor affecting the basic yield of wheat and the response value of wheat yield to nitrogen fertilizer. Clay soils have poor drainage, but generally have high fertility (Melero et al., 2007); silt soils have moderate drainage and water retention and fertility (Sasal et al., 2006). Therefore, these two soil types also have a high level of importance. Soil organic carbon content is of high importance because it is an important indicator of soil fertility.

The impact of sub-continental precipitation on wheat production varies by region and specific climatic conditions. In some areas, adequate winter precipitation may help wheat growth, but summer moisture may lead to an increase in pests and diseases. In other areas, winter dryness may be a limiting factor for wheat growth. The wet winter characteristics of oceanic precipitation help provide sufficient moisture for wheat, but it also increases the risk of pests and diseases. In addition, oceanic precipitation keeps the soil moist, which may affect soil aeration and root development. From the perspective of climate zone, temperate areas have sufficient sunshine and suitable temperatures, which are the most suitable climate areas for wheat growth (Asseng et al., 2015).

Genetic and management factors are relatively less important than environmental factors in this study. The basic yield of wheat is influenced by irrigation, and the kind of wheat affects the value of wheat yield response to nitrogen. One reason is that the data collected from the literature have few genetic and management factors, only a total of three traits, and many other traits that affect wheat basic yield and nitrogen utilization were not included in the study. Such as wheat plant characteristics, grain protein content (Liu et al., 2023), type of nitrogen fertilizer used (Ghafoor et al., 2021), etc. Follow-up studies require more dimensions of data to further improve the model to explore the importance of more genes and management characteristics.

Conclusion

This study investigated the estimation of basic wheat yield and the wheat yield response to nitrogen fertilizer across six major global regions through Bayesian Hierarchical Model. The results revealed significant regional variations in both basic yield and nitrogen response, historical wheat cultivation practices and nitrogen fertilizer inputs were identified as key factors contributing to these regional differences. Additionally, climate variations, such as high temperatures in Africa, also played a role in shaping yield discrepancies.

The study explored the importance of G×E×M factors in influencing wheat production. Environmental factors, particularly soil type and precipitation patterns, emerged as dominant determinants of wheat basic yield and wheat yield response to nitrogen. Sandy soil was identified as the most influential factor affecting both basic yield and nitrogen response, likely due to its drainage performance and water permeability.

In conclusion, this study can contribute to the understanding of wheat yield and yield-nitrogen response characteristics in different regions of the world and explore the complex interactions between genotype factors, environmental factors and management practices, and wheat production. By understanding and addressing these factors, policymakers, farmers, and researchers can work towards improving wheat yields and ensuring food security in diverse agricultural contexts worldwide.

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