Nitrogen economy in corn-soybean farming systems

by

Adrian Alejandro Correndo

B.S., Universidad de Buenos Aires, 2011
M.S., Universidad de Buenos Aires, 2018

AN ABSTRACT OF A DISSERTATION

submitted in partial fulfillment of the requirements for the degree

DOCTOR OF PHILOSOPHY

Department of Agronomy
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Manhattan, Kansas

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Abstract

Nitrogen (N) is the most limiting nutrient for producing maize (*Zea mays* L.) and soybean [*Glycine max* (L.) Merr.] crops. The complex system governing the soil-plant N dynamics requires exploring multiple perspectives. Concomitantly, there is a marked need to deploy data-driven models that account for uncertainty in the processes of interest to provide improved N recommendations in both crops. Therefore, the objectives of this dissertation were: (i) to assess the contribution of environmental and crop management factors on the prediction of inherent maize productivity without N fertilizer; (ii) to identify the main drivers of both, expected values and uncertainties, of key components describing the process models for the maize yield response to N fertilizer; (iii) to summarize the impact of N and water management practices in maize grain quality; (iv) to study the residual effects of N management in maize on the following soybean crop; and, (v) to evaluate statistical techniques for the assessment of agreement between predictions and observations.

In a joint effort between different academic and industry institutions in the US and Canada, a database with more than 1,200 maize N fertilization experiments (1999-2019) was built. Crop management factors such as previous crop and irrigation in combination with soil organic matter contributed to explain half of the variability of maize yield without N fertilization, while including spring weather variables (March-May) resulted in a similar performance than a framework including weather during the entire season. Crop management factors largely affected the prediction of the expected yield without N fertilizer, but just slightly impacted (<5%) the uncertainty of the response (and their components) of yield to N fertilizer. Conversely, weather variables were, undeniably, the most relevant factors and roughly contributing to 80% of the explained variance to predict the uncertainties on the yield response to N. On the other hand, a

meta-analysis using a database of 92 site-years revealed that N fertilization not only increases yields but also shows a positive impact on the grain protein concentration, however, both starch and oil remained relatively constant under contrasting N fertilization levels. In contrast, water stress resulted in an erratic effect on all the evaluated grain quality components, possibly due to changes in the moment, severity, and extent of the stress. Evaluating two case studies under a maize-soybean rotation in Kansas, we documented that N fixation and soybean yields were marginally or not affected by the N management in the previous crop. Lastly, a novel and simple methodology on the use of linear regression to assess the prediction ability of simulation models is presented, also suggesting a derived decomposition of the prediction error into lack of accuracy and lack of precision along with the R-code to assist potential users.

Forthcoming projects on N economy in maize and soybean farming systems should expand, provide incentives, and discuss standards in collaborative research, which represented a foundational component of this project. This dissertation highlights the advantages of deploying cutting-edge data analysis techniques for addressing research gaps on the N economy in maize-soybean farming systems. Machine learning, meta-analysis, and Bayesian statistics bring new horizons for improving forecast models as well as their interpretability. Future generations of predictive models in agriculture must be able to capture complex interactions as well as to emulate how farmers deal with uncertainties in the real world. Under this context, the awareness about uncertainties and their drivers should become one of the pillars of the dynamic N recommendations, which is crucial to convey wise information to stakeholders. Undoubtedly, we must move from static to dynamic crop models in order to design optimized GxM adaptation strategies under future climates.

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hand, a meta-analysis using a database of 92 site-years revealed that N fertilization not only increases yields but also shows a positive impact on the grain protein concentration, however, both starch and oil remained relatively constant under contrasting N fertilization levels. In contrast, water stress resulted in an erratic effect on all the evaluated grain quality components, possibly due to changes in the moment, severity, and extent of the stress. Evaluating two case studies under a maize-soybean rotation in Kansas, we documented that N fixation and soybean yields were marginally or not affected by the N management in the previous crop. Lastly, a novel and simple methodology on the use of linear regression to assess the prediction ability of simulation models is presented, also suggesting a derived decomposition of the prediction error into lack of accuracy and lack of precision along with the R-code to assist potential users.

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Dedication

To my daughter *Amelie* and my wife *Milagros*, who give me my sense of purpose every day. To my parents, *Margarita* and *Pedro*, and my sister, *Yanina*, who gave me their all and provided me with the best family I could have ever asked for.

A mi hija *Amelie* y mi esposa *Milagros*, quienes me dan mi sentido de propósito cada día. A mis padres, *Margarita* y *Pedro*, y mi hermana Yanina, quienes me lo dieron todo y me brindaron la mejor familia que podría haber pedido.

Chapter 1: General Introduction

Nitrogen (N) is the most limiting nutrient for crop production worldwide and probably the most complex nutrient to study due to the set of spatio-temporal interactions governing plant growth dynamics, soil processes cycling, and environmental effects on the plant-soil system (Mesbah et al., 2017; Lemaire and Ciampitti, 2020; Briat et al., 2020). Therefore, characterizing the degree to which the N supply fails to meet crop N demand results imperative to the development of more efficient and environmentally sound N management guidelines. In North America, maize (*Zea mays* L.) - soybean [*Glycine max* (L.) Merr.] rotation is among the most common cropping sequences (Gaudin et al., 2015; Vanhie et al., 2015). For both crops, improving the prediction ability of N economy components and identifying their sources of uncertainty should be of a high priority for current and future research efforts.

Deploying modern yield forecast tools

In spite of decades of research, addressing the uncertainty on the crop growth and N demand in maize is still a major concern due to the collateral impacts of misuse of fertilizer and low N use efficiency (Morris et al., 2018; Sela et al., 2018). Refining the management of a complex system such as the one governing soil-plant N dynamics requires understanding the processes generating the yield response to N using multiple perspectives. In parallel, there is a clear need to develop data-driven predictive algorithms that account for uncertainty in the processes of interest, underpinning the maize yield response to N to provide new fertilization guidelines. By using state-of-the-art statistical and machine learning models, this project aimed to tackle the development of unprecedented maize yield forecast models with yield response to N and its uncertainty components at the center of the attention. In a joint effort between fourteen researchers pertaining to ten different academic and industry institutions in the US and Canada, a database with more than 1,200 maize experiments (1999-2019) was built. Thus, in chapters 2 and 3, we made use of these massive experimental database to develop yield and N responsiveness forecast models while assessing the role of crop management, soil, and weather variables.

Maize yield response to N

A first key component of yield responsiveness to N fertilization, is the inherent maize productivity without N fertilizer. The N responsiveness depends on both the yield under non-limiting N supply as well as on the inherent productivity under zero N fertilizer, herein expressed as Y0. Developing predictive frameworks while disentangling the driving factors of Y0 will enhance the optimization of N fertilization in maize. Using a conditional random forest algorithm, in Chapter 2, we assess the predictability of Y0 while identifying the most determinant factors related to crop management, soil and weather.

As an appropriate summary of the N responsiveness process, the response to N fertilizer rates in maize is normally described using regression models (Kyveryga et al., 2007). Nevertheless, the degree of uncertainty on the parameters (e.g. intercept, slope, curvature) and derived quantities (e.g. optimum rate, maximum yield, fertilizer N efficiency) describing these models is extensively overlooked in the scientific literature (Hernandez et al., 2007). For this review, using a refined database of 779 studies, a hierarchical Bayesian framework was applied in combination with extreme gradient boosting algorithm (machine learning) to study the influence of soil, weather, and crop management factors on both the value and the magnitude of uncertainty on the parameters and quantities describing the N responsiveness process in maize.

Maize grain quality response to N and water management

Concomitantly pursuing superior maize productivity with grain quality is essential for food security (Motukuri, 2019). In parallel with the impact of N nutrition, water stress is one of the major limiting abiotic factors related to climate change, adversely impacting the yield and quality of many field crops (Butts-Wilmsmeyer et al., 2019). Even tough maize grain quality have received more emphasis in recent years, yet the published data have not been synthesized to better understand generalized effects across all the studies. For this purpose, meta-analysis is a method that can help with integrating knowledge and results from diverse studies and evaluate the impact of treatment on sets of target variables and provides quantitative estimates of effect sizes (Borenstein et al., 2009). Consequently, in Chapter 4, we aimed to evaluate the effects of water and N fertilization on the following three main components of maize grains: protein, starch, and oil concentrations.

Footprints of maize N management on the following soybean

Historically, literature have concentrated most of the attention to the concept of N credits from the preceding soybean to maize crops (Bundy, 2008; Morris et al., 2018). However, the consequences of the N management for maize on the following soybean crop have received less attention. The N fertilizer management in the preceding maize crop could affect multiple process directly or indirectly impacting soybean N nutrition, and eventually seed yields. Besides the contribution to plant N demand from soil N supply, soybean establishes a symbiosis with Bradyrhizobium spp. that may contribute, in average, with 50-60% of N requirements (Salvagiotti et al., 2008; Di Ciocco et al., 2011), via the symbiotic N fixation (SNF) process. Nonetheless, there is a well-documented antagonism between the soil N supply and N derived from SNF process (Allos and Bartholomew, 1955; Sinclair and De Wit, 1975). Thus, soil N changes induced by different N management in the preceding maize may affect how the soybean crop satisfies its N requirements. In Chapter 5, we used two cases studies in Kansas to assess the residual effects of maize N fertilization management on the seed yields, and the seasonal contribution of SNF and soil N supply to the N nutrition in the following soybean crop.

A novel and simple approach to evaluate models' performance

Lastly, assessing the quality of predictions is a crucial step in models' evaluation (Wallach and Makowski, 2019), either using machine learning or other prediction frameworks. However, the use and interpretation of statistical models and error metrics to evaluate performance are still controversial in the literature. A myriad of scoring rules and statistical criteria have been developed for model evaluation (Gupta et al., 2009; Moriasi et al., 2007; Willmott et al., 2012). Before this overwhelming world of model evaluation criteria, modelers and users might feel submerged under "The Paradox of Choice", and then simply choose the most popular metric (e.g. linear regression, R2). In the agricultural research and related disciplines, using a scatter plot and a regression line to visually and quantitatively assess agreement between model predictions and observed values is an extensively adopted approach (Piñeiro et al., 2008), even more within the simulation modeling community (Yang et al., 2014). Thus, in Chapter 6, a novel and simple perspective about the use of linear regression to assess the prediction ability of simulation models is offered. Concomitantly, we suggest a simple decomposition of the prediction error into lack of accuracy and lack of precision. In order to assist potential users, an open-access code tutorial to compute the proposed assessment of agreement using R-software is presented.

General Objectives

Therefore, the following five chapters of the present dissertation are aligned with the following five general objectives:

1) to assess the contribution of soil, weather, and crop management factors on the prediction of inherent maize productivity without N;

2) to identify the main drivers of both, expected values and uncertainties, of key components describing the process models for the maize yield response to N fertilizer;

3) to summarize the impact of water and N management practices in maize grain quality;

4) to study the residual effects of N management in maize on the following soybean crop; and,

5) to evaluate statistical techniques for the assessment of agreement between predictions and observations.

Chapter 2: Assessing the uncertainty of maize yield without nitrogen fertilization

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Abstract

Maize (*Zea mays* L.) yield responsiveness to nitrogen (N) fertilization depends on the yield under non-limiting N supply as well as on the inherent productivity under zero N fertilizer (Y0). Understanding the driving factors and developing predictive algorithms for Y0 will enhance the optimization of N fertilization in maize. Using a random forest algorithm, we analyzed data from 679 maize N fertilization studies (1031 Y0 observations) conducted between 1999–2019 in the United States and Canada. Predictability of Y0 was assessed while identifying determinant factors such as soil, crop management, and weather. The inclusion of weather variables as predictors improved the model efficiency (ME) from 51 up to 64 %, and reduced the root mean square error (RMSE) from 2.5 to 2.0 Mg ha^{-1}, 34 to 27 % in relative terms (RRMSE). The most relevant predictors of Y0 were previous crop, irrigation, and soil organic matter (SOM), while the most influential weather data was linked to the radiation per unit of thermal time (Q quotient) around flowering and spring precipitations. The crop rotation effect resulted in Alfalfa (Medicago sativa L.) as the previous crop with the highest Y0 level (IQR = 11.5–15.0 Mg ha^{-1}) as compared to annual legumes (IQR = 5.6–10.0 Mg ha^{-1}) and other previous crops (IQR = 3.6–7.8 Mg ha^{-1}). The Q quotient around flowering positively affected Y0, while spring precipitations and extreme temperature events during grain filling showed a negative association to Y0. Overall, these results reinforce the concept that yields are controlled not only by soil N

supply but also by factors modifying plant demand and ability to capture N. Lastly, we foresee a promising future for the use of machine learning to address both prediction and interpretation of maize yield to obtain more reliable N guidelines.

2.1. Introduction

Decades of research on yield response to N application has not yet produced accurate algorithms to issue N recommendations for maize in North America. Addressing the uncertainty on N needs for maize (*Zea mays* L.) is still a major concern (Morris et al., 2018; Raun et al., 2019) because of the unintentional impacts of misuse of N and low N use efficiency (Sela et al., 2018a, 2018b). Estimations of N recovery efficiency in the region are typically below 50 % of the applied N, which may reflect a higher uptake efficiency from indigenous sources (soil) than for applied fertilizer (Cassman et al., 2002). This scenario is linked to the complex process of fertilizer N losses such as leaching, denitrification, and volatilization (Baker and Johnson, 1981; Francis et al., 1993; Bowles et al., 2018). Despite genetic improvement for N use efficiency (Mueller et al., 2019) there are further opportunities to develop prescription algorithms to improve N management and fertilizer recommendations.

For most of the twentieth century, N recommendations in North America have been mostly based on estimation of yield and production goals (Stanford et al., 1966; 1973), that is the N demand dictated the amount of N to be added as fertilizer after the estimation of a simplified N balance that considered N credits and other subtractions and additions (Morris et al., 2018). Refined N guidelines for maize has been addressed following different systems over time and across states (Heady and Pesek, 1954; Bundy and Andraski, 1995; Scharf et al., 2005; Kyveryga et al., 2007; Kitchen et al., 2010; Setiyono et al., 2011; Wortmann et al., 2011; Yost et al., 2014; Sindelair et al., 2015). Lory and Scharf (2003) have described an approach using delta yield, as the yield difference between non-N-limited and non-N-fertilized plots (Y0), assuming the latter as a proxy of indigenous soil N supply (Cassman et al., 1996). More recently, utilizing a large database of N response trials, the "maximum return to N (MRTN) recommendation system represented an approach to adjust estimations of the economic optimum N rate (EONR) grouping response functions according to several factors of interest including management and soil features (Sawyer et al., 2006). Likewise, the integration of multiple site-years expanding combinations of soil, crop management and weather scenarios, might lead to the use of complementary predictive models (e.g., supervised learning techniques) with more focus on forecasting the N needs for maize crop rather than an ex-post analysis.

The dissection of the yield response to N can inform decisions to manage a complex system such as the one governing the soil-plant N dynamics. For a given site-year, we may depict the Y0 as the intercept of the function that along with non-N-limited yield (plateau) defines a yield response to N fertilization for a given curvature. Thus, defining realistic expectations for EORN predictions will inevitably rely on accurate predictions of Y0. Recent attempts to address the problem of forecasting yield response to N have been pursued with limited datasets that restrict our inference space (Puntel et al., 2019) or used yield simulations that restrict the inference to the set of parameters and model assumptions (Shahhosseini et al., 2019; Archontoulis et al., 2020). Yield under non-N-limiting scenario is largely determined by temperature and solar radiation (van Ittersum et al., 2013) and it is adequately captured within dynamic crop growth model frameworks (Monteith, 1972; Messina et al., 2009). In contrast, soil processes governing N cycling and its interactions with the plant and environment system are complex and less well represented in models. Predicting N deficiency level and Y0 poses a much difficult problem to solve than non-N-limited yield (Puntel et al., 2018; Archontoulis et al., 2020), in particular for experiments conducted in small plots (Tao et al., 2018). The combination of mechanistic models for predicting non-N-limited yield and data-driven machine learning models for predicting Y0 could open up opportunities to increase the predictability of complex systems (Messina et al., 2020).

Methodologically, science is entering an entirely new phase that involves data-intensive practices (Tolle et al., 2011). Machine learning is one method, laying at the intersection of computer science and statistics (Jordan and Mitchell, 2015) useful to identify repeatable patterns in large datasets. Belonging to the family of supervised learning techniques, tree-based methods such as decision trees, boosting and random forest (RF) are robust and versatile techniques as demonstrated in remote sensing applications (Belgiu and Drãgut, 2016; Schwalbert et al., 2018) and more recently in agriculture (Khaki and Wang, 2019; Ramanantenasoa et al., 2019). For forecasting purposes, a minimum set of candidate predictors including as early as possible metadata during the crop growing season is desirable. Since most substantial uncertainties are inherent to weather, with very limited predictability beyond 10−15 days (Stern and Davidson, 2015; Zhang et al., 2019), then those variables are the main candidates to perform a sensitivity analysis. A model with no-weather, assuming it as completely unknown and stochastic, may serve as a reference prediction framework to later assess the value of adding weather information. On the other hand, spring weather is likely to be known by the time of planting and including weather predictors may be useful in forecasting applications for N availability in production fields (Puntel et al., 2016). Lastly, defined seasonal weather patterns could serve as model limits.

The main goal of this work is to describe properties of Y0 on a large database of maize fertilization studies performed in the United States and Canada, an develop a prediction model with potential to improve N management systems. The specific goals for this manuscript are to i) rank and identify the main soil, management and weather features impacting Y0, and ii) assess the prediction performance of different frameworks involving soil and management factors but varying the inclusion of weather features: a) no weather variables; b) spring weather known around planting; and c) weather known for the entire crop growing season.

2.2. Material and methods

2.2.1. Data collection

A database was built through meeting certain requirements as follows: i) experiments performed during the last two decades (1999–2019) in order to reduce the noise related to different hybrids eras (Woli et al., 2016); ii) only replicated field trials having N treatments either on small plots or strip-plots; iii) absolute yield data reported for the zero-N control treatment; iv) top-soil analysis results and/or soil series reported; v) data of previous crop and tillage system; vi) latitude and longitude coordinates, or nearest town reported in order to retrieve weather and missing soil data; vii) starter-N and manure treatments were excluded to minimize confounding effects; and viii) general crop management (e.g., planting date, row spacing, other nutrients, weed and pest management) was assumed to have been set to maximize yield under each site-specific condition. Published manuscripts were the first source of data through an engine-search in Web of Science® filtering by the following keywords: “corn/maize” and “nitrogen fertilizer” or “nitrogen fertilization” and “United States” and/or “Canada”. In order to reduce publication bias effect (Dickersin and Min, 1993), unpublished data (e.g., dissertations, field reports, unpublished experiments) were also included in the database as long as they met the established criteria. After filtering and selection processes, 679 site-years resulting in 1031 treatments of maize without N fertilizer were gathered from 59 different data sources, including published and unpublished studies (Supplementary Table 1).

2.2.2. Data analysis

2.2.2.1. Response and explanatory variables

Yield that resulted from treatments receiving zero-N application (Y0, Mg ha^{-1}) was used as the response variable in the analysis. Grain yield was standardized at a water content of 155 g kg^{-1}. Average values (3–5 replications) were considered as an unbiased central tendency-values of Y0.

A set of weather, soil, and crop management variables were considered as explanatory variables, predictors or features. Soil related variables were topsoil (0−15 cm) soil organic matter (SOM, %) and soil texture (clay, silt and sand, %). Soil data were collected from original sources, accessed from authors' records when not reported in manuscripts, or retrieved from gridded POLARIS soil data engine (Chaney et al., 2016), a raster optimization based on SSURGO data with a spatial resolution of 1 km^2. When SOM data were reported at 0–20 or 0−30 cm, values were standardized to 0−15 cm using stratification factors based on data from previous research on grain crops trials (Al-Kaisi et al., 2005; Varvel and Wilhelm, 2011; Franzluebbers, 2010; Villamil et al., 2015).

Daily weather data were accessed via the Google Earth Engine platform (Gorelick et al., 2017) using reported latitude-longitude coordinates of the trials or nearest town. With a spatial resolution of 1 km^2, precipitation (PP), temperature (T, ºC, maximum and minimum) and vapor pressure deficit (vpd, kPa) were obtained from the Parameter-elevation Regressions on Independent Slopes Model -PRISM- (Daly et al., 2015); while incident shortwave solar radiation during daylight period –Rad, MJ m^{-2}- plus day-length were retrieved from Daymet (Thornton et al., 2018). Weather data were transformed into bi-monthly basis (as sum or average) following Carter et al. (2018a). We divided the weather data into three main periods: i) April-May (AM) as proxy of the early-growth period; ii) June-July (JJ) as proxy of the flowering period; and iii) and August-September (AS) as a proxy of grain filling period. In addition, we also considered PP and mean temperature of March as spring weather with the intent to represent typical weather data accessible to farmers when planting and N fertilizer decisions are made.

A series of additional weather variables were calculated in order to capture environmental differences that might not be captured by analyzing standard weather information. For example, the Shannon Diversity Index (SDI) as described by Tremblay et al. (2012) was included to describe the distribution of PP during each period. Extreme PP events were included as the number of days with precipitations greater than 25 mm as a proxy of excessive rainfall events (Puntel et al., 2019). Crop development was described by crop heat units (CHU; Tremblay et al., 2012). Extreme temperature events (ETE, defined as the number of days with mean maximum temperature over 30 °C) were also included as a proxy of heat stress risk (Butler and Huybers, 2013; Ye et al., 2017). The photo-thermal quotient (Q) was calculated as the ratio between cumulative Rad and CHU, as an indicator of the solar radiation available to the crop per unit of thermal time during each period, related to yield potential (Bannayan et al., 2018).

2.2.2. Prediction models

Three prediction models were tested with models differing in the weather features included:

i. a “No-weather” model includes only management and soil features;

ii. a “Spring-weather” model includes precipitations and mean temperature during March and April-May as proxy of pre-plant and early vegetative periods; and

iii. a "Full-weather" model includes all features from April 1st through September 30th (Table 1). This model is descriptive and enables assessing the relevance of seasonal weather and interactions with soil properties and management on Y0.

2.2.2.3. Machine learning algorithm

A tree-based algorithm was selected over other learning alternatives because as a non-parametric tool, it allows constructing prediction rules based on the simultaneous use of categorical and continuous predictors without making prior assumption on normality or on the form of associations with the response variable (Probst et al., 2019). While a single regression tree might be easier to interpret, its prediction power is normally low (and easy to overfit), so it is considered a "weak learner". As an ensemble of trees, the RF is considered as a "strong learner" being much more capable in terms of prediction power (Breiman, 2001). Random Forest is primarily used here for two purposes: i) as a prediction tool, and ii) to assess the relevance of features on prediction.

Among the RF alternatives, we used conditional inference trees to build the ensembles (forests) using the party package (Hothorn et al., 2006) for R software (R Core Team, 2021). The function cforest() from party implements safeguards at the tree level to ensure the feature selection is not biased towards continuous predictors and/or those with many possible splits (Strobl et al., 2009; Probst et al., 2019), which is not available in randomForest() and ranger() functions. The permutation variable importance measure (Breiman, 2001; Strobl et al., 2007) has been demonstrated to reduce bias as compared with other alternatives (Strobl et al., 2007; Boulesteix et al., 2012). Moreover, since our dataset includes correlated features (Supplementary Figures 2 and 3), we evaluated the variable importance with a "conditional" permutation test to minimize the overestimation on importance scores of correlated features (Strobl et al., 2008; Probst et al., 2019).

2.2.2.4. Cross-validation scheme

For each prediction model, a nested cross-validation (CV) scheme was applied to avoid over-fitting during the model selection process (Zhang and Yang, 2015). This type of CV encompasses the use of an inner-loop for optimization and an outer-loop to assess the generalization performance (Krstajic et al., 2014). Acknowledging our dataset as relatively small for machine learning purposes (Zhang and Ling, 2018), we increased the k value (folds) with respect to the traditional 5 or 10-folds as a safeguard to reduce potential bias on the generalization error (Cawley and Talbot, 2010). Thus, an outer 20-fold scheme was used, setting aside a different 5 % of observations at a time to be used later as the testing data. At the inner loop, a 10-fold-CV was applied over each outer-training set, dividing 90 % for training and 10 % for validation. A grid-search was performed to optimize model hyper-parameters of interest: i) ntree, as the number of trees in the forest, and ii) mtry, as the number of random variables considered at each tree node-split across the forests. Best combinations were selected based on average performance on the inner-validation set. With the optimized hyper-parameters, performance metrics and features importance were assessed using the outer-training sets (20) to predict the observations on the outer-testing sets.

Six complementary metrics were used to evaluate models performance: i) the mean absolute error (MAE, Mg ha^{-1}) as an average magnitude of the errors; ii) the root mean square error (RMSE, Mg ha^{-1}) as an average squared errors-based statistic that penalizes large residuals more heavily than MAE; iii) the normalized or relative RMSE (RRMSE, %) as a metric of percentage deviation from the average yield (Yang et al., 2014); iv) the mean bias error (MBE, Mg ha^{-1}) as the average difference of predicted values with respect to observed, for which positive values mean a systematic over-prediction while negative mean under-prediction; v) the Nash–Sutcliffe model efficiency (ME) as a normalized analogous statistic to the coefficient of determination (Nash and Sutcliffe, 1970; Krause et al., 2005); and vi) the concordance correlation coefficient (CCC) as a normalized metric that weighs the Pearson correlation coefficient (r) by an index of accuracy (Lin, 1989). The medians (50th percentile) of each metric based on the 20-folds-CV were selected as their unbiased central-tendency statistic.

2.3. Results

2.3.1. Database description

Maize experiments were distributed across 21 US states (AL, AR, IA, IL, IN, KS, KY, MI, MN, MO, NC, ND, NE, OH, OK, PA, SD, TN, TX, VA and WI) and two Canada provinces (ON and QC) (Figure 2.1A). In temporal terms, 19.7 %, 31.0 %, 31.2 %, and 18.1 % were distributed between 1999–2004, 2005–2009, 2010–2014, and 2015–2019, respectively (Supplementary Figure 2.1). A total of 831 (81 %) and 200 trials (19 %) were conducted under rainfed and irrigated conditions, respectively. Under rainfed conditions, Y0 ranged from 0.73 to 17.7 Mg ha^{-1}, with a mean of 6.97 Mg ha^{-1} and a median of 6.41 Mg ha^{-1} (inter-quartile range, IQR_{25-75} = 4.21−9.49 Mg ha^{-1}). Under irrigation, Y0 varied from 1.29 to 16.1 Mg ha^{-1}, with a mean of 9.10 Mg ha^{-1} and a median of 9.50 Mg ha^{-1} (IQR_{25-75} = 6.84-11.65 Mg ha^{-1}). Based on available observations of above-ground plant N uptake at maturity (n = 279), estimations of apparent indigenous soil N supply varied from at least 23 kg N ha^{-1} to 411 kg N ha^{-1}, representing apparent N requirements from 11. 8–22.1 kg N Mg grain yield^{-1} (Figure 2.1B). Complementary, observations of grain N uptake and grain dry biomass (n = 305) were used to estimate a grain N nutrition index (NNI) following the ear-N dilution curve (%Nc = 2.22 *

Grain−0.26; Zhang et al., 2020), which was able to portray the positive effect of alfalfa as previous crop on maize N nutrition (Figure 2.1C).

In terms of soil, experiments represented 11 soil textural groups (Soil Survey Staff, 2014) (Figure 2.1D). Soil organic matter at topsoil (%, 0−15 cm) ranged from 0.46 % to 11.3 %, with a mean of 3.49 % and a median of 3.40 % (IQR25−75 = 2.12 %–4.91 %). In terms of weather, studies were exposed to a wide range of mean seasonal temperatures (Figure 2.1E) that ranged from 13.5 °C to 26.6 °C, with a mean of 18.9 °C and a median of 18.7 °C (IQR25−75 = 17.2–20.9 °C); and seasonal precipitations -April-September- (Figure 2.1F) ranged from 165 mm to 1167 mm, with a mean of 613 mm and a median of 593 mm (IQR_{25-75} = 502–703 mm). A total of 630 (61 %) and 401 trials (39 %) were reported under conventional tillage (TI) and no-tillage (NT) systems, respectively. Previous crops were alfalfa (n = 83), soybean and annual legumes (n = 497), and cereals and others (n = 451). Planting dates were reported in 643 cases (62 % of database), which in 95 % of cases ranged between March-20th to May-28th and were centered around May-5th (IQR_{25-75} = April-23rd to May-11th).

Exploratory correlation matrix was calculated (Supplementary Figure 2.2) and principal components analysis (Supplementary Figure 2.3) conducted to understand the main relationship patterns between the continuous explanatory variables. The first component, explaining 36 % of variability, can be interpreted a temperature-dimension where temperature variables (Temp, CHU, ETE) showed a high correlation to each other and were negatively correlated with latitude and Q index. The second component, explaining 11 % of variability, discriminates levels of precipitation and radiation. In total, five interpretable components explained about 70 % of variability in both, rainfed and irrigated conditions (Supplementary Figure 2.3).

2.3.2. Prediction performance

Performance metrics improved with increasing number of weather predictors accessible to the model (Full > Spring > No Weather, Figure 2.2). The model “No weather” that did not include weather predictors accounted for roughly half of the variation in Y0 (ME = 0.51), with CCC = 0.66, MAE = 1.94 Mg ha^{-1}, RMSE = 2.46 Mg ha^{-1}, RRMSE = 33.7 %, and MBE = -0.107 Mg ha^{-1}. The “spring model” improved the accuracy relative to “No weather” model by adding mean temperature and precipitations of March and April-May periods. Prediction metrics medians were ME = 0.59, CCC = 0.75, MAE = 1.72 Mg ha−1, RMSE = 2.16 Mg ha−1, RRMSE = 29.3 %, and MBE = -0.036 Mg ha−1. The “Full weather” model accounted for 64 % the variation in Y0 (ME = 0.64), with CCC = 0.77, MAE = 1.56 Mg ha−1, RMSE = 2.01 Mg ha−1, RRMSE = 27.1 %, and MBE = –0.043 Mg ha−1.

2.3.3. Features importance

Conditional importance analysis indicated that the most important factors driving Y0 variability were previous crop and irrigation for all models (Figure 3). These factors were several times more relevant than the evaluated soil and weather features. Regarding the previous crop effect, Y0 levels were the greatest with alfalfa as previous crop, followed by annual legumes and others, respectively (Figure 4A). Irrigation positively influenced Y0 of maize, especially with annual legumes as previous crop, increasing yields differences over other previous crops that did not reflect a positive effect of irrigation as annual legumes (Figure 4A). Soil factors decreased in relative importance as weather features were introduced. However, SOM ranked as the most important soil variable for Y0 regardless of the model (Figure 3). Regarding soil texture, its relevance resulted inconsistent with no fraction resulting particularly relevant.

When the weather features were introduced to the model, they improved the prediction accuracy, reduced the relevance of soil factors, and increased the relevance of management factors (Figure 3B; C). Precipitations and mean temperature during April-May ranked as the most important features for the Spring weather. Although including all weather variables still refined the prediction accuracy (Figure 2), signs of redundant features with only a marginal effects on performance were observed. Since importance scores were estimated conditional to the presence of correlated features, general low scores and a considerable fragmentation was observed across all the weather variables. Thus, relative importance of weather in the Full-weather model did considerable not increase with respect to the Spring-weather model. Notwithstanding, it is noticeable that the Full model allowed better ensemble structures that increased the relevance of previous crop and Irrigation factors (Figure 2.3C), which resulted in increased prediction accuracy (Figure 2.2). Moreover, several important insights emerged from the ranking of weather predictors. The occurrence of extreme precipitation events (EPE_AM, daily PP>25 mm) during early-growth stages exhibited a negative effect on Y0 (Figure 2.4C). The amount of radiation per unit of thermal time (Q quotient) during April-May (Figure 2.4D) but particularly during June-July (Figure 2.4E) exhibited a positive effect on predicted Y0 until reaching an optimum level (about 1.0 unit for Q_AM, and 0.6 units for Q_JJ). Likewise, a negative association of Y0 with extreme temperature events (>30 °C) during August-September (ETE_AS) (Figure 2.4F) as well as with the mean temperature of April-May (data not shown), as both weather features are moderately correlated (Supplementary Figures 2.2 and 2.3). Although, only simple dependencies are shown, this did not preclude existence of significant higher-level interactions.

High-level interactions arose from this analysis. However, it is remarkable that two out of the five most important weather variables in the full model were from early stages (EPE_AM, and Q_AM), plus the high relevancy of PP_AM and Tm_AM for the Spring weather model. These results indicate that early spring weather data already provides relevant information relative to the interaction between plant N demand and soil N supply.

2.4. Discussion

This study combined a comprehensive collection of maize experiments and advanced analytics to: i) describe properties of Y0 under a large variation of production conditions, and ii) to assess the importance of environmental and agronomic determinants of variation in this important descriptor of maize productivity. The outlined model could be used in combination with mechanistic models to improve prediction accuracy and decision making in N fertilization (Messina et al., 2020). This study also determined uncertainty levels for the forecast of Y0 under alternative prediction frameworks, which defines limits of predictability. Awareness about uncertainty on Y0 is crucial to set realistic expectations on prediction accuracy for yield response to N, EONR, and ex-ante N recommendations.

Further insights on the main driving factors of Y0 have implications for its use as a proxy of indigenous soil N supply (Cassman et al., 2002) or as a metric of biological buffering capacity (Morris et al., 2018). Available data on plant N uptake at crop maturity (R6) on this database indicates that under zero-N fertilizer, a maize crop needed at least between 11.8–22.1 kg available N ha^{-1} per Mg of grain yield (Figure 2.1B), acknowledging that the crop is not a merely passive sink for N (Fox and Piekielek, 1995; Vanotti and Bundy, 1994; Meisinger et al., 2008; Soufizadeh et al., 2018). Undoubtedly, addressing the soil-N-supply and plant-demand trade-offs (Briat et al., 2020) from complementary perspectives plays a key role for the design of N management strategies in maize crop. For a reduced portion of our dataset (<30 %), Figure 2.1C shows that following the concept of N dilution curves (Plénet and Lemaire, 2000; Lemaire and Ciampitti, 2020), estimates of N nutrition index (NNI) could provide a mechanistic-approximation of N uptake satisfied by a given soil condition (Devienne-Baret et al., 2000). This estimation of grain NNI at harvest using ear-N dilution curve as reference (Zhang et al., 2020) was able to portray differences of zero-N maize under different previous crops. However, a major limitation at a regional scale relies on the lack available and relevant data (co-variables) such as on whole-plant biomass and plant N uptake at specific stages (e.g., flowering) in order to represent contrasting management, soil, and weather conditions.

For the above-mentioned purposes, it is noteworthy that collecting field data on Y0 would be fairly scalable. Similarly, collecting initial soil data and obtaining precise spring weather data for building a simple but an effective prediction approach would also be fairly scalable. The reasonable performance of our data assessment framework across a wide geographic region suggests that cross-state guidelines could be pursued, a pending aspect for most of current N guidelines (Morris et al., 2018). Further efforts should recognize the value of combining collaborative research with increasing computational resources, data sources and type of models (Messina et al., 2020).

This study also offers an ex-ante approach using a large database of field studies to develop forecast models for Y0. Past efforts were mostly focused on: i) describing N response curves ex-post (Morris et al., 2018); ii) predicting the EONR via simulation models (Melkonian, 2008; Setiyono et al., 2011; Puntel et al., 2018); or iii) predicting EONR via machine learning using datasets of limited size that constrain the generalization of outcomes (Qin et al., 2018;

Ransom et al., 2019). The vast majority of models in literature use all the available data for training, but not out-of-sample data is used for testing how well they predict unseen observations. Predicting EONR faces the issue of defining a reference value, and its degree of uncertainty is generally overlooked (Hernandez and Mulla, 2008), highly depending on the best fitted model (Jaynes, 2011) and on the fertilizer to grain price ratio (Kim et al., 2013). Machine learning with small datasets (up to few hundred observations) is likely to suffer of high bias, limiting the detection of patterns and restricting the predictive ability in unexplored domains (Zhang and Ling, 2018). Still yet, limited efforts were focused specifically on the prediction of Y0 (Puntel et al., 2019), also with constraints on data availability to explore benefits of machine learning-type models.

We acknowledge issues limiting the scope of this approach: i) achieving a balanced and more detailed dataset, ii) research plot data has limitations, and iii) the trade-off between prediction power and interpretability of machine learning. For the first point, our dataset suffered from unevenly reported metadata and a lack of relevant features such as soil N availability tests, plant biomass and N uptake, planting and maturity dates, among other data descriptors that could eventually result in improved performance. From the scalability perspective, yields in well-managed research experiments are generally greater than yield with the same practices applied by farmers in production fields (Cassman et al., 2002). Regarding the interpretability limitations, this is currently shared by most of the machine learning algorithms (Khaki and Wang, 2019). Nonetheless, as computing power and algorithms exponentially grow, we will likely overcome the “black-box” limitation in the foreseeable future with refined methods to assess features role on prediction (Springenberg et al., 2015). Meta-learning models as ensembles of learning algorithms (Makowski et al., 2015) coupled with simulations (Shahhosseini et al., 2019; Messina et al., 2020) and cross-scales models (Wu et al., 2019) may contribute to this process. Finally, Bayesian statistics are also likely to contribute to yield forecast models as they offer more inference options on dealing with yield uncertainty (Iizumi et al., 2009).

A noteworthy outcome of this study is that a large fraction of the Y0 variability was explained just by management and soil factors (∼50 %). Weather contributed to improving the overall performance (+15 %). The “Full weather” and the “Spring weather” models reduced the RRMSE by 7 % and 4 %, respectively, with respect to the “No weather” model. While the reduction in RRMSE of the “Spring weather” model is lower than the “Full weather” model, it could be utilized for prediction. Prediction errors in the range of RMSE ∼2 Mg ha^{-1} (RRMSE from 27 % to 34 %) still represent a moderate performance and significant remaining uncertainty (Liu et al., 2013). Taking into consideration the observed range of apparent N requirement to produce 1 Mg yield ha−1 (Figure 2.1B), those values can be translated into an uncertainty in soil N supply of at least from 23 to 44 kg N ha^{-1} (considering an ideal, 100 %, N uptake efficiency). However, this also represents an opportunity for improvement. For example, a similar research approach on the prediction of rainfed maize yield using 2267 field studies across the US obtained a RRMSE up to 11 % using deep neural networks (Khaki and Wang, 2019), although encompassed more than 140,000 observations for training, as well as a much a more balanced and detailed database in terms soil, weather, in addition to the use of genetic markers data.

Across all models, the positive influence of legumes residues into crop rotations is clearly highlighted among management factors. The effect of alfalfa on the following maize N response has been well documented affecting soil N availability as well as soil physical conditions (Yost et al., 2012, 2013; 2014; Riedell, 2014). At the cropping system level, better coupling of C and N cycling processes can be achieved by relying more on organic rather than inorganic nutrient inputs (Drinkwater and Snapp, 2007). On the other hand, as one of the most limiting factors of maize yields (Mueller et al., 2012; Elliott et al., 2013; Meng et al., 2016), water supply was also a critical management factor for Y0, particularly enhancing yields of annual legumes as previous crops more than for cereals (Figure 2.4A), as the first group is comparatively less likely to suffer N-limitations. Counter-intuitively, our analysis did not show the expected influence of factors such as tillage on improving the estimation of Y0. Nonetheless, a lack of differences in yield response was also noted from the MRTN database (Sawyer and Nafziger, 2005). At a regional scale of our analysis, marginal effects are likely distorted by higher level interactions and by systematic differences in experimental methods. At a field level, however, it is well documented that tillage can modify soil aggregation, water holding capacity, soil temperature, and consequently soil N mineralization (Bruce et al., 1990; Andraski and Bundy, 2008; Coulter and Nafziger, 2008).

Considered an essential part of the soil and farming systems (Lal, 2004), SOM played the most influential role among soil features. A recent global meta-analysis documented a positive trend of maize yields with SOM with leveling off at ∼3.4 % (Oldfield et al., 2019). This study estimated that the same yield would be achievable with zero-N input in a soil with SOM of 3.4 % as with 50 kg N ha^{-1} with SOM of 0.9 %. However, N mineralization and the total organic carbon pool shows inconsistent relationship across the literature (Fox and Piekielek, 1984; Narteh and Sahrawat, 1997; Schomberg et al., 2009; Soon et al., 2007; Sainz Rozas et al., 2008), potentially related to differences in the most active of SOM fractions (Schmidt et al., 2011). In this sense, indices of soil N mineralization would theoretically improve the utilization of SOM and a simple index from soil-test biological activity appears noteworthy (Franzluebbers, 2018). Lastly, the soil texture is sometimes presented in association with soil N mineralization, but the relationship is variable across studies in the literature (Hassink, 1997; Franzluebbers et al., 1996; Yoo and Wander, 2006; Zhu et al., 2009; Dessureault-Rompré et al., 2010; Ros et al., 2011; Cai et al., 2016). For instance, a meta-analysis including 51 experiments in North-America have reported higher maize N responses under finer soil textures (Tremblay et al., 2012), while only marginal effects of spatial variability for soil texture relative to variation across years were also reported in other studies (van Es et al., 2005v; Tremblay and Bélec, 2006; Kyveryga et al., 2009).

Weather factors are determinants of both N supply and demand (Soufizadeh et al., 2018). In this study, the excess of rainfall early in the season enter in prediction models consistent with the negative impact of high precipitation on drainage, water-logging and increased N losses (Cameron et al., 2013; Wang et al., 2014). Spring precipitations have been reported to account for 74 % of inter-annual variation in mean soil residual N at pre-sidedress (Balkcom et al., 2003). Similarly, every 10 mm of April precipitation above historical average delayed planting date for 1 day in the main 12 central US states (Kucharik, 2008). Although it is unlikely that yields under N limitations were limited by solar radiation (DeBruin et al., 2013; Soufizadeh et al., 2018), radiation per unit of thermal time (Q quotient) during June-July (JJ) and early in the season (AM) positively affected yields (Andrade et al., 2000; Carter et al., 2018; Soufizadeh et al., 2018) until variable optimum levels, exhibiting the trade-off with the temperature effects on radiation use efficiency (Andrade et al., 1993) and biomass partitioning to the ear (Wilson et al., 1995). Regarding temperature, the occurrence of extreme temperatures during the reproductive period (ETE_AS) resulted in one of the most relevant features suggesting that the positive effect of temperature on soil N mineralization (Dalias et al., 2002; Wu et al., 2008; Fernández et al., 2017) could be offset by a negative impact of supra-optimal temperatures on plant growth (e.g., shortening the grain filling duration) and plant N demand (Muchow et al., 1990; Soufizadeh et al., 2018). Overall, the high relevance of weather features at early stages (spring) appraises to invest more resources in the aggregation and analysis of massive databases that allow to further explore the development of prediction frameworks for Y0 that can be applied in practice.

2.5. Conclusions

Management factors such as previous crop and irrigation in combination with top-soil SOM accounted for the largest portion of variation in Y0, while the inclusion of weather features refined the prediction accuracy. In a practical sense, a simple framework including weather variables of spring (March-May) might result comparable in performance to a framework including all-season weather. Future attempts should assess alternative statistical and machine learning approaches offering performance and interpretability improvements. Refined prediction frameworks for Y0 could provide new insights on N responsiveness and represent a step-forward towards more collaborative and regional-scale N recommendation guidelines.

Table 2.1. Explanatory variables included for the prediction of maize yield under N omission (Y0). *Periods: AM = April-May, JJ = June-July, AS = August-September.

	Management	
Previous Crop	alfalfa; annual legumes; others (maize, sorghum, wheat, barley, rye, sunflower)	
Tillage system	Till; no-till	
Irrigation	Irrigated; Rainfed	
	Soil	
Variable	Units	Depth
SOM = Soil Organic Matter	%	0-15 cm
Clay		
Silt		
Sand		
	Weather	
Variable	Units	Periods
PP = Precipitations	mm	March, AM (Apr-May), JJ (Jun-Jul), AS (Aug-Sept)
Tm = Mean Temperature	ºC	
SDI = Shannon Diversity Index	0-1 (uneven - even)	AM (Apr-May), JJ (Jun-Jul), AS (Aug-Sept)
EPE = Extreme PP Events	# days PP > 25 mm	
vpd = Vapor Pressure Deficit (sum)	KPa	
Rad = Incident radiation (sum)	MJ m^{-2}	
CHU = Crop Heat Units	ºC	
Q = Photothermal quotient	MJ m^{-2} / CHU	
ETE = Extreme T Events	# days T_{max} > 30ºC	JJ, AS

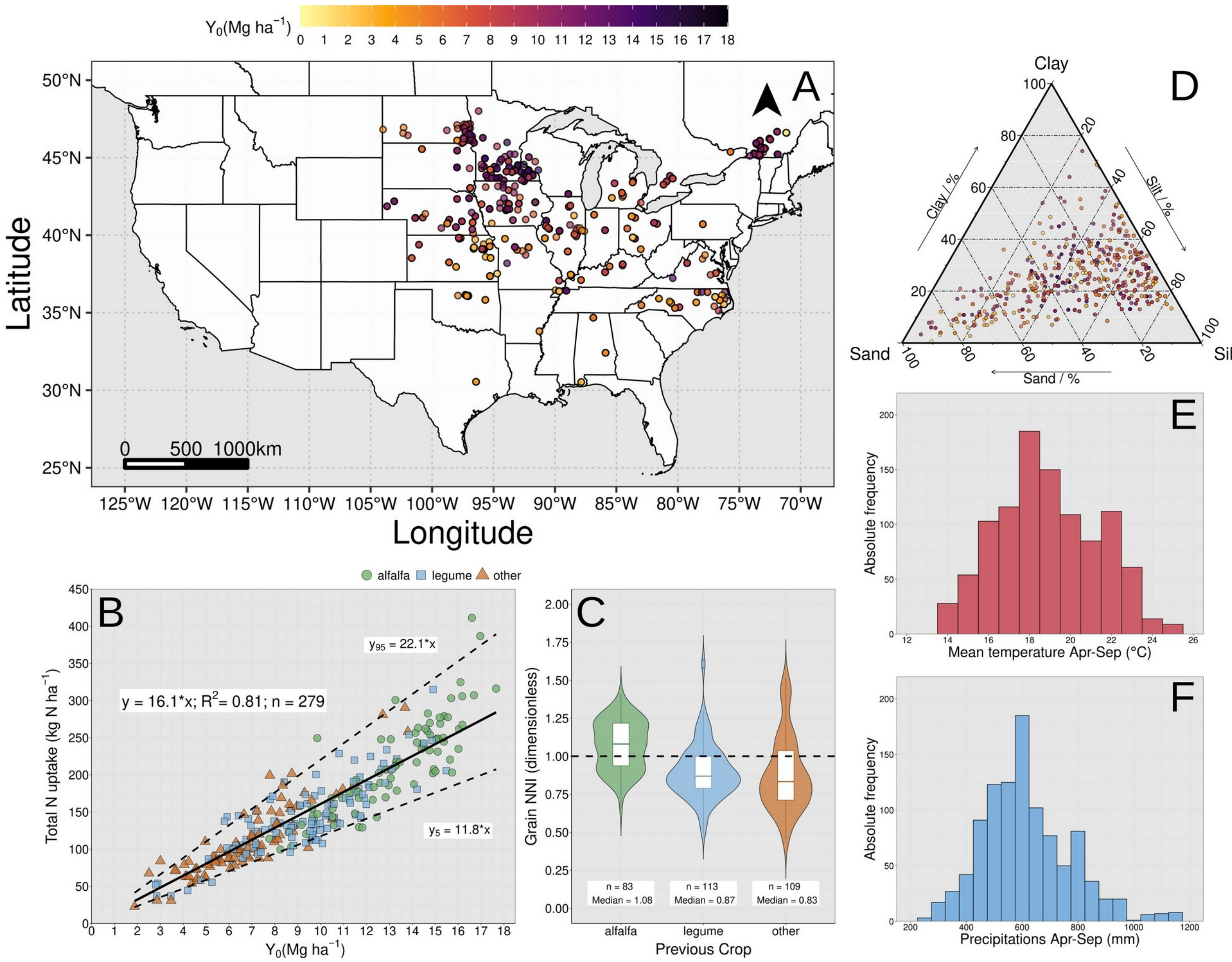

Figure 2.1. A: Geographical distribution of maize nitrogen fertilization trials under study (1031 Y0 observations from 679 site-years) performed in the USA and Canada during the period 1999-2019. B: Relationship between total above-ground N uptake at crop maturity (R6, n = 279) and yield under zero-N (Y0). C: Estimated grain N Nutrition Index (NNI, n = 305) of zero-N maize for different previous using ear N dilution curve as reference (Zhang et al., 2020). D: variability of soil texture (0-15 cm), E: distribution of mean temperature, and F: total precipitation (mm) from April 1st to September 30th.

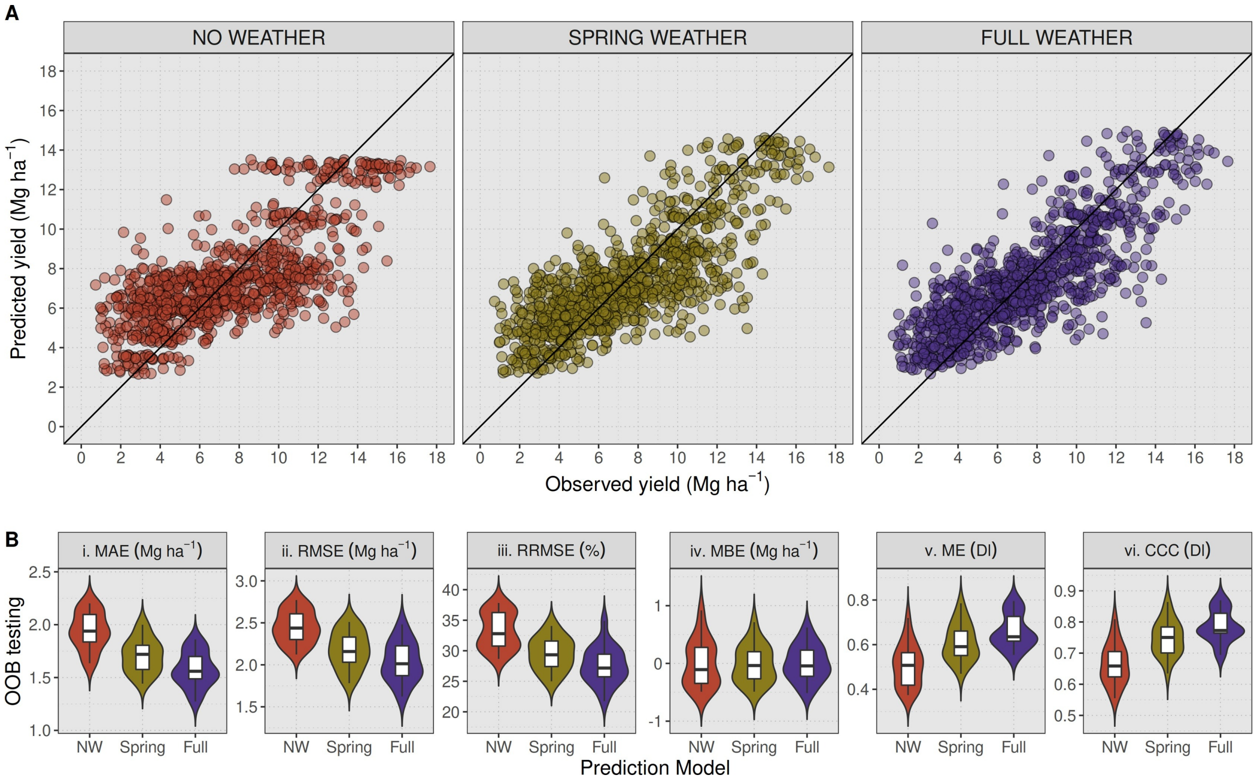

Figure 2.2. Out of bag (OOB) prediction performance of conditional random forest considering three alternative models: NW – No weather, only soil and crop management features; Spring weather – including March, April and May mean temperature and precipitations; and Full weather – including all weather variables during the cropping season (April-September). Violin plots represent variability of performance metrics assessed on a 20-fold cross-validation scheme. Internal boxes represent the inter-quartile range (25th to 75th percentile) and whiskers the 5th to 95th percentiles. Model Efficiency (ME) and concordance correlation coefficient (CCC) are dimensionless (Dl) indices.

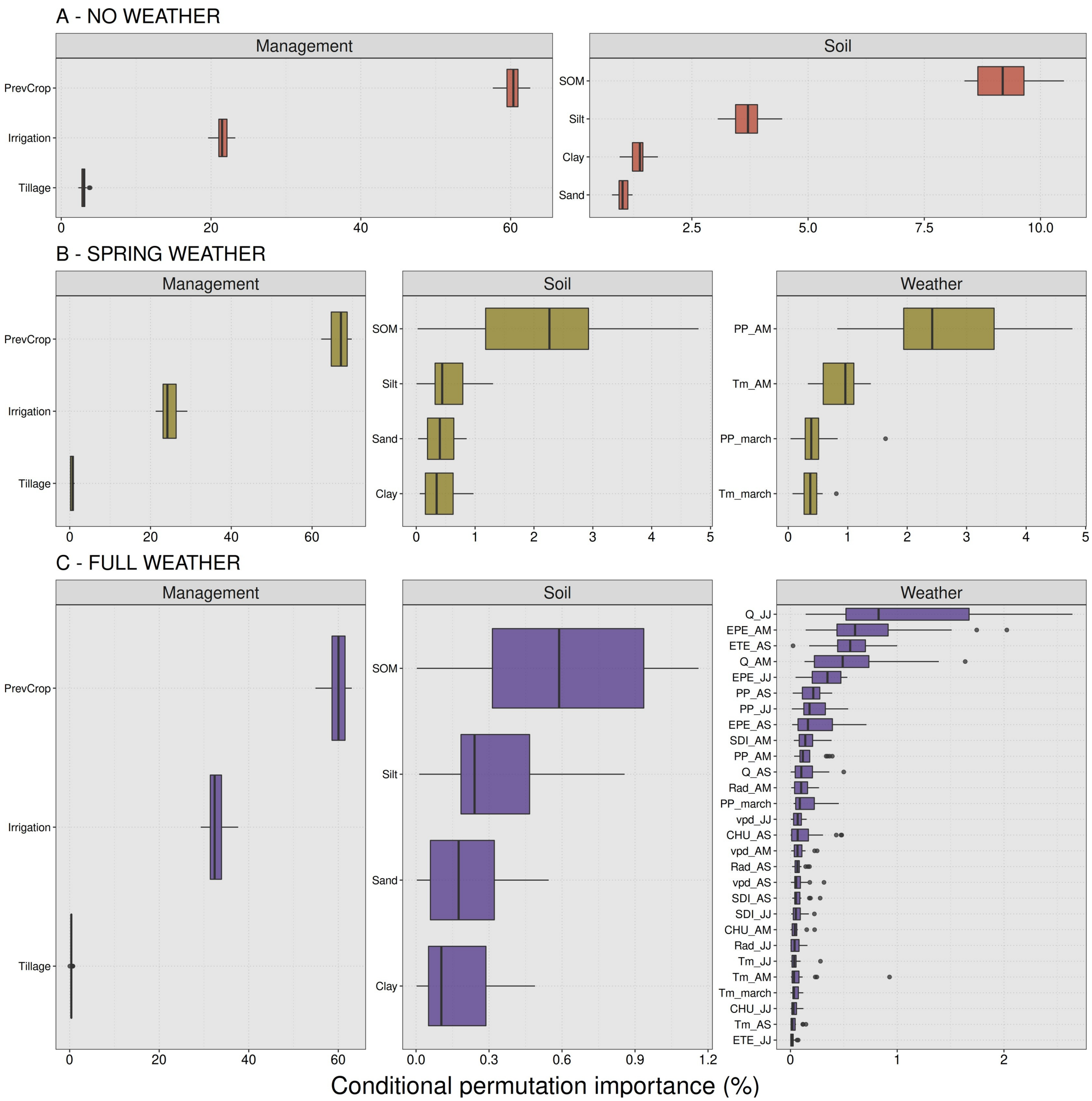

Figure 2.3. Variable importance of management, soil, and weather features on the prediction of Y0 at three alternative frameworks assessed via conditional permutations on random forest models (Strobl et al., 2008) re-scaled to percentage. Within each framework, boxes represent the inter-quartile range (25th to 75th percentile) and whiskers the 5th to 95th percentiles of conditional importance under a 20-fold cross-validation scheme. Abbreviations from Table 2.1.

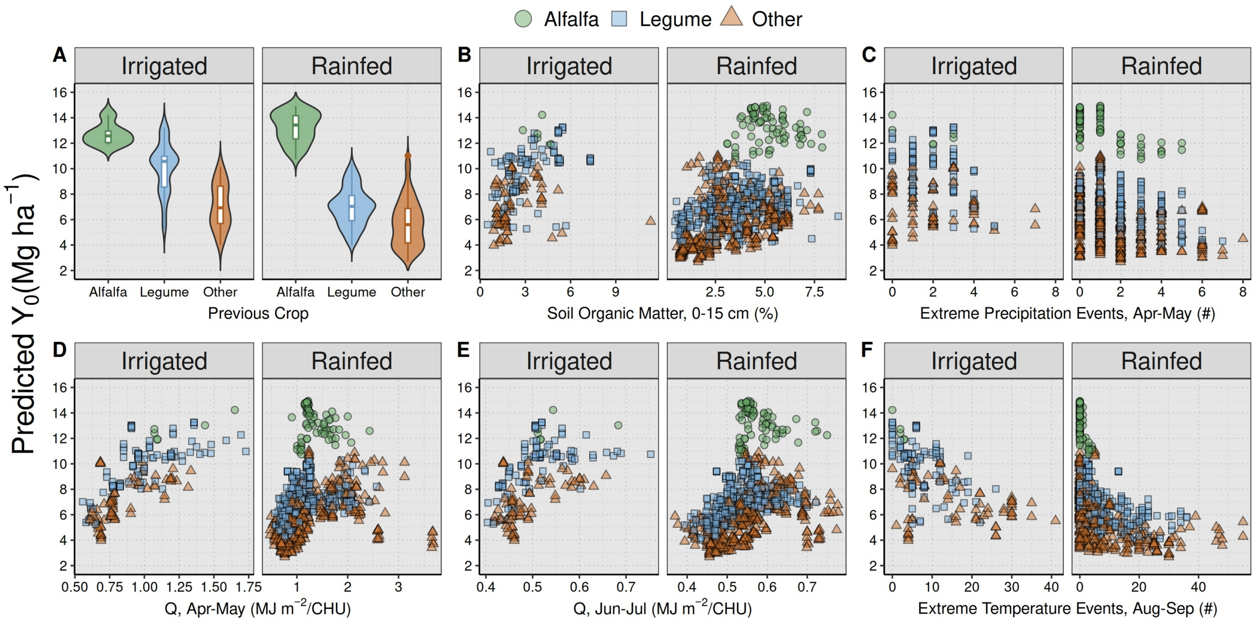

Figure 2.4. Partial main dependencies of predicted maize grain yield under N omission (Y0, Mg ha−1) on the most relevant features related to management, soil, and weather (Figure 3). In A, Boxes represent the inter-quartile range (25th to 75th percentile) and whiskers the 5th to 95th percentiles. Out-of-bag predictions from 20-fold cross-validation for the Full weather framework.

Chapter 3: Unraveling uncertainty drivers of the maize yield response to nitrogen: A Bayesian and machine learning approach

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Abstract

Development of predictive algorithms accounting for uncertainty in processes underpinning the maize (*Zea mays* L.) yield response to nitrogen (N) are needed in order to provide new N fertilization guidelines. The aims of this study were to unravel the relative importance of crop management, soil, and weather factors on both the estimate and the size of uncertainty of the main components of the maize yield response to N: i) yield without N fertilizer (B0); ii) yield at economic optimum N rate (YEONR); iii) EONR; and iv) the N fertilizer efficiency (NFE) at the EONR. Combining Bayesian statistics to fit the N response curves and a machine learning algorithm (extreme gradient boosting) to assess features importance on the predictability of the process, we analyzed data of 730 response curves from 481 site-years (4297 observations) in maize N rate fertilization studies conducted between 1999 and 2020 in the United States and Canada. The EONR was the most difficult attribute to predict, with an average uncertainty of 50 kg N ha^{-1}, increasing towards low (<100 kg N ha^{-1}) and high (>200 kg N ha^{-1}) EONR expected values. Crop management factors such as previous crop and irrigation contributed substantially (~50%) to the estimation of B0, but minorly to other components of the maize yield response to N. Weather contributed about two-thirds of explained variance of the

estimated values of YEONR, EONR, and NFE, and governed the uncertainty (72% to 81%) of all components. Soil factors provided a consistent but limited (10% to 23%) contribution to explain both expected N response as well as its associated uncertainties. Efforts to improve N decision support tools should consider the uncertainty of models as a type of risk, potential in-season weather scenarios, and develop probabilistic frameworks for improving this data-driven decision-making process of N fertilization in maize.

3.1. Introduction

Nitrogen (N) is probably the most complex plant nutrient to study due to an intricate set of spatio-temporal interactions governing plant growth dynamics, soil biogeochemical cycling, and environmental effects on the plant-soil system (Mesbah et al., 2017; Briat et al., 2020). Despite decades of research, addressing the uncertainty on the growth and demand of N in maize (*Zea mays* L.) is still a major concern (Babcock, 1992; Morris et al., 2018, Raun et al., 2019), as indicated by the collateral impacts of misuse of fertilizer and low N use efficiency due to uncertainty of fertilizer rate needed (Sela et al., 2018a; 2018b). Refining the management of a complex system such as the one governing soil-plant N dynamics requires understanding the processes generating the yield response to N using multiple perspectives (Lory and Scharf, 2003; Martinez-Feria et al., 2018; Correndo et al., 2021a).

Yield responses to N fertilizer are often modeled using non-linear regression models, which are considered a practical way to provide summaries of the N response. Field trials with various fertilizer N rates are used to estimate optimum rates, mostly under the economic return criteria. Under this scenario, uncertainty is inevitable due to the multiple interactions between the crop with the agronomic management, soil processes, and weather factors (Kyveryga et al., 2007). The degree of uncertainty on the parameters describing the N response functions (*e.g.*, intercept, slope, curvature) and derived quantities (*e.g.*, intercept, optimum N rate, maximum yield, efficiencies) represent a measure of risk (Babcock, 1992), however, they are typically overlooked in the scientific literature (Hernandez and Mulla, 2008). The unpredictable nature that environment has on N dynamics and crop yield dictate the need for models accounting for stochastic components (Tmusiime et al., 2011; Raun et al., 2019).

From the statistical standpoint, the N response curves have been mostly studied using a frequentist approach, for which only the data are considered random, and unknown parameters of interest are treated as fixed variables. In contrast, the Bayesian approach treats the unknown model parameters and derived quantities as random variables. Within the Bayesian framework, we aim to estimate the best model parameters given two main components: i) prior knowledge of the process of interest (the N response curve), and ii) the available observed data (Wakefield, 2013). Literature or expert knowledge is used to define prior distributions of model parameters, and the data are used as new evidence to update our prior beliefs through inferences based on probability distributions (posteriors). Therefore, not only the estimates of the parameters but also their uncertainties are components of interest in a Bayesian framework. Given the increasing computational power and development of new algorithms, Bayesian methods are becoming more common, and are increasingly being used in agricultural research (Lacasa et al., 2020; Laurent et al., 2020; Ciampitti et al., 2020).

Machine learning algorithms are suitable to identify complex association patterns in large datasets (Jordan and Mitchel, 2015). Belonging to the family of supervised learning techniques, classification and regression tree-based methods such as decision trees, random forests and boosting are robust and powerful techniques as recently demonstrated in agricultural research (Shahhosseini et al., 2019; Schwalbert et al., 2020). For example, Correndo et al.

(2021a) used conditional random forests to compare forecast frameworks for predicting maize yield without N fertilization while evaluating the contribution of management, soil, and weather features on those predictions. Alternatively, boosting methods consist of fitting multiple decision trees to the data, where each tree is *sequentially* grown using the residuals from previous trees (James et al., 2013). Extreme gradient boosting (*xgboost*; Chen and Guestrin, 2016), one of the implementations of gradient boosting machines (Friedman, 2001), is known as one of the best performing algorithms for both regression and classification problems (Osman et al., 2021; Park and Kim, 2021). Besides its prediction capabilities, *xgboost* allows the estimation of a permutation-based feature importance, which serves as a useful interpretation tool to examine the decrease in a scoring rule (*e.g.*, mean square error) when features values are randomly shuffled (Breiman, 2001).

The objectives of this research were to study the importance of crop management, soil, and weather factors on both estimate and the magnitude of uncertainty of the main components —a yield without N (B0), economic optimum N rate (EONR), yield at the EONR (YEONR), and N fertilizer efficiency (NFE) at the EONR— describing the maize yield response to N.

3.2. Materials and methods

3.2.1. Review

A database was built by including experimental data that met certain requirements as follows: 1) Collected on experiments during the last two decades (1999-2020) in order to reduce the yield variability associated with genetic advancement of yield potential (Woli et al., 2016); 2) Collected from replicated field trials with N treatments in small plots or field strips; 3) A minimum of four N rate treatments, including a control (zero-N) and a maximum rate of at least

Corn 168 kg N ha^{-1} in order to limit the chances of N limitation for achieving an environmentally attainable yield maximum; 4) Trials with positive response but without reaching a yield-plateau were removed from the analysis since EONR and YEONR expected values resulted out of the data range and their uncertainties extremely high, and no associations with specific soil or weather conditions were found, indicating a most likely experimental design limitation (data not shown); 5) Absolute yield data; 6) Planting date; 7) Topsoil crop nutrient analysis results and/or soil series; 8) Previous crop and tillage system; 9) Latitude and longitude coordinates, or report the nearest town in order to retrieve archived weather and/or missing soil series data; 10) No manure as treatments or as a past management input. General crop management (hybrid, row spacing, other nutrients, weed and pest management) was assumed to have been chosen to maximize yield under each site-specific condition.

Published manuscripts were the first source of data, accessed using an engine-search in Web of Science® filtering by the following keywords: "corn/maize" and "nitrogen fertilizer" or "nitrogen fertilization" and "United States" and/or "Canada". In order to reduce publication bias effect (Dickersin and Min, 1993), unpublished data (*e.g.*, dissertations, field reports, unpublished experiments) that met criteria were also included. After filtering and selection processes, 481 site-years distributed across United States and Canada (Figure 3.1A) resulting in 730 N response curves of maize were gathered from 32 different data sources (Supplementary Table 1), including published and unpublished studies (Supplementary Table 3.1). Grain yield was standardized at a water content of 155 g kg^{-1}, and each yield point at a given N rate was the average value of 3 to 5 replications.

The database used partially coincides with a previous study by Correndo et al. (2021a), who focused solely on developing a predictive algorithm to forecast maize yield without N.

However, this current study is dissimilar mainly in the following points: 1) this study pay special attention on assessing the uncertainty on the entire N response process rather than on a single component, maize yield without N (Correndo et al., 2021a); 2) the present work uses function parameters of the N response process (Bayesian regression analysis) and their uncertainties as the object of study, while Correndo et al. (2021a) used observed yields without N as the only response variable; 3) the current manuscript considers only experiments with a set of fertilizer N rate treatments satisfying certain minimum requirements (481 site-years, 4297 yield observations), while Correndo et al. (2021a) only considered studies presenting observed maize yields without N fertilization (679 site-years, 1031 yield observations); and lastly, 4) this study only uses trials that reported "sowing date" in order to produce more refined weather variables with the planting date as a reference to adjust the weather summaries (Table 3.1), while Correndo et al. (2021a) used only weather variables summarized by calendar months.

3.2.2. Metadata

Soil related variables were topsoil (0-15 cm) soil organic matter (SOM, %) and soil texture (clay, silt and sand, %). Soil data were collected from original sources, accessed from authors' records when not reported in manuscripts, or retrieved from gridded POLARIS soil data engine (Chaney et al., 2016), a raster optimization based on SSURGO data with a spatial resolution of 1 km^2. When SOM data were reported at 0-20 or 0-30 cm, values were standardized to 0-15 cm using stratification factors based on data from previous research on grain crops trials (Al-Kaisi et al., 2005; Varvel and Wilhelm, 2011; Franzluebbers, 2010; Villamil et al., 2015).

Daily weather data were accessed via the Daymet (Thornton et al., 2019) API-client source developed for R-software (package daymetr) using reported latitude-longitude coordinates of the trials or nearest town. With a spatial resolution of 1 km2, precipitation (PP), maximum and minimum temperature (T, °C,), vapor pressure deficit (vpd, kPa), incident shortwave solar radiation during daylight period (Rad, MJ m^{-2}) and day-length. Weather data were transformed into monthly basis (as sum or average) using reported sowing dates as the reference (das: days after sowing). We divided the weather data into five main periods: i) pre-sowing, as the weather of 30 days before sowing; ii) 1st month after sowing (0-30 das), as proxy of the establishment period; ii) 2nd month after sowing (31 to 60 das), as a proxy of the most active growth vegetative period; iii) 3rd month after sowing (61 to 90 das), as proxy of the period around flowering; and iv) 4th month after planting (91-120 dfs), as a proxy of the grain filling period.

A series of additional weather variables were calculated to capture environmental differences that might not have been captured by analyzing standard weather information. For example, the Shannon Diversity Index (SDI) as described by Tremblay et al. (2012) was included to describe the distribution of PP during each period. Extreme PP events were included as the number of days with precipitations greater than 25 mm as a proxy of excessive rainfall events (Puntel et al., 2019; Correndo et al., 2021a). Crop development was described by crop heat units (CHU; Tremblay et al., 2012). Extreme temperature events (ETE, defined as the number of days with maximum temperature greater than 30°C) were also included as a proxy of heat stress risk (Butler and Huybers, 2013; Ye et al., 2017). The photo-thermal quotient (Q) was calculated as the ratio between cumulative Rad and CHU, as an indicator of the solar radiation available to the crop per unit of thermal time during each period, related to yield potential (Bannayan et al., 2018).

3.2.3. Data analysis

3.2.3.1. Nitrogen response process

We fit quadratic and quadratic-plateau regression models using grain yield as the response variable and N rate as the explanatory variable. The quadratic and the quadratic-plateau models are the most extensively used in the literature as they have parameters with a clear interpretation for developing N recommendations (Cerrato and Blackmer, 1990; Wortmann et al., 2011; Kyveryga et al., 2007). Besides its simplicity, the quadratic model presents a great flexibility in terms of possible shapes of the response including flat-, negative or positive linear-, and bell-shaped curves. For each particular case, we selected the model that resulted in the best performance (>R^2 median from Bayesian posteriors). Overall, we have observed a better performance of the quadratic model in the majority of cases (n=513) (Supplementary Figure 3.1), with less uncertain estimates, especially in terms of key descriptors of interest such as EONR and NFE (Supplementary Figure 3.2). The quadratic-plateau model resulted the best option in 217 cases, particularly when the response curve was very well defined -high R^2 for both models- (Supplementary Figure 3.1). In contrast, with less defined N responsiveness patterns, the quadratic-plateau model may result in a more erratic convergence. Since many of the sites used in this study are in areas of the USA where high wind is possible, the quadratic response for maize may also be most appropriate due to yield decrease due to high-wind-induced ‘green snap’ under high N conditions, while the quadratic-plateau model assumes there is no penalty for greater N rates.

The N response measured through a quadratic model is normally estimated as follows [Eq. (3.1)]:

$$y_i = B_0 + B_1 x_i - B_2 x_i^2 \qquad \textbf{(3.1)}$$

where, for the ith observation, y represents the maize yield (Mg ha^{-1}), x represents the N rate (kg N ha^{-1}), B_0 is the intercept (yield without N fertilizer), B_1 is the linear slope, as the response in yield per unit of change in initial N availability, and B_2 is the quadratic coefficient.

Sharing the same parameters than Eq. (3.1), the N response measured through a quadratic-plateau model is normally estimated as follows [Eq. (3.2)]:

$$y_i = B_0 + B_1 x_i - B_2 x_i^2, if\ x_i < AONR, \\ B_0 + B_1 AONR - B_2 AONR^2, if\ x_i \geq AONR \qquad \textbf{(3.2)}$$

where, AONR stands for the agronomic optimum N rate, which corresponds to the level of xi when the first derivative of the function is equal to zero (AONR = B_1 / $2B_2$)).

Once the model was selected, we considered four main descriptors of the N response process (Figure 3.2: i) B0 (yield without N fertilizer); ii) the grain yield at the economic optimum N rate (YEONR, Mg ha^{-1}); iii) the EONR (kg N ha^{-1}); and iv) N fertilizer efficiency at the EONR (NFE, kg yield (kg applied N)$^{-1}$). The B0 was estimated as the intercept of the response curves. The YEONR and the EONR were estimated as the level of y, and x, respectively, when the first derivative of Eq. (1) is equal to the nitrogen:maize prices ratio (Mg grain kg N^{-1}). Lastly, the NFE was estimated as the quotient between the N responsiveness (YEONR - B0) and the EONR.

A novelty of this analysis was to include an uncertainty component associated with maize grain and fertilizer N prices. For this purpose, we considered the prices ratio as a random variable. Thereby, each time the EONR was estimated, instead of considering a fixed ratio, the value was sampled from a probability distribution. Including a gamma prior distribution into the Bayesian framework, we simulated the historical prices ratio variability observed during the period 1998-2018 (USDA-ERS, 2021a; 2021b). For maize grain we considered the future price at each April, whereas for fertilizer N we considered the average price of anhydrous ammonia (82-0-0) and urea (46-0-0) at each April or March. The historical average prices of maize were 152 \$ Mg grain^{-1} and 0.763 \$ kg N^{-1}, with an average prices ratio of 0.0053 Mg grain kg N^{-1} (standard deviation of 0.0014 Mg grain kg N^{-1}). With a mean of 0.0055 kg grain kg N^{-1} and a standard deviation of 0.0016 Mg grain kg N^{-1}, the simulated prior for the prices ratio (~ gamma (shape = 11, rate = 2)) showed a distribution equivalent to the actual historical PR variability (Supplementary Figure 3.3).

3.2.3.2. Bayesian N response models

The four descriptors of interest were obtained by fitting the quadratic or the quadratic-plateau regression model under a hierarchical Bayesian framework using the following priors [Eq. (3.3-3.8)]:

$$y_i \sim Gaussian\left(\mu_i, \sigma_i^2\right) \quad \textbf{(3.3)}$$

$$u_i = B_0 + B_1 x - B_2 x^2 \quad \textbf{(3.4a)}$$

$$u_i = B_0 + B_1 x_i - B_2 x_i^2, if\ x_i < AONR, \quad B_0 + B_1 AONR - B_2 AONR^2, if\ x_i \geq AONR \quad \textbf{(3.4b)}$$

$$B_0 \sim U(0{,}18); \quad \textbf{(3.5)}$$

$$B_1 \sim U(0{,}0.2); \quad \textbf{(3.6)}$$

$$B_2 \sim gamma(1{,}10); \quad \textbf{(3.7)}$$

$$\sigma_i^2 \sim gamma(2{,}2); \quad \textbf{(3.8)}$$

where for each trial, y_i represents the yield at the i^{th} N rate, u_i represents the underlying process (3.4a if quadratic, 3.4b if quadratic-plateau), σ_i^2 is the variance of the process, and Gaussian, *U*, and *gamma* stands for normal, uniform, and *gamma* distributions for priors. Weakly informative priors were defined following previous experience on maize observed yield without N fertilization (B_0) (Correndo et al., 2021a), linear response to N of quadratic models (B_1), and curvature (B_2) (Correndo et al., 2021b; Lacasa et al., 2020). Uniformly distributed priors for B_0 and B_1 were used to ensure adaptability of the priors to each case. In the case of B_2 and σ_i^2, gamma priors were used to support positive values of the parameters, similar to Lacasa et al. (2020) in a study maize yield response to plant density. Particularly for , a *gamma* prior provides a more suitable alternative than uniform priors, which are proven to lead to a positive miscalibration (overestimation) of the variance (Gelman, 2006).

From each model, the expected estimates of the descriptors were retrieved as the median (50^{th} percentile) of the posterior distributions. Similarly, the magnitude of uncertainty for each descriptor was obtained as the length of the 95%-credible intervals (2.5^{th} to 97.5^{th} percentile) from the posterior distributions.

Bayesian models were fit in R-software (R Core Team, 2021), using the rjags package v4-10 (Plummer et al., 2019), which applies Gibbs sampling (Geman and Geman, 1984), a Markov Chain Monte Carlo (MCMC) algorithm to generate a sequence of samples approximated to a posterior probability distribution function of parameters. We used 4 parallel chains with 20,000 iterations, including 5,000 as burn-in, and a thinning interval of 10.

3.2.3.3. Feature importance assessment

In order to reproduce complex association patterns between the descriptors of the N response process and crop management, soil, and weather variables, we applied the *xgboost* algorithm (Chen and Guestrin, 2016). The target variables were eight, as both the estimate (median) and the uncertainty (95%-credible interval length) of the four N response descriptors: B0, YEONR, EONR, and NFE (Figure 3.2). The model inputs were the crop management, soil, and weather variables described in Table 3.1. Since *xgboost* only handles numerical matrices, categorical variables such as previous crop, tillage and irrigation were transformed using one-hot-encoding. As a result, previous crop -containing three levels (Table 3.1)-was split into two dummy variables: i) ALF, equal to 1 if previous crop was “alfalfa” (*Medicago sativa* L.), or equal to 0 if not, and ii) LEG, equal to 1 if previous crop was an “annual legume”, equal to zero if previous crop was “other”, otherwise (ALF = 1) always equal to 0.

Since the main purpose of using *xgboost* here was to assess features importance rather than developing a forecasting model, we considered the entire seasonal weather as if these data were known or perfectly predictable.

For each model, a nested cross-validation (CV) that encompassed the use of an inner-loop for optimization and an outer-loop to assess the generalization performance (Krstajic et al., 2014). We used an outer 20-fold scheme, setting aside a different 5% of observations at a time to be used later as the testing data. At the inner loop, a 10-fold-CV was applied over each outer-training set, dividing 90% for training and 10% for validation. For each model, we performed a grid-search to optimize the hyper-parameters of interest: i) *nrounds*, as the number of trees in the forest, ii) *eta*, as the gradient or learning rate, iii) *maxdepth*, as the maximum depth of trees in the forest, iv) *alpha*, as the L1 (LASSO) regularization coefficient, and v) *lambda*, as the L2 (Ridge) regularization coefficient. Regularization through *alpha* and *lambda* was used to reduce the influence of collinearity due to the presence of correlated covariates (Supplementary Figure 3.4). We fixed *ncolsamples* at 0.7 (70% of features randomly selected) and early_stopping_rounds at 3. The rest of parameters were set to default options. Best combinations were selected based on average performance on the inner-validation set. With the optimized hyper-parameters, performance metrics and features importance were assessed using the outer-training sets (20) to predict the observations on the outer-testing sets. The importance of data input features was quantified using permutation tests (Breiman, 2001).

To evaluate models performance, we used: i) the root mean square error (RMSE, Mg ha-1) as an average squared errors-based statistic that penalizes large residuals; ii) the normalized or relative RMSE (RRMSE, %) as a metric of percentage deviation from the average yield (Yang et al., 2014); iii) the mean bias error (MBE) as the average difference of predicted values with respect to observed, for which positive values mean a systematic over-prediction while negative mean under-prediction; iv) the Nash–Sutcliffe (ME), and v) the Kling-Gupta (KGE) model efficiencies, as a normalized analog to the coefficient of determination (Nash and Sutcliffe, 1971; Kling et al., 2012); vi) the concordance correlation coefficient (CCC) as a normalized metric that weighs the correlation coefficient (precision) by an index of accuracy (Lin, 1989); and vii) the classical coefficient of determination (R^2) that represents a measure of precision (not accuracy). Formulae of metrics can be found at Supplementary Table 3.2. The medians (50th percentile) of each metric based on the 20-folds-CV were selected as their unbiased central-tendency statistic.

3.3. Results

3.3.1. Database description

Maize N rate trials under study were distributed across 19 US states (AL, IA, IL, IN, KS, MI, MN, MO, NC, ND, NE, OH, OK, PA, SD, TN, TX, VA, and WI) and two Canada provinces (ON and QC) (Figure 3.1A). The majority of experiments were concentrated during the period 2004-2014 (n=499, 68%), 103 trials were conducted between 1999-2003 (14%), and 128 between 2015-2020 (18%). A total of 601 (82%), and 129 (18%) trials were under rainfed and irrigated conditions, respectively. In terms of tillage management, 466 trials were reported under conventional tillage (64%), and 264 under no-tillage (36%). Previous crops were alfalfa (n=82), annual legumes (n=368), and cereals or others (n=280). Sowing dates (day of the year) varied from days 61 (March 1st) to 155 (June 4th), with a median at day 120, and inter-quartile range (IQR, percentiles 25th to 75th) between days 103 to 136. From sowing to 120 das, mean temperature ranged from 15.7 ºC to 25.9 ºC, with a median of 20.6 ºC (IQR = 19.4 ºC – 21.9 ºC), and accumulated precipitations ranged from 117 mm to 727 mm, with a median of 420 mm (IQR = 350 mm – 480 mm). Soils represented 11 soil textural classes (Soil Survey Staff, 2018) (Figure 6.1B), and SOM values (%) ranged from 0.5% to 7.9% with a median of 3.6% (IQR = 2.4%-5.2%).

Maximum N rates varied from 168 to 366 kg N ha^{-1}, with a median of 248 kg N ha^{-1}. The reported metadata concerning N fertilization strategy resulted incomplete in the majority of cases. Thus, only 284, 490, and 642, and 284 reported details on fertilizer application form, source, and timing, respectively. Reported forms of N application were broadcasted (n=94), injected (n=176), banded (n=7), and incorporated (n=7). Reported N sources were urea-ammonium nitrate (32-0-0, n=238), ammonium nitrate (34-0-0; n= 169), urea (46-0-0, n=35), calcareous-ammonium nitrate (15-0-0, n=24), and anhydrous-ammonia (82-0-0; n=23). Lastly, reported N application timings were between V2-V6 (n=280), at sowing (n=198), pre-sowing (n=81), split applications between planting and V4-V6 (n=58), and between V7-V9 (25).

Observed yields varied from a minimum of 0.35 Mg ha^{-1} to a maximum of 19.0 Mg ha^{-1}. Yield without N averaged 7.93 (IQR = 5.31-10.24 Mg ha^{-1}), maximum yield averaged 12.23 (IQR = 10.61-14.16 Mg ha^{-1}), and the apparent N responsiveness (maximum yield minus yield without N) averaged 4.30 Mg ha^{-1} (IQR = 2.28-6.20 Mg ha^{-1}).

3.3.2. Bayesian analysis of N response descriptors

The analysis of the 730 regression curves using the Bayesian approach produced most probable values of the four maize N response descriptors as well as their corresponding uncertainties (Figure 3.3A-D). For B0, the estimates ranged from 0.5 to 17.5 Mg ha^{-1} with a median of 7.9 Mg ha^{-1}, and uncertainty ranged from 0.3 to 4.0 Mg ha^{-1} with a median of 1.4 Mg ha^{-1}. For YEONR, estimates ranged from 1.5 to 19.0 Mg ha^{-1} with a median of 12.4 Mg ha^{-1}, and uncertainty ranged from 0.2 to 8.2 Mg ha^{-1} with a median of 1.6 Mg ha^{-1}. For EONR, estimates ranged from 0 to 368 kg N ha^{-1} with a median of 158 kg N ha^{-1}, and uncertainty ranged from 8 to 261 kg N ha^{-1} with a median uncertainty magnitude of 49 kg N ha^{-1}. Lastly, NFE estimates ranged from 4.2 to 68.8 kg yield kg N^{-1} with a median of 22.1 kg yield kg N^{-1}, and uncertainty ranged from 2.1 to 39.5 kg yield kg N^{-1} with a median uncertainty of 7.1 kg yield kg N^{-1}. The uncertainty in B0, YEONR and NFE showed a poor association with the estimated values (Figure 3.3E, F, H), while EONR uncertainty was more closely related to estimates, with a trend of higher uncertainties with at both low as well as at high EONR estimated values (Figure 3.3G).

3.3.3. Prediction performance

As expected, the xgboost algorithm showed better performance in predicting estimated values than in predicting uncertainties (Figure 3.4). The prediction of estimates showed RMSE medians of 1.90 Mg ha^{-1} for B0 (RRMSE = 24%), 1.68 Mg ha^{-1} for YEONR (RRMSE = 14%), 52 kg N ha^{-1} for EONR (RRMSE = 34%), and 10.2 kg yield kg fertilizer N $^{-1}$ for NFE (RRMSE = 40%). The prediction of uncertainties resulted in RMSE of 0.52 Mg ha^{-1} for B0 (RRMSE = 36%), 1.17 Mg ha^{-1} for YEONR (RRMSE = 72%), 44 kg N ha^{-1} for EONR (RRMSE = 69%), and 6.2 kg yield kg fertilizer N $^{-1}$ for NFE (RRMSE = 66%). The rest of the dimensionless metrics, although with different error penalization rules, indicated that the uncertainty magnitudes were much more complex to predict than the estimates (Figure 3.4). For example, R^2 ranged from 0.36 to 0.71 when predicting estimates, while varied from 0.08 to 0.22 in the case of predicting uncertainties.

3.3.4. Features contribution

The permutation importance test served as an indicator of the relative contribution of features (Figure 3.5) to explained variability by the xgboost algorithm (Figure 3.4). Results indicate that the crop management factors under study were more relevant to predict the estimates rather than the uncertainties of the N response process. Particularly for the estimate of B0, crop management contributed 50% of explained variability (Figure 3.4A), while it only contributed about 1% of explained uncertainty (Figure 3.4B). For YEONR, EONR and NFE estimates, crop management contributed 16%, 19%, and 12%, respectively, of explained variance. In contrast, crop management contributed only 4%, 4%, and 3% of explained variance of YEONR, EONR, and NFE uncertainties, respectively. Regardless of the descriptor estimate or uncertainty, the contribution of soil variables to explained variances was more consistent, ranging from 10% to 23% of explained variance of the N response. Lastly, and as expected, the contribution of weather variables to explained variance was more relevant for prediction of uncertainties than for prediction of estimates. Regardless of the N response descriptor, weather contributed from 72% to 81% of explained variance of uncertainties. In the case of estimates, weather was particularly useful for the prediction of YEONR (64%), EONR (67%), and NFE (78%) components.

Among the crop management components affecting B0 value prediction, previous crop contributed about 37% of explained variance, while irrigation contributed about 13%. In terms of

B0 uncertainty, however, previous crop and irrigation showed a negligible influence (Figure 3.5). The most influential weather variable for the B0 expected value was vpd during the pre-sowing period (6%), while precipitations during the late vegetative period (Pp_2) and vpd during grain filling (vpd_4), and clay content, respectively, were the most relevant variables, each contributing about 6% of explained variance of B0 uncertainty. In the case of YEONR estimates, the most relevant feature resulted SOM with ca. 11% of explained variance, while irrigation and previous crop contributed with ca. 14%. Although precipitations and radiation around the flowering period (Pp_3, 6%; Rad_3, 5%) and distribution of precipitations during the late-vegetative period (SDI_2, 3%) resulted among the most important weather features, importance patterns highlight an evenly distributed contribution of evaluated weather variables. Similarly, although precipitations during late vegetative period (PP_2) resulted the most important weather variable (ca. 6%), most of features evenly contributed to explain YEONR uncertainty. Lastly, soil variables contributed with ca. 23% of explained variance, with silt (9%) and SOM (6%) as the most important features, while crop management variables showed an insignificant contribution to YEONR uncertainty (5%).

Previous crop was the most important variable to predict expected EONR values, explaining about 17% of variance. Nonetheless, as stated above, crop management showed a trivial contribution to explain EONR uncertainty. The silt fraction contributed with ca. 5% of explained variance of EONR estimates and ca. 10% of EONR uncertainty. However, we were not able to observe a clear set of most important weather variables defining either estimates or uncertainties, denoting the complex association patterns involving EONR. Similarly, previous crop exerted the most important influence on NFE estimates (ca. 11%), however, the rest of evaluated variables evenly contributed to predict NFE. In terms of the NFE uncertainty, as the most important variables,precipitations around grain filling period (Pp_4) contributed with ca. 5% of explained variance, while clay, SOM, and clay contributed with ca. 5%, 4%, and 4% of explained NFE-uncertainty variance, respectively.

3.4. Discussion

This study provides an unprecedented assessment of the N response in maize, combining Bayesian statistics with machine learning to unraveling the contribution of crop management, soil, and weather factors to the prediction of both the expected response and its related uncertainties. Highlighting the stochastic nature of the process, this work offers a decomposition of the N response into simple and interpretable components (Figure 3.2A). In the scientific literature, scarce attempts can be highlighted related to considering the parameters of the yield response to N supply as random variables (Hernandez and Mulla, 2008; Tembo et al., 2016; Boyer et al., 2013). However, none of the existing literature on this topic has addressed the investigation of the drivers behind the uncertainty magnitude in the estimated parameters of the maize yield to N supply responses for a given environment.

Improving the awareness of the uncertainties is critical to convey wise information to stakeholders, moving from a static/experience based to a more dynamic/data-driven decision-making process. Similar insights have been recently offered by Laurent et al. (2020) when discussing the benefits of reporting credibility intervals and probability of mean effect size for on-farm network trials. Enhancing the capability of current models to capture uncertainty and to provide sensitivity analysis is the foundation for deploying Bayesian frameworks (Makowski et al., 2004; van de Schoot et al., 2014) to become one of the new pillars for the improved crop N recommendation systems around the globe.

A valuable novelty in our approach is considering the stochastic nature of prices when estimating the EONR. In this regards, although the uncertainties in maize and fertilizer N prices are both major factors deciding fertilization strategy (Blackmer and Kyveryga, 2012), the clear majority of the literature studying the EONR only considered fixed prices for simplicity (e.g., Scharf et al., 2005; Kyveryga et al., 2007; Alotaibi et al., 2018), missing a relevant random component when developing N guidelines. Hence information on historical series of prices at local and/or regional levels should be considered when estimating the EONR (Yost et al., 2014; Nigon et al., 2019). From an economic standpoint, an *ex-ante* approach is the most adequate when estimating EONR (Bullock and Bullock, 2000; Hernandez and Mulla, 2008), for which the evaluation of uncertainties is crucial. In addition to model the uncertainty on the yield response components, we have demonstrated that employing Bayesian statistics also allows to model the variability on the prices ratio by using available historical prices data as a prior.

From the main factors linked to the estimates of the maize N response curves, previous crop (alfalfa) and irrigation have been already identified as critical for B0 (Correndo et al., 2021a) mainly due to the effect of soil N supply and soil physical conditions (Yost et al., 2014; Riedell, 2014) and water as critical factor limiting productivity for field crops and maize (Mueller et al., 2012; Meng et al., 2016). Likewise, for YEONR, water and previous crop were quite relevant from a management standpoint, but with a larger role of SOM with a minor influence of clay as key soil factors for attaining high yields (Lal, 2004; Tremblay et al., 2012). For both EONR and NFE, the influence of weather on the estimation of these factors is more relevant in agreement with previous reports highlighting the impact of this factor on N supply and demand (Soufizadeh et al., 2018).

This study provides relevant insights on the importance of weather (72 to 81%) for improving forecast models that enhance our ability to predict the uncertainties in N response. From a weather standpoint, the most relevant features were evident 60 days after planting time. On the one hand, this emphasizes the importance of further improving the in-season diagnosis tool for crop N status (Scharf et al., 2011). In that regard, combining sensor data with machine learning techniques appears as a promising approach (Wang et al., 2021a). On the other hand, this denotes the need for improving our understanding of future weather conditions and our ability of developing probability scenarios (using historical weather as a proxy)when deciding optimal N rates to be applied in our diverse (*e.g.*, different crop rotation, tillage, management) farming systems. Lack of adequate spatial resolution weather data is a large constraint not only for developing more precise forecasts but also for improving relevant decision support tools (Van Wart et al., 2015). The main challenges for estimating the economic production potential for large field regions is generally linked to the uncertainty of weather forecasts and changes of agricultural landscapes (Jones et al., 2000). In addition, the uncertainty of weather data and its interpolation greatly depend on the density and distribution of weather stations within a region (Mourtzinis et al., 2017). However, future challenges for weather data are mainly connected to the ease of access, data quality, and comprehensiveness/evaluation for this information for relevant use on decision tools and research in agriculture (Overpeck et al., 2011).

The minor role of the evaluated crop management factors (previous crop, irrigation and tillage) on predicting the uncertainties of the yield response to N implies the need of testing the relevancy of other practices (e.g., fertilization strategy, hybrid, plant density) for explaining residual variance. Our results also remark a consistent but limited contribution of the evaluated soil features to understand the uncertainty of N response process. Nonetheless, the inference related to SOM and soil texture fractions results limited since they are not direct and perhaps inconsistent estimators of soil N mineralization (Schomberg et al., 2009; Ros et al., 2011; Cai et al., 2016) and they may also carry confounding effects regarding geographical differences. Thus, further soil indicators regarding soil N supply may be valuable inputs for N response prediction models (Franzluebbers, 2018; McDaniel et al., 2020). Both results may reflect limitations in our approach. As described in Correndo et al. (2021a), our database presents unevenly reported metadata and a lack of relevant features such as pre-plant and/or in-season soil N supply, plant growth determinations, N concentration in tissues or overall plant N uptake, maturity dates, genetic material, among other data descriptors that could ultimately result on improved prediction performance.

Historically, fertilizer N recommendations have been based on estimated production functions treated as the “true” underlying model, largely ignoring the inherent uncertainty existent in any relationship and its associated errors. The estimated uncertainties in our research serve as a measure of risk magnitude when modeling the yield response functions to generate N recommendations. Our main finding is that the EONR presents an significant inherent uncertainty, typically about 50 kg N ha^{-1}, with an increasing risk of erratic estimates at both low (< 100 kg N ha^{-1}) and high (> 200 kg N ha^{-1}) expected EONR values. Empirical evidence indicate that the majority of US maize farmers prefer in-field management strategies as a method of adapting to climate-based risk (Mase et al., 2017). Thus, producers commonly consider N fertilizer as a risk reducing factor (Babcock, 1992; Scharf et al., 2005). In other words, the uncertainty derived from weather or soil N supply most likely leads to increased N rates as risk-neutral farmers perceive profitable to reduce the probability of being caught short of N. Notwithstanding, our evidence indicates that increasing the N fertilizer rate “just in case” (without a clear rationale) under high EONR uncertainty would result both environmentally and economically riskier.

Lastly, this study also provides insights on the opportunity to model the uncertainties of the yield response functions, with the challenge of enhancing the quality of in-season weather forecasts and generating robust prediction frameworks. Crop simulation tools such as DSSAT (Jones et al., 2003), APSIM (Holzworth et al., 2018), or more specific models such as Adapt-N (Melkonian et al., 2008; Sela et al., 2016) combining crop management, soil, and in-season weather data to optimize split applications of N fertilizer are a robust foundation. For example, Adapt-N offers estimates of the uncertainty around the recommended rate and allows to use a set of risk considerations related to market prices and N dynamics. Still, the challenge is to transform the simulation frameworks from deterministic to more probabilistic. Decision support tools focusing on N recommendations should ideally provide potential seasonal weather scenarios and their probabilities to understand the level of risk taking by agronomists, farmers, and stakeholders. The data-fusion approach of integrating observed weather data during the early vegetative period and historical weather to create potential scenarios during the late vegetative and reproductive periods represent a unique opportunity to evaluate risks when deciding the N rate (Wang et al., 2021b). The inclusion of stochastic dominance analysis (studying conditional distributions instead of just means) may also provide valuable insights about key factors to manage risks on N decisions, as it has been made for other production factors such as genetics (Nolan and Santos, 2019). Therefore, still major efforts on risk research should be the main focus when fine-tuning decision tools for input utilization in farmer fields, conducting scenarios for combinations of types of risk based on probabilities of historical data (Pannel, 1997) and/or based on better seasonal weather forecasts.

3.5. Conclusions

This study provides relevant insights on understanding the estimation of the N response for maize, with the additional component of assessing the level of uncertainty for those parameters of the response models. One of the main conclusions of this work is that the expected values of N response components and, although more challenging, their related uncertainties are both susceptible to be modeled. More precisely, yield without N (B0), YEONR and NFE are the most predictable components of N response, while the biggest difficulties were found for predicting the EONR component. Although challenging, broadly variable and susceptible to change by weather, we foresee that uncertainties can be modeled, especially for the B0 and NFE components.

Weather features contributed with roughly two-thirds of explained variance of YEONR and NFE. In addition, weather variables were, undeniably, the most relevant metadata (72% to 81%) to predict the uncertainty of N response (mainly reflected in the EONR). Crop management factors largely affected the prediction of the expected B0, but slightly influenced all the other parameters of the maize N response model. Likewise, crop management displayed a trivial influence (<5%) on the uncertainty of the N response components. Soil factors exerted a consistent but limited contribution to explain both expected N response as well as their uncertainties.

Overall, this research suggests that improvement on the decision support tools should consider the uncertainty of yield response to N supply models as a type of risk, potential in-season weather scenarios, and develop probabilistic frameworks for improving the data-driven decision-making process for N fertilization in maize. The combination of improved modeling approaches along with artificial intelligence tools and advance statistical frameworks (e.g. Bayesian) can provide more dynamic options for N management in maize and other major field crops.

Table 3.1. Meta-data included for studying their influence on selected descriptors of the N response process in maize. *CHU = crop heat units (Tremblay et al., 2012). †das = days after sowing.

Management		
Variable	*Levels*	
Previous Crop	alfalfa; annual legumes (soybean); others (maize, sorghum, wheat, barley, rye, sunflower)	
Tillage system	Tilled; no-till	
Irrigation	Irrigated; Rainfed	
Soil		
Variable	*Units*	*Depth*
SOM = Soil Organic Matter	%	0-15 cm
Clay		
Silt		
Sand		
Weather		
Variable	*Units*	*Periods*
Pp = Precipitations (sum)	mm	pre = -30 – -1 das†, 1 = 0-30 das, 2 = 31-60 das, 3 = 61-90 das, 4 = 91-120 das,
Tm = Mean Temperature (average)	ºC	
SDI = Shannon Diversity Index	0-1 (uneven - even)	
EPE = Extreme PP Events (count)	# days PP > 25 mm	
vpd = Vapor Pressure Deficit (average)	KPa	
Rad = Incident radiation (sum)	MJ m^{-2}	
Q = Photothermal quotient	MJ m^{-2} / CHU*	
ETE = Extreme T Events (count)	Days w T_{max} > 30ºC	2,3,4

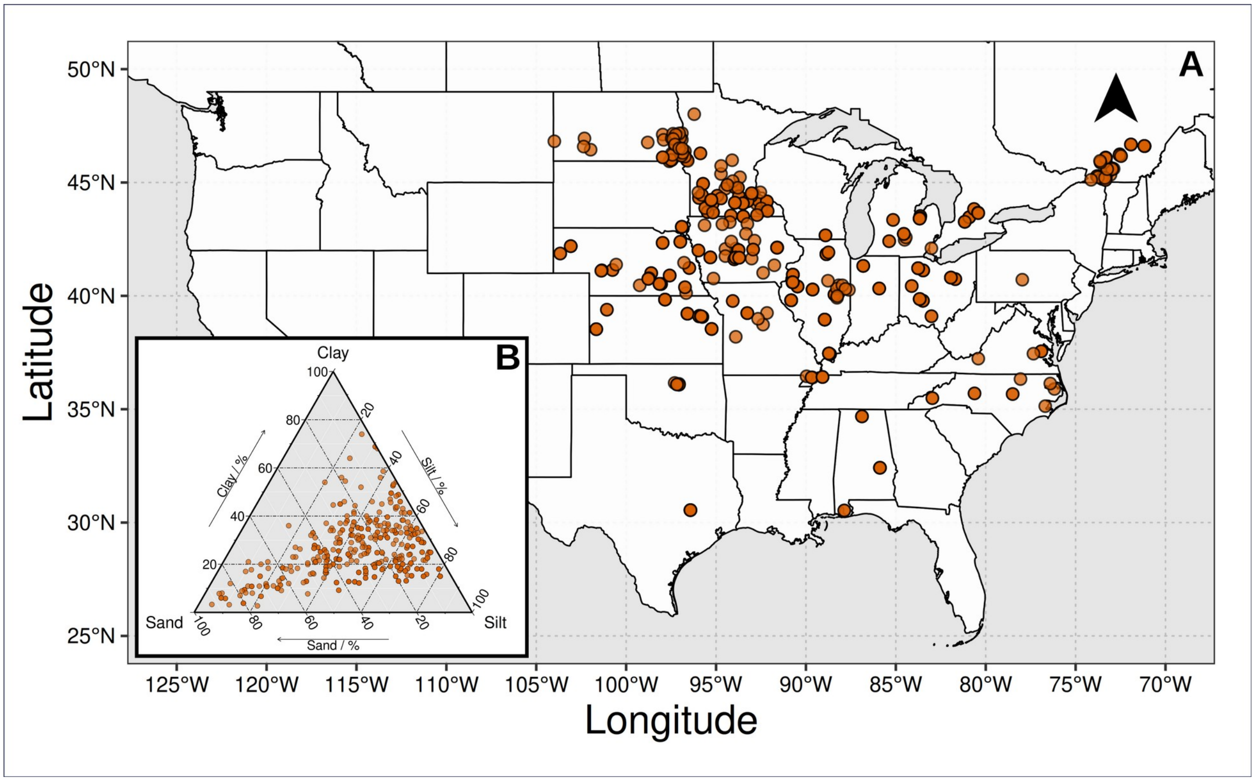

Figure 3.1. A: Geographical distribution of maize nitrogen fertilization trials under study (730 response curves from 481 site-years) performed in the USA and Canada during the period 1999-2020. B: soil texture distribution (0-15 cm).

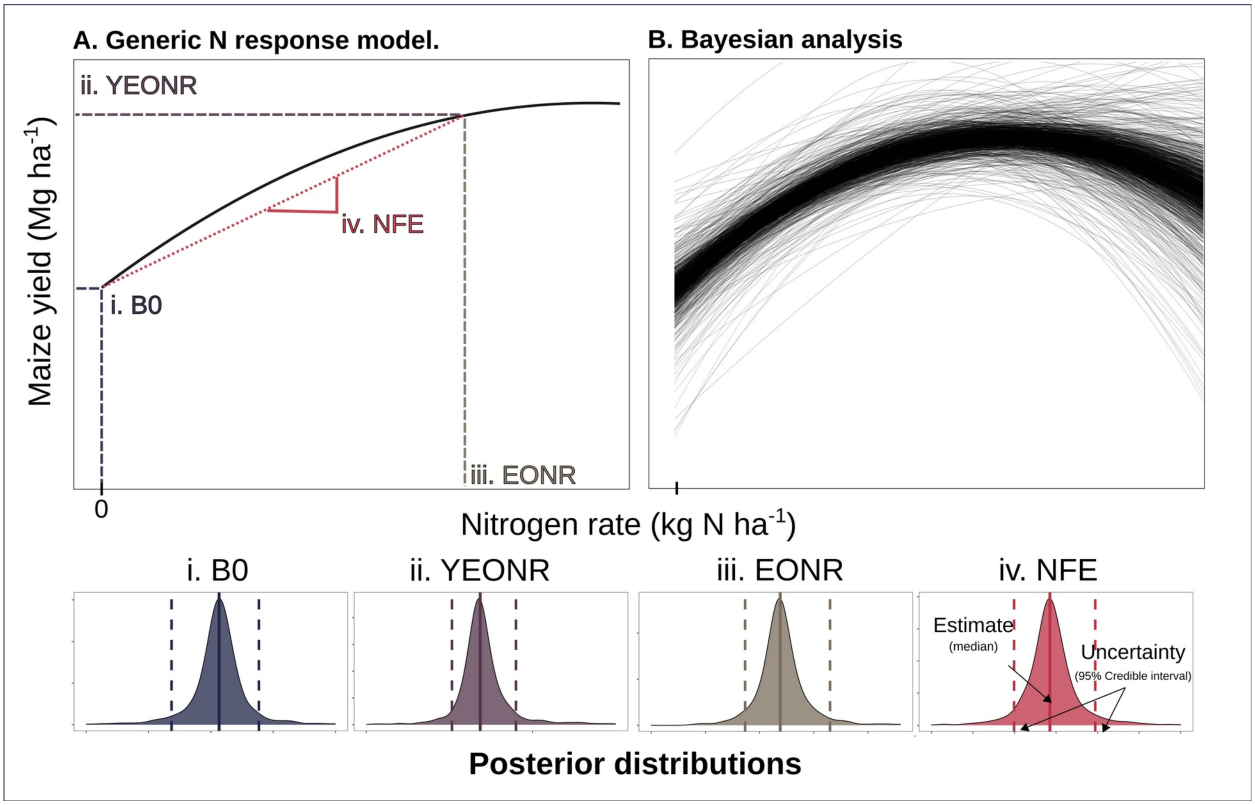

Figure 3.2. Conceptual representation of the N response process descriptors of interest (A), and the applied Bayesian analysis framework (B) to obtain both estimates and uncertainties from posterior distributions of: i. B0 (yield without N, Mg ha^{-1}), ii) YEONR (yield at EONR, Mg ha^{-1}), iii) EONR (kg N ha^{-1}), and iv) NFE (kg yield response kg N^{-1} at EONR).

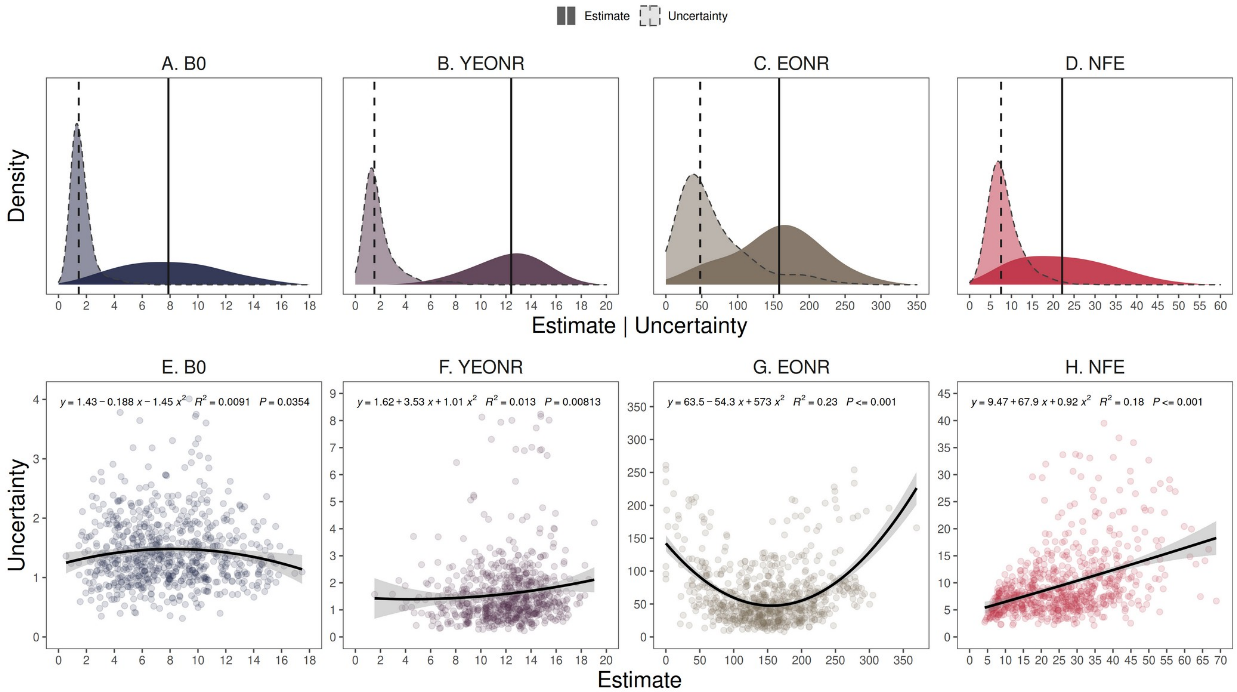

Figure 3.3. Distribution of estimates and their corresponding uncertainties (A-D) of the four selected maize nitrogen response descriptors (A: intercept (B0, Mg ha^{-1}); B: yield at the economic optimum N rate (EONR)(YEONR, Mg ha^{-1}); C: EONR (kg N ha^{-1}); and D: N fertilizer efficiency to the EONR (NFE, kg yield kg fertilizer N^{-1}); and the relationship between the uncertainty of each descriptor and its estimate (E-H). In A to D, vertical lines indicate the medians of the distributions (solid: estimate, dashed: uncertainty).

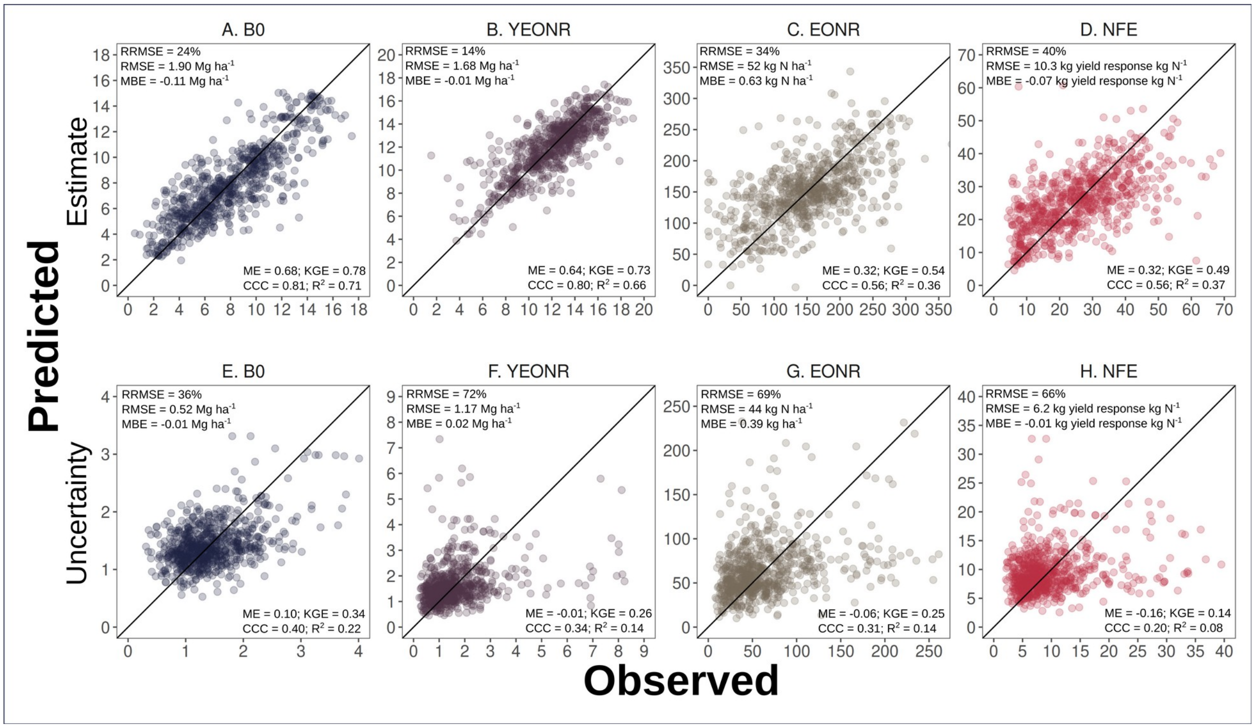

Figure 3.4. Extreme gradient boosting performance for the prediction of estimates (A-D) and uncertainties (E-H) of four descriptors of the maize nitrogen response process: i) intercept (B0, Mg ha^{-1}), ii) yield at economic optimum nitrogen rate (EONR) (YEONR, Mg ha^{-1}), iii) EONR (kg N ha^{-1}), and iv) nitrogen fertilizer efficiency (NFE = kg yield response kg N^{-1}). Data points are pooled from 20 out-of-bag (OOB) testing samples from cross-validation procedure. Metric values represent the medians of the OOB samples. RMSE: root mean square error; RRMSE: relative RMSE; MBE: mean bias error; ME: Nash-Sutcliffe model efficiency; KGE: Kling-Gupta model efficiency; CCC: concordance correlation coefficient; R^2: coefficient of determination.

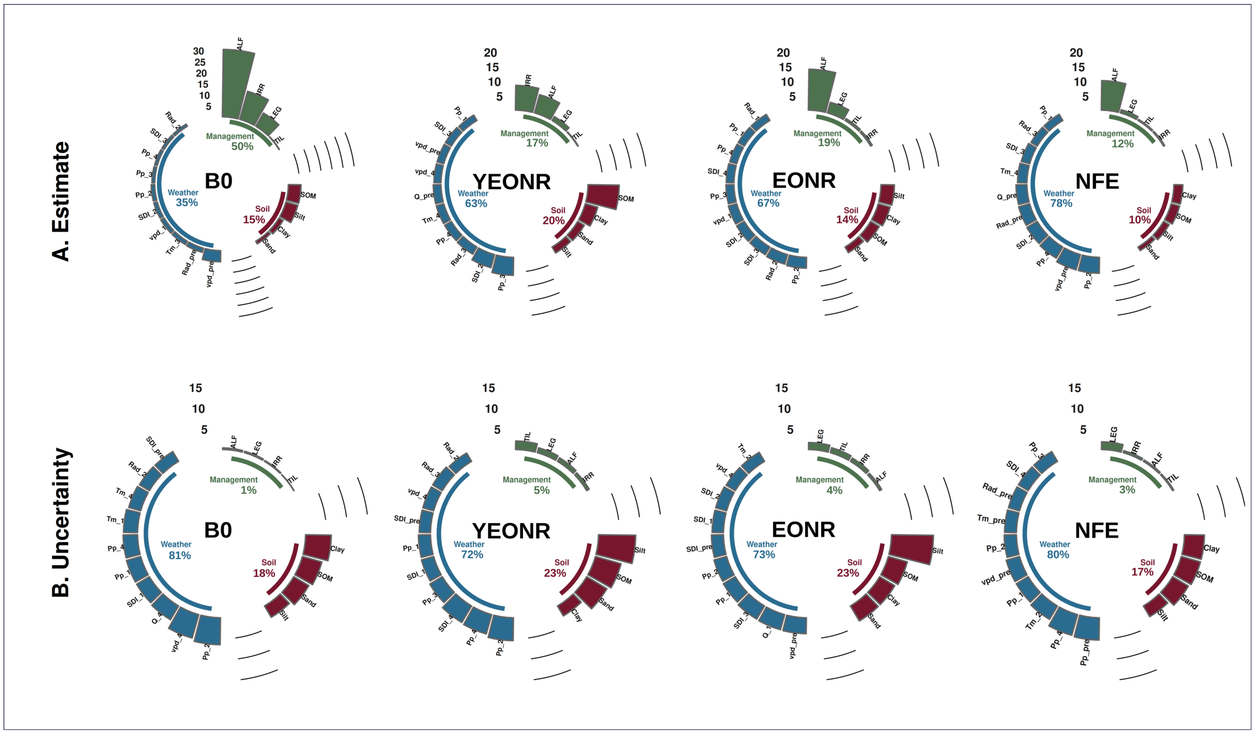

Figure 3.5. Relative contribution (%) of crop management, soil, and weather variables (10 most important) to expected estimates (A) and uncertainties (B) of main descriptors of the maize nitrogen responsiveness process: i) intercept (B0), ii) yield at the economic optimum N rate -EONR- (YEONR), iii) EONR, and iv) nitrogen fertilizer efficiency (NFE = (YEONR – B0) / EONR).

Chapter 4: Do water and nitrogen management practices impact grain quality in maize?

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Abstract

Concomitantly pursuing superior maize (*Zea mays* L.) productivity with grain quality is essential for food security. Therefore, this study provides a meta-analysis of 21 studies assembled from the scientific literature to tackle the effect of the two most limiting factors for maize production, water and nitrogen (N), and their impacts on grain quality composition, herein focused on protein, oil, and starch concentrations. Water stress levels resulted in erratic responses both in direction and magnitude on all grain quality components, plausibly linked to different duration, timing, and intensity of water stress treatments. Nitrogen fertilization more consistently affected grain protein concentration, with a larger effect size for protein as fertilizer N levels increased (protein change of +14% for low, ≤ 70 kg N ha^{-1}; +21% for medium, >70-150 kg N ha^{-1}; and +24% for high, >150 kg N ha^{-1}). Both starch and oil grain concentrations presented less variation to fertilizer N levels. The positive protein-oil correlation (r = 0.49) permitted to infer that although oil concentration may reach a plateau (8%), further increases in protein are still possible. Augmented research on grain quality is warranted to sustain food production but with both high nutritional and energetic value for the global demand.

4.1. Introduction

The overgrowing demand for improved quality of agricultural products has stressed the already need for food, feed, fuel, and fibers. In recent years, there have been greater emphasis on quality of cereal grain in addition to yield. For this study, we use the term ‘grain quality’ to explore impacts on protein, oil, and starch compounds of cereal grains. From the perspective of crop improvement, plant breeders are dauting task to create more nutritious crops (‘biofortification’) without compromising further yield gains (Vyn and Tollenaar, 1998; Morris and Sands, 2006). However, development of nutritious crops requires a joint effort of multiple disciplines, from agronomy to food scientists (Diepenbrock and Gore, 2015).

Cereals contribute to roughly 60% of the total world food demand (Darra et al., 2019). Within the cereals, maize (*Zea mays* L.) plays a significant role in animal feed and human nutrition, as the main source of both energy and protein for tropical and sub-tropical regions (Motukuri, 2020). It is also one of the most important staple food crops for humans and key for global food nutritional security in both developed and developing countries. During the last decades, it has also gained significance as a source of vegetable oil (Ali et al., 2010). In 2019, global maize harvested area was roughly of 197 million ha, with a total production of 1148 million tons and average yield of 5.8 Mg ha^{-1} (FAO, 2021). From a grain composition, mature grain of dent maize presents 60% to 72% starch, 8 to 11% protein, and 4 to 6% oil (Jahangirlou et al., 2021). Starch and protein are mainly stored in the endosperm (ca. 90% of the grain weight), while the oil is mainly in the embryo (ca. 10% of the grain weight) (Flint-Garcia et al., 2009). For this study, grain quality is investigated as the changes in grain protein, oil, and starch concentrations.

Maize grain yield and quality attributes are interrelated and are highly influenced by environmental conditions (Butts-Wilmsmeyer et al., 2019). One of the major abiotic stresses related to climate change is water stress (drought), adversely impacting yield and quality of many field crops (Alqudah et al., 2010). It has been demonstrated that drought could decrease the starch concentration and increase the protein concentration in grains of many crops (Lu et al., 2014). Non-limiting water availability during flowering and grain filling periods increased grain yield and protein concentration in maize (Butts-Wilmsmeyer et al., 2019). Severe water stress decreased grain yield and starch but increased protein concentration in maize relative to no stress conditions (Ge et al., 2010). Water stress during grain filling stages decreased grain yield but may present no major changes in protein and oil concentration (Barutçular et al., 2016). Drought stress after pollination significantly decreased grain yield, increased grain protein concentration but not starch (Lu et al., 2014). While water stress during late vegetative stages stress increased seed oil concentration in maize (Ali et al., 2010).

Management practices modifying the availability of resources, especially during critical periods, are also likely to alter the grain components (Martinez et al., 2017) mainly through changes in the source/sink ratios (Borras et al., 2002). Among other key practices such as sowing date (Abdala et al., 2018), nitrogen (N) management is indisputably one of the most limiting factors not only for grain productivity but also for the grain quality attributes (Miao et al., 2006; Cirilo et al., 2011). Besides the well documented effects of N deficiencies in biomass and grain production, they are also likely to impact the grain quality composition. For instance, Jahangirlou et al., (2021) reported that high N applications (184 kg N ha^{-1}) not only increased yield but also grain quality mainly due to increments in the concentration of non-essential amino acids. The same authors also observed that more frequent irrigation events (6 day intervals) and a high fertilizer N rate increased oil and starch concentrations. This emphasizes the existence of interactions of water x N management and co-limitations (Sadras, 2005) on grain yield and quality traits, with impacts dependent upon timing, duration, and intensity of stress. Although few studies have quantified the impacts water stress and nitrogen fertilization levels on grain quality trains (protein, starch, and oil concentrations) under field and controlled environmental conditions, those investigations were all conducted under different genotype, environment, and management (GxExM) scenarios. These published data have not been synthesized to better understand generalized effects across all studies. For this purpose, meta-analysis is a method that can help with integrating knowledge and results from diverse studies and evaluate the impact of treatment on sets of target variables and provides a quantitative estimates of effect sizes (Tremblay et al., 2012; Laurent et al., 2020; Fernandez et al., 2020).

The overall objective of this study was to execute a meta-analysis to evaluate the effects of water and nitrogen levels on the three main components of maize grains: protein, starch and oil concentrations. The specific goals of this study were to employ a meta-analytic model to: i) study the effect of water stress levels on grain protein, oil, and starch concentrations, ii) investigate the effect of N fertilization and quantify the impact of N (sub-level of N level) added (low, <70 kg N ha^{-1}, medium, >70-150 kg N ha^{-1}, and high, >150 kg N ha^{-1}) on grain protein, oil, and starch concentrations for maize crop.

4.2. Materials and Methods

The source of data were only published manuscripts under the peer-review process. Using the Web of Science®, CAB-Abstracts®, and Scopus® search-engines, the following keywords were applied as a filter: corn or maize, and grain quality or grain composition, and nitrogen fertilization or water stress or drought stress. The search was also constrained to journal articles, and to the agricultural and biological sciences areas. Therefore, we also applied the following keywords in the search equation: not fodder, not animal, not soil. After the initial results, a screening of titles was applied in order to reduce the number of candidate studies. A total of 91 manuscripts were downloaded and revised, with only 21 retained based on the following criteria: i) replicated experiments, ii) treatments of interest included either N fertilization (control vs. fertilized) or water management treatment (irrigated as control and water stressed as the treated plot), iii) variables of interest reported at the treatment level including grain yield, and/or nitrogen (N) concentration, and/or protein, and/or starch, and/or oil concentrations. In addition to the engine search, a set of experiments belonging to a comprehensive database on +30 N trials in maize (Wortmann et al., 2011) was included. Although these trials were not particularly designed to evaluate maize grain quality, the database met the criteria. When protein data were not reported, protein was calculated as the grain N concentration multiplied by a factor of 5.6x following Mariotti et al. (2008), Sosulski and Imafidon (Mariotti et al., 2008; Sosulski and Imafidon, 1990).

The final database consisted of 21 data sources (92 site-years) comprising experiments published between 1972 and 2019, and distributed across 11 countries (Argentina, Brazil, Canada, China, India, Iran, Pakistan, Serbia, Turkey, United States, and Venezuela) (Table 4.1). In terms of the factors of interest, a total of 12 studies (75 trials) only evaluated the effect of N on grain quality, 7 studies (15 trials) only evaluated the effect of water stress on grain quality, and 1 study (2 trials) evaluated their interaction. Most of the experiments were performed under field conditions, and one study was carried out under controlled environmental conditions (Lu et al., 2014). This controlled study was included as it satisfied our search criteria and to expand the database. In terms of variables of interest, a total of 20 studies accounted for protein concentration, 14 studies evaluated starch concentration, and 14 reported oil concentration.

Grain yields were adjusted to dry basis (0 g moisture kg^{-1}), and protein, starch, and oil were standardized to percentage (%) units. The final database consisted in 510, 570, 279, and 265 data points for grain yield, protein, starch, and oil concentration, respectively.

4.2.1. Statistical analysis

Descriptive statistics provide a summary of variables of interest in the compiled database (Table 4.2). Simple correlation (Figure 4.1) and regression analyses were performed in order to study the relationships among the grain quality components (Figure 4.1) and the components and yield (Figure 4.2).

4.2.1.1. Meta-analysis

Meta-analysis models are particularly useful identifying patterns when data from multiple sources are combined and analyzed (Fernandez et al., 2020; Philibert et al., 2012). Thus, for the comparison of water stress and N fertilization effects on grain quality components, random effects meta-analysis models were fit following the log response ratio (lnRR) approach (Hedges et al., 1999). This type of meta-analysis allows to acknowledge that the effect of a single study come from a distribution of effects rather than cdautingonsidered as fixed. The meta-analyses were performed with the metafor package (Viechtbauer, 2010) in R software (R Core Team, 2021). Each model consisted into the evaluation of specific effect sizes of the treatments of interest. The three models to analyze the water stress effect were split into: i) protein concentration, ii) starch concentration, and iii) oil concentration. The effect sizes of water stress on these quantities were estimated following Eq. (4.1) and Eq. (4.2):

$$y_{i(j)} = \ln\left(\frac{z_{stress}}{z_{control}}\right) \quad \textbf{(4.1)}$$

$$v_{i(j)} = \frac{1}{w_{i(j)}} = \frac{n_{stress} + n_{control}}{n_{stress} * n_{control}} \quad \textbf{(4.2)}$$

where $y_{i(j)}$ is the water stress effect size for the ith observation nested within the jth study, and $z_{i(j)}$ is the concentration of protein, starch, or oil in the water stressed (z_{stress}) or the in the water-controlled ($z_{control}$) treatments. Each y_i were subsequently weighted using the inverse sample variance of each case ($v_{i(j)}$), using the corresponding sample sizes (n) to estimate the weights ($w_{i(j)}$).

Similarly, for the N models, the effect sizes of N fertilization on the grain quality components were estimated following Eq. (4.3) and Eq. (4.4):

$$x_{i(j)} = \ln\left(\frac{z_{N_f}}{z_{N_0}}\right) \quad \textbf{(4.3)}$$

$$v_{i(j)} = \frac{1}{w_{i(j)}} = \frac{n_{N_f} + n_{N_0}}{n_{N_f} * n_{N_0}} \quad \textbf{(4.4)}$$

where $x_{i(j)}$ is the N fertilization effect size for the ith observation nested within the j^{th} study, and $z_{i(j)}$ is the concentration of protein, starch, or oil in the N-fertilized (z_{Nf}) or the in the control (z_{N0}) treatments. Each $x_{i(j)}$ were subsequently weighted using Eq. (4.4).

Since the studies presented a wide range of N fertilization rates (30 to 280 kg N ha^{-1}, Table 1), a second meta-analysis was fit for the N models in order to assess the effect of the N level as follows: i) low N (< 70 kg N ha^{-1}) ii) medium N (>70-150 kg N ha^{-1}), and high >150 kg

N ha^{-1}). Thus, the effect size of N fertilization (x_i) was also assessed at the sub-level of N level within each study.

In order to estimate the confidence intervals (CI, 95%) of the mean effect sizes at the study and overall levels, we used non-parametric bootstrapping stratified by study in order to conserve the original data structure. Thus, at the study level (j), the available observations (i) were resampled with replacement (n=5000) (Adams et al., 1997; Van Den Noorgate et al., 2005) using the *boot* package (Canty et al., 2021) in R-software. The heterogeneity between studies was calculated using the I2 statistic to detect whether all of them are assessing the same effect (Borenstein et al., 2009).

Forest plots were used to summarize the effects of water and N fertilizer, re-expressing the y_j, x_j (ln ratios), and their respective confidence intervals (95% CI) to percentage units (%) using Eq. (4.5) and Eq. (4.6).

$$\textit{Water Stress Effect}\,(\%) = \left(\exp^{y_j} - 1\right) * 100 \qquad \textbf{(4.5)}$$

$$\textit{N fertilizer Effect}\,(\%) = \left(\exp^{x_j} - 1\right) * 100 \qquad \textbf{(4.6)}$$

4.3. Results

The descriptive analysis of the database indicates that maize grain yield showed a wide range of values, with an average of 8.7 Mg ha^{-1}, ranging from 1.8 to 18 Mg ha^{-1}, and with a standard deviation of 2.8 Mg ha^{-1} (Table 4.2). Although only 3 studies reported yield data on water stress, limiting the comparison, water limited treatments resulted in average yields of 8.4 Mg ha^{-1} relative to full irrigation with yields of 11.6 Mg ha^{-1}. Similarly, in average, N-limited yields were of 6.4 Mg ha^{-1}, while N fertilized were of 9.2 Mg ha^{-1}.

Protein concentration varied between 2.8 to 18%, with a mean of 8.0% and a standard deviation of 2.0%. While water stress appears not to exert an effect on maize grain protein, the N-limited scenario resulted in a mean of 7.0% while the N-fertilized averaged a protein of 8.2%. Starch concentration ranged from 44% to 80%, with a mean of 70% and a standard deviation of 5.4%, but with starch neither affected by water stress nor by N fertilizer. Finally, oil concentration ranged from 0.6 % to 7.9%, with a mean of 4.4% and a standard deviation of 1.3%, but also with trivial effect of both evaluated factors (Table 4.2).

In terms of trade-offs between grain quality components (Figure 4.1), protein and oil concentrations displayed an overall moderate positive correlation ($r = 0.49$), followed by a low but negative correlation between protein and starch ($r = -0.25$), and low but positive correlation between oil and starch ($r = 0.17$). A particular remark to the protein-oil relationship (Figure 4.1) is that oil concentration seems to reach a plateau about 8%, while it is still possible to achieve further increases in protein levels. Nonetheless, specific trade-offs were observed at each particular study (Supplementary Figure 4.1).

Even though significant relationships were observed between the quality components and grain yield (Figure 4.2), the strength of associations were characterized by their weakness ($R^2 < 0.1$). Besides the weak relationships, it is noteworthy to highlight that all three components presented large variability when yields were below ca. 10 Mg ha^{-1}. For instance, at a yield level of ca. 4 Mg ha^{-1}, protein ranged between < 4% to ca. 12%. In contrast, the range of protein, starch, and oil concentrations is considerably narrower with yield levels above ca. 10 Mg ha^{-1} (Figure 4.2).

4.3.2. Meta-analysis results

4.3.2.1. Water stress

The impact of water stress was contrasting across components and with high heterogeneity among studies (Figure 4.3). Although an overall null effect is expected, the effect was variable depending on the study and reflected by I2 values of 96, 99 and 93%, for protein, starch, and oil, respectively. Only two out of eight studies observed a significant reduction in protein (ca. 17%), one showed a small but yet significant reduction (ca. 4%), two showed a non-significant effect, and two studies presented a significant increase (7-10%) (Figure 4.3A). Three out of eight studies evaluating starch showed a significant increase under water stress (4.7% to 9.2%), four studies showed no effect, while two presented significant reductions of 7.0% and 18% (Figure 4.3B). Finally, three out of six studies evaluating oil showed a significant decrease in oil concentration (12% to 30%), three studies resulted in minor water stress effect, while one study observed a significant increase of ca. 45% (Figure 4.3C).

4.3.2.2. Nitrogen fertilizer

Regarding the N fertilizer effect, its impact on each grain quality component was relatively more consistent as compared to the water stress effect (Figure 4.4). Still the effect size was highly heterogeneous across studies, with I2 values of 90, 91 and 98%, for protein, starch, and oil, respectively. Although an overall positive effect of ca. 21% in protein is expected as a result of N fertilization (Figure 4.4A), across studies, the mean effect size varied from ca. +8% to +37%, being significant in the majority of the cases (12 out of 13). An overall small but yet negative N fertilizer effect (-1.5%) is expected in starch concentration (Figure 4.4B), while an overall null effect on the oil fraction (Figure 4.4C). Nonetheless, the effect on the two latter components differed across studies. Only three out of six studies observed a small (ca. -1.7 to -

2.7%) but yet significant reduction in starch (Figure 4.4B), while the remaining expressed a null effect. Out of the seven studies evaluating oil, two showed a decrease of oil (ca. -3.7 to -5.9%), one showed a small positive effect (+2.0%) while no significant effect on the remaining (Figure 4C).

Considering N fertilizer levels (Figure 5), low N rates (≤ 70 kg ha^{-1}) showed a significant mean effect on protein of +13.8%, while medium (>70-150 kg N ha^{-1}) and high rates (>150 kg N ha^{-1}) showed a similar but significantly greater effects than low N rates, with +21% and +24%, respectively. In terms of starch, all N fertilizer levels produced a low but yet significant starch reduction, with an overall effect of -1.7%. Finally, none of the N levels produced a significant impact of the oil concentration. Nonetheless, it is important to highlight the effect on the quality components differed across studies (Supplementary Figure 4.2).

4.4. Discussion

This meta-analysis offers a novel summary with focus on the effect of the two most limiting factors for maize production, water and N, on grain quality (protein, oil, and starch concentrations). Historically, water and N management studies have mainly focused on yield as the response variable, with less attention paid to the grain quality components [18]. In this regard, combining and weighing the results from multiple studies, our analysis represents a valuable contribution to the literature. This meta-analysis synthesized two-fold more data for protein relative to both starch and oil, highlighting the lack of research studies focused on quality, mainly in non-protein factors.

One of the first lessons is that a not clear trade-off was apparent between yield levels and the most expensive components in energetic terms (oil > protein > starch). Unexpectedly, we were neither able to confirm a negative association between the most (oil) and the less (starch) expensive components, nor between protein and starch concentrations (Borrás et al., 2002). Moreover, the positive association observed between protein and oil was somewhat surprising, although oil concentration remained relative constant at ca. %8 while protein levels could still be increased. This scenario remarks the stability of the oil fraction, which is mostly located in the embryo (Flint-Garcia et al., 2009), and the possibility of concomitantly high protein levels. Likewise, (Zhang et al., 1993) reported stable oil concentrations across N fertilization levels, also suggesting that an increase in protein could not necessarily imply a decrease in energy concentration.

The water stress effect on maize grain quality was mainly characterized by its inconsistency. Most likely, we could not distinguish noise from signal as the database encompasses stress treatments applied at different timing during season (e.g. entire season, around flowering, during grain filling), with different intensity and duration, as well as different environments (soil and weather conditions), genetic materials (e.g. dent, semident, flint, wax), and management practices (planting dates, tillage systems, etc.). For example, the severity of drought impact on crops production generally depends on the soil moisture status and nutrients availability (Gandah et al., 2003). As these unaccounted factors were basically pooled in the meta-analysis, there is a risk of obscuring the actual impact of drought stress on the quality components. As water stress remains an undesirable scenario, when irrigation is not possible, the risk of water shortage should be managed with other crop practices such as sowing dates, hybrid selection, among others. We should also consider that the genetics, environment, and management (GxExM) factors may interact with the response to either water stress or N fertilizer levels (Tsai et al., 1992). It is also worth to remark that only one study evaluated combinations of water stress and N fertilizer, factors that are largely known for interacting and exert co-limitations (Sadras, 2005; Tremblay et al., 2012; Lemaire et al., 2020).

The effect of N fertilizer on grain quality showed, in contrast, a more consistent trend across studies, particularly for protein, as this fraction is generally expected to show increments with increasing resources, particularly N availability (Miao et al., 2006). Nonetheless, further research is needed regarding the effect not only in the protein concentration but also in its amino acids quality (Zhang et al., 2017). For example, diets with essential amino acids as the only N source are used less efficiently than diets with better ratio of essential to nonessential amino acids (Allen and Baker, 1974), which may ultimately modify the fate of N in the animal production (Lenis et al., 1999). Synergistic applications of N and S cannot only increase protein concentration but increase protein quality via increments in the concentration of essential amino acids, such as methionine, tryptophan, and lysine (Liu et al., 2020).

Our results suggest that N fertilizer rates within a medium-range (>70-150 kg N ha^{-1}) may be sufficient to saturate the response on protein (+21% with respect to a control), which will also cover a wide range of economic optimum N recommendations (Morris et al., 2018). However, more accurate interpretations on the effect of N on grain quality present the same challenge than research on grain yield (Morris et al., 2018): more accurate estimations of the soil N supply (Rain et al., 2019; Correndo et al., 2021a). Improved estimations of quantity (and timing) of soil N supply will help producers reducing the risk of losing efficiency with either a N deficiency or a N surplus. Other N sources such as mineralization and carryover from the previous year (Dhakal., 2019) may exert a significant influence on both grain yield and quality. In that regard, research on splitting the N fertilizer should expand the current focus on yield and efficiency improvements (Fernandez et al., 2020) to explore the role of late N applications on improving grain quality components as well.

Increases in protein may be concomitant with decreases in starch and/or in oil (Miao et al., 2006; Tamagno et al., 2016; Singh et al., 2002). However, we found an overall small reduction in starch due to N fertilizer, and oil resulted a stable fraction against changes in either water or N availability. In the scientific literature, a negative trade-off between protein and starch is generally reported for specific conditions [Butts-Wilmsmeyer et a., 2019; Borrás et al., 2002; Singh et al., 2002; Seebauer et al., 2010), while maize oil concentration is normally found as the most stable grain compound under varying environmental conditions (Borrás et al., 2002; Zhang et al., 1993; Singh et al., 2002; Genter et al., 1956).

Future research steps should seek to overcome certain limitations encountered in our work. A first shortcoming was related to very limited number of cases (11) reporting all three grain quality components and grain yield, constraining the evaluation and inference about potential trade-offs. A second deficiency was linked to the lack of studies reporting more detailed grain quality compounds such as amino- and fatty-acids, in order to expand our database and synthesis analysis. Prospective research should also explore the effect of heat stress on grain quality [10], either isolated or in combination with water and N management. Similarly, effect of other nutrients besides N and their interactions (co-limitations) is a relevant topic that warrants further investigation. Moreover, the explored literature presents a lack of standard practices reporting the laboratory protocols used to determine protein, starch, and oil concentrations (e.g., chemical extraction procedures, near infrared). Finally, from a methodological standpoint, the lack of presentation of measures of variation at the treatment level in the studies gathered by this meta-analysis restricted the possibilities regarding weighing procedures of the effect sizes (Weir et al., 2018).

4.5. Conclusions

Accompanying maize grain productivity increases with a high nutritional quality is essential towards the main goal of global food security. This meta-analysis reported that i) water stress resulted in erratic direction of the grain quality response, plausible to changes in timing, intensity, and duration of the stress; and ii) N fertilization not only increases yields but also grain protein concentration, while both starch and oil remained relatively stable under contrasting N levels. In the current context of an emerging food crisis, this study documented a remarkably important scenario for maintaining oil concentration while increasing the protein fraction. Under an adequate management of N fertilizer, this represents a unique opportunity of producing maize crops with both higher quality and energetic value.

Table 4.1. Data sources, measured grain quality variables, country, number of site-years per study (SY), water or nitrogen treatments, and other factors evaluated. PRO = protein, STA = starch, OIL = oil, FC = field capacity, RSMC = relative soil moisture content. *Performed under controlled conditions.

No.	Authors	Variables	Country	Years	SY(#)	Treatments	+Factors
			Water				
1	Ali et al., 2010	PRO, STA, OIL	Turkey	2007	1	Irrigated (15d intervals), Water stress (21d intervals)	Hybrid
2	Ali et al., 2011	PRO, STA, OIL	Turkey	-	1	Irrigated (15d intervals), Water stress (21d intervals)	Hybrid, Hormones
3	Barutcular et al., 2016	PRO, STA, OIL	Turkey	2014-2015	2	Irrigated (full), Water stress (reproductive)	Hybrid
4	Ge et al., 2020	PRO, STA, OIL	China	2002-2003	2	Irrigated (full), Water stress (mild-severe, 3rd leaf to maturity-)	-
5	Hussain et al., 2020	PRO, STA, OIL	Pakistan	2013-2014	2	Irrigated (full), Water stress (mild-severe)	-
6	Kresovic et al., 2007	PRO, STA, OIL	Serbia	2012-2014	3	Irrigated (full), Water stress (75% FC - 50% FC - rainfed)	-
7	*Lu et al., 2014	PRO, STA	China	2011-2012	2	Irrigated (75% RSMC), Water stress (60% RSMC, flowering to harvest)	Hybrid (wax)
8	Mason and Mason, 2002	STA	United States	1991-1994	4	Irrigated, rainfed	Hybrid, Plant density
9	Jahangirlou et al., 2021	STA, OIL	Iran	2018-2019	2	Irrigated (6d intervals), Water stress (12d intervals)	N
			Nitrogen				
9	Jahangirlou et al., 2021	PRO, STA, OIL	Iran	2018-2019	2	0, 184	Water Stress
10	Barrios and Basso, 2018	PRO, STA	Venezuela	2013	1	0, 100, 150, 200	Hybrid
11	Duarte et al., 2005	PRO, OIL	Brazil	2000-2001	3	0, 60, 120, 240	-
12	Ma and Biswas, 2016	PRO	Canada	2006-2010	5	0, 30,60,90,120,150,180	-
13	Miao et al ., 2006	PRO, STA, OIL	United States	2001-2003	6	0, 112, 168, 224, 336	Hybrid
14	O’Leary and Rehm, 1990	PRO	United States	1984-1986	8	0, 75, 150, 225	-
15	Perry and Olson, 1975	PRO	United States	1972-1973	2	0, 90, 180, 270	-
16	Simić et al., 2020	PRO, STA, OIL	Serbia	2016-2018	3	0, 180, 240	Tillage
17	Tamagno et al., 2016	PRO, STA, OIL	Argentina	2012-2013	2	0, 70, 165	Hybrid
18	Tsai et al., 1992	PRO	United States	1984-1986	3	0, 67, 134, 201, 268	Hybrid
19	Uribelarrea et al., 2004	PRO, STA, OIL	United States	2001-2002	2	0, 30, 60, 90, 120, 160, 200, 240	Hybrid
20	Wortmann et al., 2011	PRO	United States	2002-2004	32	0, 84, 140, 196, 280	-
21	Zhang et al., 1993	PRO, OIL	Canada	1989-1991	6	0, 90, 180	N timing

Table 4.2. Descriptive statistics of the reported data on maize grain yield (dry basis), protein, starch, and oil concentration split by the treatments of interest (water and nitrogen fertilizer). Main statistics are: sample size (n), mean, median, minimum (min), maximum (max), standard deviation (sd), and coefficient of variation (%).

Variable	**n**	**mean**	**median**	**min**	**max**	**sd**	**cv(%)**
Grain yield, Mg ha^{-1}	510	8.7	8.4	1.3	18.1	2.8	32
Water, Control	*7*	*11.6*	*12*	*3.9*	*18.1*	*5.3*	*46*
Water, Stress	*9*	*8.4*	*7.9*	*1.3*	*15.7*	*4.8*	*58*
N, Control	*103*	*6.4*	*5.7*	*2.4*	*13.1*	*2.3*	*36*
N, Fertilized	*391*	*9.2*	*8.9*	*1.8*	*14.4*	*2.5*	*27*
Protein, %	562	8.990	7.79	2.8	18.4	2.0	24.5
Water, Control	*29*	*8.1*	*7.80*	*5.75*	*12.4*	*1.2*	*14.9*
Water, Stress	*31*	*8.1*	*8.17*	*6.24*	*12.0*	*1.1*	*14.3*
N, Control	*107*	*7.0*	*6.8*	*2.8*	*11.3*	*1.7*	*24.7*
N, Fertilized	*395*	*8.2*	*8.05*	*3.2*	*18.4*	*2.0*	*24.6*
Starch, %	279	70.2	72.2	43.8	80.2	5.3	7.6
Water, Control	*37*	*64.7*	*64.1*	*56.7*	*71.4*	*3.9*	*6.1*
Water, Stress	*39*	*63.9*	*64.1*	*43.8*	*75.5*	*6.1*	*9.5*
N, Control	*43*	*72.7*	*73.6*	*65.2*	*78.6*	*3.2*	*4.4*
N, Fertilized	*160*	*72.3*	*72.9*	*63.0*	*80.2*	*3.5*	*4.8*
Oil, %	265	4.4	4.1	0.6	7.9	1.3	30.0
Water, Control	*29*	*3.5*	*3.1*	*2.5*	*6.4*	*1.1*	*31.5*
Water, Stress	*31*	*3.5*	*3.0*	*0.6*	*6.1*	*1.2*	*34.9*
N, Control	*45*	*4.4*	*4.1*	*3.2*	*7.2*	*1.0*	*23.2*
N, Fertilized	*160*	*4.8*	*4.7*	*2.9*	*7.9*	*1.3*	*26.9*

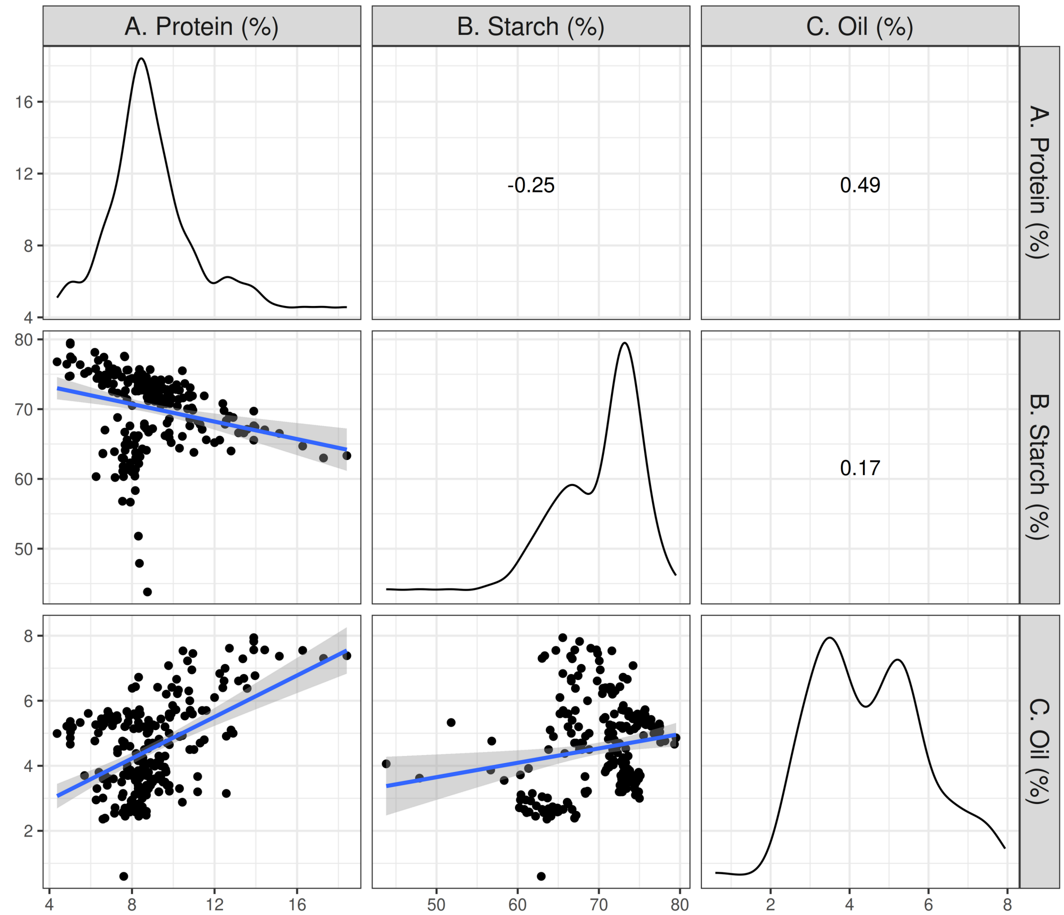

Figure 4.1. Correlation matrix between protein (%), starch (%), and oil (%), all expressed in concentration (%), considering a subset of studies (11) where the three variables were quantified (n = 239) (**Table 4.1**).

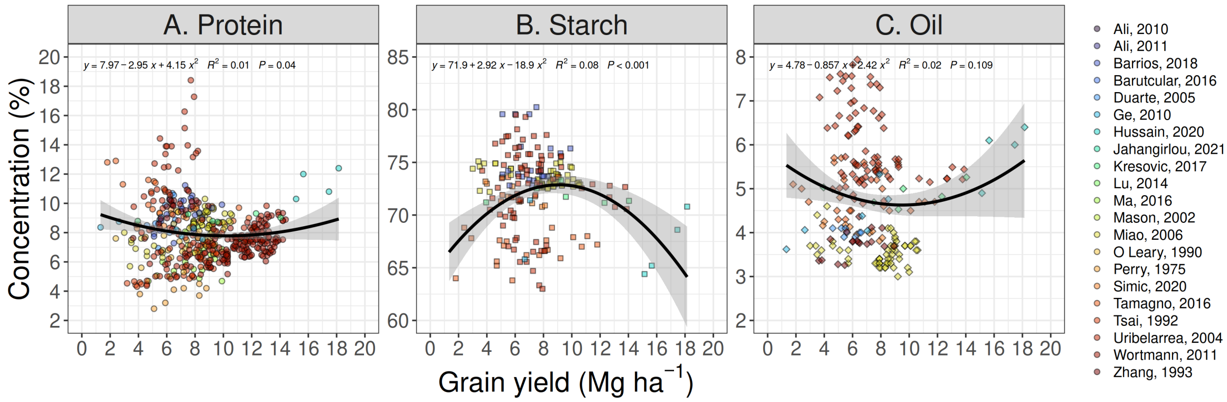

Figure 4.2. Simple relationships between grain yield (Mg ha^{-1}, expressed in dry basis) and grain concentration (%) of protein, starch, and oil (all adjusted to dry basis). For each component, data points belong to multiple studies where both grain yield and the component of interest were quantified.

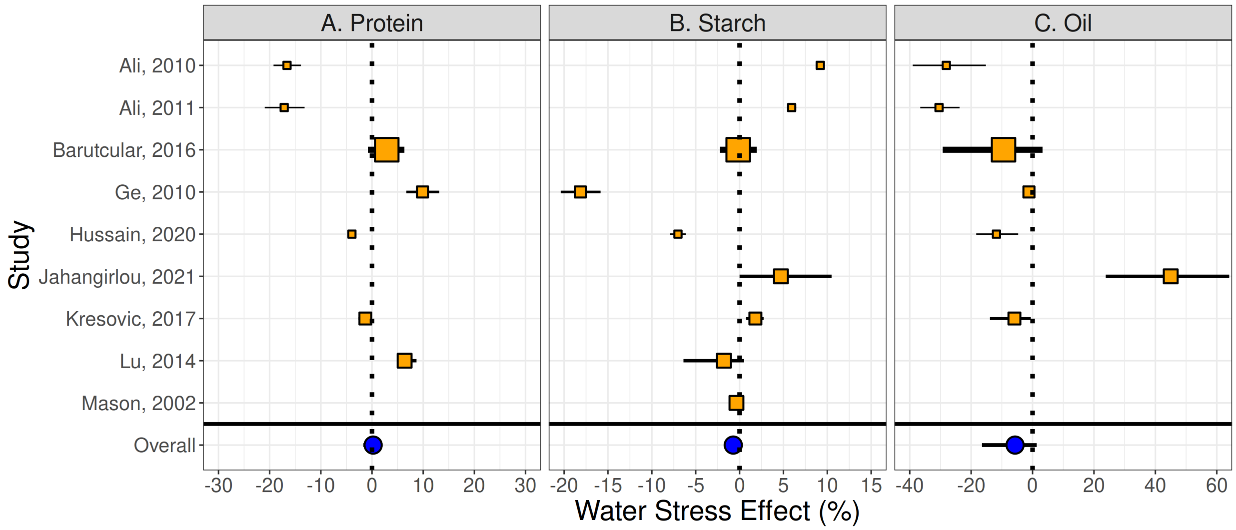

Figure 4.3. Summary of water stress effect (%) on maize grain quality components (A – Protein, B – Starch, and C – Oil, all expressed in concentrations, %). Effect sizes and 95% confidence intervals (CI) were transformed from lnRR into percentage (exp(lnRR)-1*100), as the concentration variation in water-stressed with respect to well-watered control. Within each variable, orange square symbols represent the mean effect per study, while shape size and whiskers their respective weights, and uncertainties, respectively. Blue circles represent the overall random effects model with their respective uncertainties.

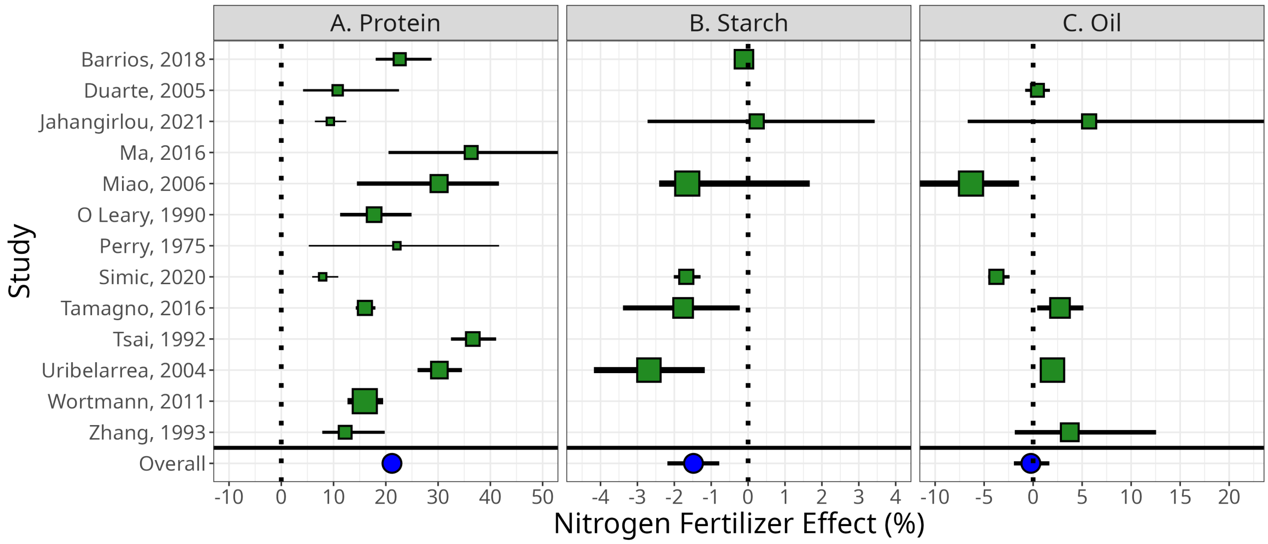

Figure 4.4. Summary of N fertilizer effect (%) on maize grain quality components (A – Protein, B – Starch, and C - Oil). Effect sizes and 95% confidence intervals (CI) were transformed from lnRR into percentage (exp(lnRR)-1*100), as the concentration variation in water-stressed with respect to well-watered control. Within each variable, green square symbols represent the mean effect per study, while shape size and whiskers their respective weights and uncertainties, respectively. Blue circles represent the overall random effects model with their respective uncertainties.

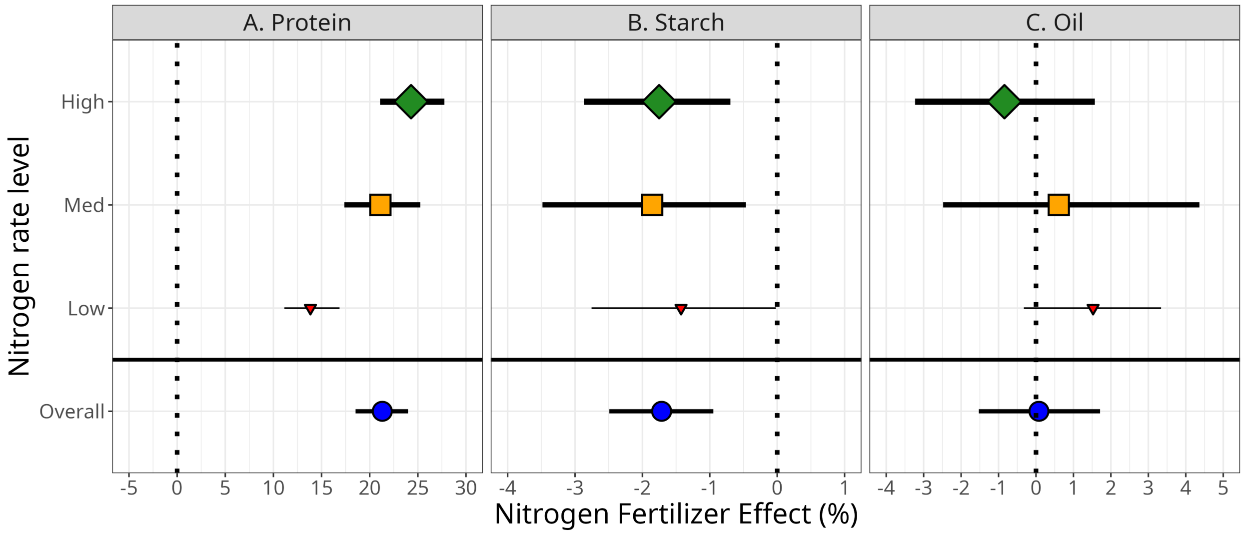

Figure 4.5. Summary of N fertilizer effect (%) on maize grain quality components (A – Protein, B – Starch, and C – Oil) pooled by the N fertilizer rate level (low -<=70 kg N ha^{-1}-, medium ->70-150 kg N ha^{-1}-, and high ->150 kg N ha^{-1}-) vs. their respective control Within each variable, green square symbols represent the mean effect per study, while size and whiskers their respective weights and uncertainties, respectively. Blue circles represent the overall random effects model with their respective uncertainties.

Chapter 5: Footprints of maize nitrogen management on the following soybean crop

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Abstract

Maize (*Zea mays* L.)-soybean [*Glycine max* (L.) Merr.] is among the most typical crop rotations in the US Corn Belt, and nitrogen (N) is the most limiting nutrient for both crops. This study aims to assess the effects of N management for maize on the following soybean crop. Maize-soybean rotation studies, both a long-term (1983-2020, case study I) and a two-seasons (2019-2020, case study II) N fertilizer rate trials were conducted in Kansas (US). The case study I was focused on soybean seed yield as the response variable, while the case study II included a detailed seasonal characterization of soil N, symbiotic N fixation (SNF), and plant N uptake for soybean considering different N fertilizer rates on the previous maize crop. Apparent N budgets from maize (N fertilizer – grain N removal) ranged from ca. -100 to ca. +50 kg N ha^{-1}, and soybean yields were slightly or not affected by maize N management. Overall, long-term N budgets in maize crops did not impact soybean yields. Soil residual N during the soybean season was not affected by previous maize N management. Small maize N surplus did not or had slight influence on the SNF, without compromising soybean N uptake or seed productivity. Forthcoming research should further address how long-term and large soil N mining or surplus in maize may enhance or inhibit N fixation for the next soybean crop.

5.1. Introduction

Alternating soybean [*Glycine Max* (L.) Merr.] with maize (*Zea mays* L.) have been demonstrated to promote higher yields than monocrop scenarios (Crookston and Kurle, 1989; Copeland and Crookston, 1992; Howard et al., 1998; Sindelar et al., 2016). Thus, maize-soybean rotation is among the most common cropping sequence throughout the US Midwest region (Gaudin et al., 2015; Vanhie et al., 2015). For both crops, nitrogen (N) is the most limiting nutrient (Morris et al., 2018; Ciampitti and Salvagiotti, 2018), and the most complex nutrient to be investigated due to the intricate set of spatio-temporal interactions governing its dynamics on the plant-soil system (Mesbah et al., 2017; Lemaire and Ciampitti, 2020; Briat et al., 2020). Historically, literature have concentrated most of the attention to the concept of N credits from the preceding soybean to maize crops (Bundy, 2008; Morris et al., 2018). In contrast, the potential impacts of N management in the previous maize on the following soybean into the crop rotation have received much less attention in literature.

Nitrogen management in the previous maize crop could affect multiple process directly or indirectly impacting soybean N nutrition, and eventually seed yield. Besides the contribution to plant N demand from soil N supply, soybean establishes a symbiosis with *Bradyrhizobium* spp. that contributes, on average, with 50-60% of N requirements (Salvagiotti et al., 2008; Di Ciocco et al., 2011), via the symbiotic N fixation (SNF) process. Nonetheless, there is well-documented antagonism between the soil N supply and N derived from SNF process (Allos and Bartholomew, 1955; Sinclair and De Wit, 1975). Thus, soil N changes induced by different N management in the preceding maize may affect how the soybean crop satisfies its N requirements. For example, a limited soil N availability early in the season could negatively impact the crop establishment and generate considerable yield losses for the soybean crop

(Osborne and Riedell, 2006). On the other hand, an increase in soil N supply produced by a large surplus in N management on previous maize crop may decrease potential yield responsiveness of soybean to N fertilizer (Stone, 1985).

Among other variables, greater amounts of maize residue could negatively affect no-till soybean systems by impacting soil N and soybean nodulation (Vanhie et al., 2015). Soil NO_3^--N content could be affected by residue quantity and quality from the previous crop. Higher residual soil N levels at maize harvest with increasing N rates have been reported in a maize-soybean rotation (Zhu and Fox, 2003). In an crop rotation experiment in Ontario (Canada), between 9.7–13.5% of maize residue-N was recovered by the following soybean crop, with below-ground residue-N supply up to 18 times more N than above-ground residues (Taveira et al., 2020). Although soil N is essential for the establishment of a vigorous seedling during early growth stages prior to the initiation of the N fixation activity, excessive soil N supply may be detrimental to yields if the SNF is inhibited (Sinclair and De Wit, 1975; Stone, 1985). To the extent of our knowledge, the residual effects of N fertilization in previous crops such as maize, on soybean SNF and yields have not been addressed yet on the current scientific literature.

The concept of apparent nutrient budget, estimated as difference between the amount of nutrient applied and the nutrient removed by grain harvest, could be used to evaluate the residual effect of N management into a rotation sequence. Besides representing an environmental risk (Sela et al., 2018), a surplus of N fertilizer on the maize crop may cause an increase in residual soil N for the next soybean crop (Welch et al., 1973; Stone, 1985). For example, years with low attainable maize yields (due to other stress factors limiting productivity) are likely to generate a carryover of soil N to the next crop under strong cold winter conditions (Bundy and Malone, 1988). Therefore, the apparent N budget on the preceding crop could be used as a response variable to explain the yield variability on the following crop in the rotation scheme, in this case with focus on soybean crop.

The objectives of this research were to evaluate, under maize-soybean rotations, the residual effects of N fertilization management on: i) seed yields of the following soybean crop for a long-term case study, ii) yield, seasonal N supply and SNF for a case study with one sequence, and iii) apparent N budget, calculated as fertilizer N added minus harvested-N in maize, and its relationship with the following soybean yields, in both studies.

5.2. Materials and Methods

Two case studies with similar experimental designs but different duration (long-term vs. 1-sequence of maize-soybean rotation) were considered for this research. The long-term experiment established since 1983, herein termed as case study I, served as a reference to test the residual effects of N management in the previous maize on the following soybean yields. On the other hand, the single sequence of maize-soybean rotation, herein termed as case study II, under both dryland and irrigated conditions, was designed to analyze the impact of maize N management on the seasonal dynamics of SNF and soil N uptake of the following soybean crop.

5.2.1. Case Study I, Topeka.

5.2.1.1. General description

Since 1983, a long-term fertilizer application experiment has been conducted on a *Eudora* silt loam soil (Soil Survey Staff, 1999) at the Kansas River Valley Experiment Field, near Topeka, KS, USA (39°09'30.28"N, 95°46'14.60"W) as an annual maize-soybean rotation. The plots under study presented relatively low levels of soil organic matter at the topsoil (0-15 cm) over time, with an average SOM level of 1.2% in 1990 and 1.5% in 2018, without differences across treatments. Soil pH maintained at levels close to neutrality (7.2 in 1990, and

7.3 in 2018), soil test K at levels above critical levels reported in literature (320 mg kg^{-1} in 1983, and 242 mg kg^{-1} in 2018), while soil test P decreased overtime (44 mg kg^{-1} in 1983, and 16 mg kg^{-1} in 2018).

Seasonal weather data were gathered from the Kansas Mesonet (https://mesonet.k-state.edu/) (Figure 5.1B, 5.1C) from the Silver Lake weather station (Topeka, KS). Cropping seasons when soybean took place were characterized for presenting precipitation levels below the historical (1983-2020) average (568 mm), although the crops always received irrigation to avoid water stress, with an even distribution of seasonal mean temperatures both above and below historical average (21.1 ^{o}C). In contrast, maize seasons presented a more even proportion of years above and below both average precipitation and temperature (Supplementary Figure 5.1).

The experimental arrangement was a randomized complete block design with four replications in plots 4.5 m width by 9.14 m length. Soybean sowing dates varied between May 8th and May 27th (Table 5.1) using a row spacing of 0.76 m. Maize sowing dates varied between April 6th and May 6th , also using 0.76 m as row spacing (Supplementary Table 5.1). The experiment was conducted under conventional tillage (early spring) and irrigation. Plots were sprinkler irrigated with a linear move irrigation system, with an average amount of 201 mm per season (Table 5.1; Supplementary Table 5.1). The N treatments were applied during even years on the maize crops and consisted of a total of five N rates (Table 5.2). Although this study presents a factorial design including phosphorus (P) and potassium (K), for the present study, all N plots always included constant P and K fertilizer applications to reduce the risk of interactions with nutrients deficiencies (Table 5.2). All fertilizer treatments were applied at pre-sowing time before maize and incorporated with the tillage operations. After 1994, the set of fertilizer rates was modified (Table 5.2). Finally, the N rates on the previous maize crops were also used as a residual treatment for the soybean crops during the odd years.

Each year, at harvest time [between September and early October (Table 5.1; Supplementary Table 5.1)] a plot combine was used for harvesting maize grain and soybean seed from the middle two rows, then scaled to yield per hectare (Mg ha^{-1}). Maize grain samples were collected in 1991 and 1997 seasons, which were analyzed for N concentration and allowed to estimate grain N removal and apparent N budgets at the plot level (N rate minus grain N removal).

5.2.2. Case Study II, Scandia.

A long-term study under a maize-soybean rotation was initiated in the 2019 cropping season at the North Central Kansas Research Station (Scandia, KS; 39°49'41.60"N, 97°50'22.07"W) in a Crete silt loam soil (fine, montmorillonitic, mesic Typic Argiduolls/Pachic Argiustoll). Soybean served as the previous crop for maize plots in 2019. The study area is conducted under no-till management since 2015. The experiment was installed at two areas, one under dryland and the other area received irrigation with a linear move sprinkler irrigation system. In 2019, maize crop received 95 mm, while in 2020 soybean received 149 mm of irrigation.

At both maize and soybean sowing time, six cores per soil sample were collected per plot at the topsoil (0–15 cm), and three cores per sample at 0-60 cm soil depth at both dryland and irrigated areas. General soil fertility was evaluated at topsoil by testing pH, soil organic matter (SOM, %), soil texture (%), soil test phosphorus as extractable (Mehlich-3, mg kg^{-1}), soil test potassium (Mehlich-3, mg kg^{-1}), and N as nitrate (NO_3^--N) and as ammonium (NH_4^+-N)

(Table 5.3). The topsoil fertility showed similar levels between dryland and irrigated areas, with slightly acidic soil pH, adequate SOM level (ca. 3%), medium soil P, and high K. The 0-60 cm samples were used to describe both NO_3^--N and NH_4^+-N availability (kg N ha^{-1}) during the cropping season. Thus, both NO_3^--N and NH_4^+-N concentrations (mg N kg $soil^{-1}$) where transformed to kg ha^{-1} by multiplying for the corresponding bulk density, which averaged 1.32 and 1.30 g m^{-3} for dryland and irrigated areas, respectively.

Seasonal weather data were gathered from the Kansas Mesonet (Figure 5.2) from the North Central Kansas Research Station (Scandia, KS). In 2019, the total precipitation during the planting-maturity period (May-Sep) was 533 mm. In 2020, the total precipitation during the sowing-maturity period (May-September) was about 406 mm (Figure 5.2). The precipitation distribution pattern denoted a dry period at the beginning of the season. More regular and abundant precipitation events were registered during June-July, ending with a dry August but with very good radiation levels during the post-flowering period.

The experimental arrangement was a randomized complete block design with five replications in plots 6 m width by 15 m length. Maize crop was planted on May 3, 2019, and soybeans on May 15, 2020, both at row spacing of 0.76 m, with a slightly higher seeding rate under irrigation due to higher expected yields. The N treatments were applied on the maize crop and consisted of a total of five N rates (Table 5.3) using urea-ammonium-nitrate (28-0-0) as the fertilizer source, V5 as the application timing, and applied on surface bands. Under the same design, the N rate management on the previous maize crop (2019) was used as a residual treatment for the 2020 soybean crops at both dryland and irrigated areas. In 2019, maize plots were manually harvested on September 30th from the two central rows by taking four subsamples of 1m^2 then scaled to the hectare. Maize grain yields were adjusted to 155 g kg^{-1} moisture content. Maize grain samples were collected and analyzed for N concentration to estimate grain N removal and apparent N budget. In 2020, soybean plots were mechanically harvested on October 13th using a combine by collecting the two central rows then scaled to the hectare. Soybean seed yields were corrected to 140 g kg^{-1} moisture content.

5.2.2.1. Plant and soil sampling

During the 2020, the sampling schedule included a total of seven times during the soybean season, 0, 45, 59, 80, 90, 101, and 115 days after sowing (DAS), which corresponded to sowing, late vegetative (ninth leaf), full flowering (R2), pod setting (R4), beginning seed (R5), beginning of full seed (R6); and right before beginning maturity (R7; Fehr and Caviness, 1977). Only three blocks and the two most contrasting N rates applied in the previous maize were considered in 2020 for sampling during the soybean cropping season: 0 kg N ha^{-1} and 240 kg N ha^{-1} herein N0, and N240, respectively. Compound soil samples (three cores per plot) were collected at 0-60 cm depth, including a sampling time at previous maize maturity and at soybean sowing date (DAS = 0). The NO_3^--N and NH_4^+-N were extracted from 2 g of dry grounded soil (2 mm sieve) with a potassium chloride solution (KCl, 1 mol L^{-1}) and quantified (mg kg^{-3}) by colorimetric procedures in a flow analyzer (Brown, 1998). On the other hand, plant samples were collected six times during the season from 45 to 115 DAS. Shoot samples were collected cutting plants at the ground level from two adjacent rows (1 m^2 area), and a subsample of ten (45-59 DAS) or five plants (80-115 DAS) was dried in an air-forced oven (65 °C) until constant weight for estimating above-ground dry matter (Mg ha^{-1}). Dried plants were ground in a micro-mill (0.125 mm particle size) and subjected to the chemical analyses of interest.

The Ndfa (%), a time-integrated measurement of the proportion of atmospheric N within the plant tissue, was estimated using the natural abundance method according to Eq. (5.1) Unkovich et al. (2008):

$$Ndfa(\%) = \frac{\delta^{15} Nofreferenceplant - \delta^{15} Nofsoybeans}{\delta^{15} Nofreferenceplant - Bvalue} \times 100 \quad \textbf{(5.1)}$$

in which $\delta^{15}N$ is the natural excess of the ^{15}N isotope in the plant tissue. Reference plants were unfertilized corn plants from plots adjacent to the soybean plots. The B-value of -2.54, which was reported as the median of previous literature (Balboa and Ciampitti, 2020). Along with $\delta^{15}N$, tissue N concentration was estimated using an isotope ratio mass spectrometer, allowing the calculation of above-ground N uptake (kg ha^{-1}), fixed N [(N uptake * Ndfa) / 100, kg N ha^{-1}], and N uptake from the soil (as N uptake – fixed N). At maturity (R8), two central rows, covering ca. 23 m^2, were mechanically harvested from each plot, adjusted to 140 g kg^{-1} moisture basis and then scaled to seed yield per hectare (Mg ha^{-1}).

5.2.3. Apparent N budget

At the plot level, the apparent N budget for the following soybean was estimated as the difference between the N fertilizer rate applied and grain N removal for maize crop. In the case study I, grain N concentration was measured in the 1991 and 1997 cropping seasons. Taking this data into account, a global regression model was fit to estimate unobserved data of grain N concentration as a function of N fertilizer rate (Supplementary Figure 5.2A). For the case study II, maize grain N concentration was measured at all plots in 2019 (Supplementary Figure 5.2B). Similarly to case study I, a positive relationship between maize grain N concentration and fertilizer N rate was observed in Scandia.

5.2.4. Data analysis

5.2.4.1. Soybean seed yield

For case study I, soybean seed yields across treatments were analyzed using a hierarchical Bayesian approach (Wikle et al., 2019), where at the top level, yield data observations (y_i) were assumed to follow a normal distribution [$y \sim N\left(z, \sigma^2\right)$] and generated from an underlying process (z), while at a secondary level, the parameters describing the process z at the groups-level of interest (N treatments) were also assumed to be random (i.e., belonging to distributions). For the case study I, the process was defined as a linear mixed effects model with year, treatment (N rate in previous maize), and their interaction as the group-level effects (i.e., analogous of frequentist fixed factors), and block as random. Since N treatments were repeated overtime on the same plots (repeated measurements), an auto-regressive of order 1 (AR1) error-correlation structure was also incorporated into the model. Since the set of N treatments was modified after the 1994 season, this first analysis was fit split by period: i) 1984-1994, and ii) 1997-2020. Similarly, a second model considering the cumulative yield as a response variable was also studied under a hierarchical Bayesian framework, with N treatment considered as the group-level effect (fixed) and block as random.

For the case study II, similarly, a linear mixed effects model was used to fit the data with treatment (N rate in previous maize) as a fixed factor (group-level), and block as random. Since irrigation phases were not part of the treatments design but a condition assigned to different sections of the experimental field at Scandia, the analysis was split by i) dryland, and ii) irrigated scenarios.

Uninformative prior distributions (for treatment means) were applied using truncated Gaussian density functions by defining a mean 4 Mg ha^{-1} with and standard deviation of 4 Mg ha^{-1}, with a lower boundary equal to zero. In all cases, pairwise means comparisons were performed using their corresponding 95%-credible intervals (2.5% to 97.5% percentiles) from the posterior high-density distributions. All models were fit using R software (R Core Team, 2021). The posterior draws using Markov chain Monte Carlo (MCMC) were performed with the *brms* package (Bürkner, 2018). In all cases, five thousand posterior samples were generated as warm-up, with fifteen thousand iterations after warm-up, and a thinning rate equal to ten in order to reduce correlation of consecutive posterior samples and improve the chains (four) mixing (Hooten and Hefley, 2019).

5.2.4.2. Seasonal soil N and symbiotic N fixation

For the case II, to study the seasonal dynamics of soil and plant N components in the Scandia experiment, process models were non-linear equations. The response variables were: i) soil NO_3^--N test, ii) soil test NH_4^+-N test, iii) fixed N (N uptake derived from SNF), and iv) N uptake derived from soil, equal to the difference between the above-ground N uptake and the fixed N. To estimate fixed N, the above-ground N uptake dry matter was multiplied by their corresponding N concentration. In all cases, the time as DAS was chosen as the independent variable because it presents a simple interpretation for non-linear model parameters, particularly for soil processes, and because samples were taken the same year, with shared sowing date, and phenology across irrigation phases and treatments. The parameters of the model were compared using the posterior distributions in similar fashion as for the linear mixed models defined in Section 5.2.4.1.

For soil N variables, generalized additive models (GAM) were used as the process models. Compared to traditional alternatives (e.g., multiple regression), GAMs allow applying smoothing functions (e.g., multiple polynomials, splines) to the factors of interest but still expressing the model as a sum of effects (Wood et al., 2017). This characteristic enables the possibility of exploring non-linear trends in the data with still a reasonable level of interpretability. For each irrigation phase, the GAM models were defined as Eq. (5.2):

$$z = \beta_0 + \beta_1 + f(DAS) \qquad \textbf{(5.2)}$$

where z is the predicted value of soil NO_3^--N or NH_4^+-N (mg kg^{-1}), β_0 is the intercept as the overall mean, β_1 is the effect of treatment (two levels: N0, N240), while the generic expression $f(DAS)$ represents the smoothing function that transforms the effect of the regressor variable time (as days after sowing) into an additive component to the model. The models were fit using the *brms* package in R-software. The willingness of the smoothing functions [*f(DAS)*] was defined using thin-plate smooths (bs="tp") with the number of knots (k) equal to 6. The blocks were introduced as a random effect with a smooth term with the basis function specified as random (bs="re").

For dry matter, Ndfa, N uptake, fixed N, and soil-derived N were assumed to follow a non-linear mixed effects model described by a logistic equation as Eq. (5.3):

$$z = \frac{m}{1 + e^{-k(x-g)}}, \qquad \textbf{(5.3)}$$

in which *z* is the predicted value, *x* is the regressor variable (time as days after sowing date), *m* is the asymptote or maximum predicted value; *k* controls the growth rate; and *g* refers to the timing of maximum growth rate. Using the first derivative of the logistic functions, the maximum growth rate (*r*) was calculated for each variable. Uninformative truncated normal distributions were set as priors to all primary parameters, restricting the posterior samples to positive values.

5.2.4.3. Soybean seed yield vs. apparent N budget

For both case studies, a linear regression model was fit to investigate the relationship between the soybean seed yields and the apparent N budget left by the preceding maize crop. A hierarchical Bayesian framework was also applied using uninformative priors for both intercept and slope. The intercept prior was centered at 4 Mg ha^{-1} with a standard deviation equal to 4 Mg ha^{-1}, and the slope prior centered on zero with a standard deviation of 1 Mg ha^{-1} kg N^{-1}. The existence of the relationship between soybean yield and the apparent budget was tested by comparing the 95% credible intervals of the slope against the value of zero.

5.3. Results

5.3.1. Soybean seed yield

5.3.1.1. Case study I: Topeka, KS.

Average soybean yields varied between 4.2 and 5.4 Mg ha^{-1} for the first (1984-1994) and from 2.8 to 4.8 Mg ha^{-1} for the second period (1998-2020, Figure 5.3). Thus, most of the yield variability corresponded to the year factor, although yield differences among fertilizer N treatments were observed on specific years (mainly in 1992 and 2020). In 1992, soybeans fertilized with 179 kg N ha^{-1} on the preceding maize showed significantly greater yields (5.4 Mg ha^{-1}) relative to the plots where the previous maize received no N fertilizer (4.7 Mg ha^{-1}). Nonetheless, the rest of the treatments showed no differences with respect to either N0 or N179. In 2020, plots with 179 kg N ha^{-1} on the preceding maize showed significantly lower seed yield (4.1 Mg ha^{-1}) than plots where the previous maize received 135 kg N ha^{-1} (5.1 Mg ha^{-1}). However, none of the latter differed from any of the other N treatments. It results important to mention that general yields during the 2014 and 2018 seasons were negatively impacted by Sudden Death Syndrome (*Fusarium virguliforme*) (Adee et al., 2016), although the differences between treatments remained the same. In terms of accumulated soybean , no significant differences were observed among the evaluated N treatments for any of the periods of the study (Supplementary Figure 5.3).

5.3.1.2. Case study II: Scandia, KS.

In 2020, soybean seed yields varied between 4.0 to 5.4 Mg ha^{-1} under dryland and from 4.5 to 5.9 Mg ha^{-1} under irrigated conditions. With no residual effect of N rates on the previous maize (Figure 5.4A), average seed yields resulted in 4.6 Mg ha^{-1} for dryland and 5.1 Mg ha^{-1} for irrigated scenarios.

Residual soil N (0-60 cm) at maturity of the previous maize (September 2019) averaged 50 kg NO_3^--N ha^{-1} and 38 kg NH_4^+-N ha^{-1} for N0 plots (total of 88 kg N ha^{-1}), and 71 kg NO_3^--N ha^{-1} and 40 kg NH_4^+-N ha^{-1} for N240 plots (total of 111 kg N ha^{-1}) under dryland conditions. On the other hand, under irrigation, residual N values averaged 78 kg NO_3^--N ha^{-1} and 40 kg NH_4^+-N ha^{-1} for N0 plots (total of 118 kg N ha^{-1}), and 59 kg NO_3^--N ha^{-1} and 31 kg NH_4^+-N ha^{-1} for N240 plots (total of 90 kg N ha^{-1}). These residual soil N levels remained similar until the initial soil sampling in soybean (April 2020), with ca. 76 kg NO_3^--N ha^{-1} and 42 kg NH_4^+-N ha^{-1} (total of 118 kg N ha^{-1}) for both N0 and N240 plots under dryland; while under irrigation values were 65 kg NO_3^--N ha^{-1} and 46 kg NH_4^+-N ha^{-1} (total of 111 kg N ha^{-1}) for N0 plots, and 74 kg NO_3^--N ha^{-1} and 51 kg NH_4^+-N ha^{-1} for N240 plots (total of 125 kg N ha^{-1}). The GAM models were able to explain the seasonal variation of soil residual N presented with an acceptable performance for both NO_3^--N ($R^2_{dryland}$ = 0.67; $R^2_{irrigated}$ = 0.51) and NH_4^+-N ($R^2_{dryland}$ =

0.52; $R^2_{irrigated}$ = 0.43). Estimated values during the season varied between ca. 20 to 100 kg NO_3^--N ha^{-1} and between ca. 35 to 90 kg NH_4^+-N (Figure 5.4B). The fitted models indicated no major differences in soil N supply related to N management on the preceding maize. Similarly, both irrigation phases showed similar patterns of residual soil N. While soil NH_4^+-N showed a relatively stable availability until 80 DAS and a peak towards the end of the season (ca. 80 kg N ha^{-1}), soil NO_3^--N availability showed two peaks, a greater at the beginning (ca. 100 kg N ha^{-1}) and then a peak (ca. 60 kg N ha^{-1}) by end of the season.

The logistic models were able to explain the dry matter accumulation with an R^2 of 0.96 for dryland, and and R^2 0.97 for irrigated conditions. Final (115 DAS, ca. R7) above-ground dry matter values were 12.0 Mg ha^{-1} (N0) and 11.4 Mg ha^{-1} (N240) under dryland, and 12.5 Mg ha^{-1} (N0) and 12.2 Mg ha^{-1} (N240) for irrigated. Estimated Ndfa levels at R7 were 70% (N0) and 65% (N240) for dryland, and 65% (N0) and 59% (N240) under irrigation. Despite the slight differences, neither dry matter accumulation nor Ndfa values differed significantly among treatments for either irrigated or dryland conditions (Supplementary Figure 5.4). With R^2 values of 0.92 and 0.90 for irrigated and dryland, respectively, no differences in N uptake were observed under irrigation (427 kg N ha^{-1} -N0- and 424 kg N ha^{-1} -N240-) (Figure 5.4C), however, the estimated N uptake at maturity was significantly greater in N0 plots (450 kg N ha^{-1}) relative to N240 plots (382 kg N ha^{-1}) under dryland conditions. Similarly, under irrigation (R^2 = 0.91), fixed N resulted in 244 and 237 kg fixed N ha^{-1} for both N0 and N240 plots, respectively. However, under dryland (R^2 = 0.94), a significantly greater amount of fixed N was observed (Figure 5.4C) with 295 kg fixed N ha^{-1} for N0 plots, and 226 kg fixed N ha^{-1} for N240 plots. Lastly, the N uptake derived from soil resulted the same for both N treatments under dryland (R^2 = 0.72, 131 kg N ha^{-1} -N0- and 130 kg N ha^{-1} -N240-). Despite a small difference of N uptake from soil between treatments (152 kg N ha^{-1} -N0- and 172 kg N ha^{-1} -N240-) under irrigation (R^2 = 0.91), those differences resulted to be not significant. Relative to dryland, under irrigation the fitted models predicted a higher N contribution from soil, which seems to occur mainly at early stages of the crop.

5.3.3. Apparent N budget

Estimated apparent N budgets resulting from previous maize crops varied between -131 to +70 kg N ha^{-1} for the case study I and from -108 to +83 kg N ha^{-1}in the case study II. Overall, it is clear that variations in apparent N budget in maize crop did not significantly impact soybean yield as a following crop in the rotation. Similar to yields, the variability on the relationships seems highly related to year-specific conditions. Across all site-years (19), only one observed a positive relationship between soybean yield and apparent N budget from the preceding maize, with a slope of +7.7 kg yield kg N^{-1} (2018 year).

5.4. Discussion

This study highlights the lack of effect of maize N management on the following soybean crop. Most of the variation on soybean yields was mainly linked to year (weather) as the main factor. Overall, by using two datasets (a long-term maize-soybean rotation and a more detailed study) we provide insights on the minor and erratic responses of soybean yield to residual N fertilization in the previous maize, as reported in the scientific literature (Welch et al., 1973; Mallarino and Pecinovski, 2007). The soybean response to N is very inconsistent even when high N fertilization rates are directly applied to the soybean crop (Halvorson and Reule, 2006; Ortez et al., 2018; Mourtzinis et al., 2018; Tamagno et al., 2018).

The residual soil N during the following soybean season, either as NO_3^--N or NH_4^+-N, was not affected by the previous maize N management. However, significant amounts of N released in synchrony with crop uptake could be undetected by soil sampling, either due to a lack of sensitivity of regular soil N tests to small differences in N (Mueller et al., 2018), to other soil organic sources (McDaniel et al., 2020), or due to the length of intervals between sampling dates. Thus, N released from above- as well as from below-ground crop residues (Taveira et al., 2020; Pinto et al., 2021) could have differed between treatments. This might partially explain the larger contribution of SNF to N uptake on N0 plots (relative to the N240) observed under dryland conditions. Although this extra N uptake from SNF did not increased yields, this additional N supply could eventually provide a boost to raise seed protein levels since it mainly occurs during reproductive stages (Ortez et al., 2018).

Surprisingly, under irrigation, we observed a different response pattern of N uptake and SNF to previous N management compared to the results under rainfed conditions. Although similar N uptake levels, we observed a trend of slightly lower Ndfa levels during the season (and final fixed N contribution) compared to dryland conditions. Unfortunately, the experimental design of the case study II does not include irrigation as a treatment in order to statistically compared water management. Including irrigation as a treatment in future research steps, we might be able to test some hypothesis arising from our results such as: (i) a facilitated soil N uptake via mass flow (McMurtrie and Näshlom, 2018) under irrigation as compared to dryland conditions, and (ii) short-term oxygen stress events due to soil saturation when irrigating could constrain the N fixation process by down-regulating nitrogenase activity (Hunt et al., 1989; Schwember et al., 2019).

More extreme N budgets (mainly large N surplus) in the previous crop may be necessary to compromise SNF at a level that soil supply could not compensate in meeting crop N demand, and ultimately, with N limiting soybean yields. At both case studies, apparent N budgets from previous maize crops were mostly below zero or slightly positive (< 50 kg N ha^{-1}) at the highest fertilizer N rates (> 200 kg N ha^{-1}). Therefore, although N fertilizer needs may widely vary over the field and years (Bundy and Andraski, 1995; Scharf et al., 2005), it is very likely that farmers applying close to economic optimum fertilizer N rates (normally < 200 kg N ha^{-1}) for maize crop will not generate scenarios compromising the SNF levels on the next soybean crop.

Interestingly, long-term (1983-2020) N budgets, from soil N mining to N surplus, did not seem to impact soybean yields. This fact opens up the following questions: (i) Could the long-term soil N mining have reduced the environmental capacity to supply N?, (ii) Should the SNF present a larger contribution to maintain yields in plots with a long-term negative budget -soil N mining- ?, and (iii) Is the soil N supply contributing more to soybean N demand in plots with a historically positive N surplus? A priori, our results in case study II do not suggest significant short-term changes in soil inorganic N due to contrasting apparent N budgets (N0 vs N240) from the previous maize crop, resulting in similar soil N contributions to the next soybean N demand. However, the latter does not exclude long-term impacts on soil organic matter pools and N mineralization levels (Poffenbarger et al., 2017; Mahal et al., 2019). On the other, the overall SNF capacity could present a marked dependency on the seasonal pattern of soil N supply (timing and size of mineralization pulses during the season) (Moro Rosso, 2021). Clearly, many more unanswered questions are still relevant and should be further explored in more detailed next studies.

Future research should cover the current data limitation on plant-soil N dynamics, including soil residual N profile, plant N uptake, and SNF components in the long-term experiment (case study I). Similarly, although considering dryland and irrigated conditions, the irrigation factor should be ideally part of the experimental design to perform statistical comparisons, and more cropping seasons would be necessary to provide a more compelling interpretation of results in case study II. Multiple locations are also desirable, as the SNF process presents a strong dependency on environmental factors (Borja Reis et al., 2021), as well as soil N dynamics could highly be dependent on soil and weather conditions such as the occurrence of extreme precipitation events favoring N leaching beyond the root zone (Iqbal et al., 2018), among others. Lastly, including the evaluation of below-ground biomass and N components (Pinto et al., 2021) could provide key information towards a more comprehensive picture about N dynamics within a maize-soybean crop rotation.

5.5. Conclusions

Soybean yields were not affected by the previous N management in maize. The apparent N budget for maize crop was mostly negative or slightly positive, without clearly impacting the main N sources for soybean crop and thus final yields. Most likely, commercial N rates in corn following the economically optimum rate criteria will not produce a substantial N surplus to impact the next soybean performance. However, we should not discard that an extreme N surplus may generate a severe inhibition to SNF to the extent of compromising the overall plant N supply and then total N uptake and yield. Prospective research should still address how long-term and large soil N mining or N surplus in maize may be to enhance or inhibit N fixation for the next soybean crop.

Table 5.1. General soil and crop management practices at the long-term maize-soybean rotation nutrition trial. Kansas River Valley Experiment Field, Topeka, KS.

Year	Soybean Variety	Seeding rate (seeds m^{-2})	Sowing Date (Month-Year)	Harvest Date (Month-Year)	Irrigation (mm)
1984	Douglas	43.2	05-17	10-18	471
1986	Sherman	43.2	05-27	10-19	136
1988	Spencer	35.6	05-09	10-03	615
1990	Sherman	35.6	05-08	09-27	316
1992	Sherman	35.6	05-18	09-30	268
1994	Edison	35.6	05-10	09-30	0
1996	Sherman	35.6	05-20	n/a	252
1998	Sherman	35.6	05-19	10-12	148
2000	IA 3010	35.6	05-03	10-13	297
2002	Garst 399RR	35.6	05-16	n/a	227
2004	Stine 3982-4	34.3	05-24	09-17	0
2006	Stine 4302-4	34.3	05-24	10-12	133
2008	Midland 9A385	34.3	n/a	n/a	118
2010	Asgrow 4005	34.3	05-27	10-07	176
2012	Asgrow 3832	38.3	05-14	10-04	284
2014	Asgrow 3833	34.6	05-21	10-09	169
2016	Asgrow 3731	34.6	05-10	09-30	21
2018	Asgrow 38x6	34.6	05-07	10-02	145
2020	Pioneer 37A27 + ILeVO	34.6	05-19	10-07	46

n/a = not available

Table 5.2. Fertilizer treatments at the long-term (1983-2020 period) maize-soybean rotation trial at Kansas River Valley Experiment Field, Topeka, KS (US).

Nutrient fertilization	**Period**	
	1983-1994	**1997-2020**
N fertilization	0, 45, 90, 179, 269 kg N ha^{-1}	0, 90, 135, 179, 224 kg N ha^{-1}
P fertilization	15 kg P ha^{-1}	15 kg P ha^{-1}
K fertilization	56 kg P ha^{-1}	139 kg P ha^{-1}

Table 5.3. General topsoil fertility (0–15 cm) at sowing time of the preceding maize (2019) and soybean (2020) crops at irrigated and dryland areas in Scandia, KS.

Crop	0–6 in. depth	pH	SOM	Clay	Silt	Sand	STP	STK	N-NO_3	N-NH_4
		-	%				ppm			
Maize, 2019	Dryland	6.0	3.0	17	59	24	12	531	16	3.6
	Irrigated	6.3	2.8	21	57	22	10	490	15	3.6
Soybean, 2020	Dryland	5.8	3.0	23	59	18	11	511	17	8.5
	Irrigated	6.1	2.8	22	59	19	17	488	21	5.6

SOM = soil organic matter (LOI); STP: soil test phosphorus (Mehlich-3); STK: soil test potassium (Mehlich-3).

Table 5.4. Crop management practices for the preceding maize (2019) and soybean (2020) crops under dryland and irrigated conditions. Case study II. Scandia, KS, USA.

Practices	**Maize**		**Soybean**	
Irrigation	Dryland	Irrigated	Dryland	Irrigated
Tillage	No-till			
Planting date	05/03/2019		05/15/2020	
Genotype	P1197AM		P39A58X (RR2-Xtend)	
Seeding rate	7.0 seeds m^{-2}	8.5 seeds m^{-2}	26.2 seeds m^{-2}	33.3 seeds m^{-2}
Row spacing	0.78 m			
P fertilization	22 kg P ha^{-1}			
N fertilization	0, 60, 120, 180, 240 kg N ha^{-1}		No N added	

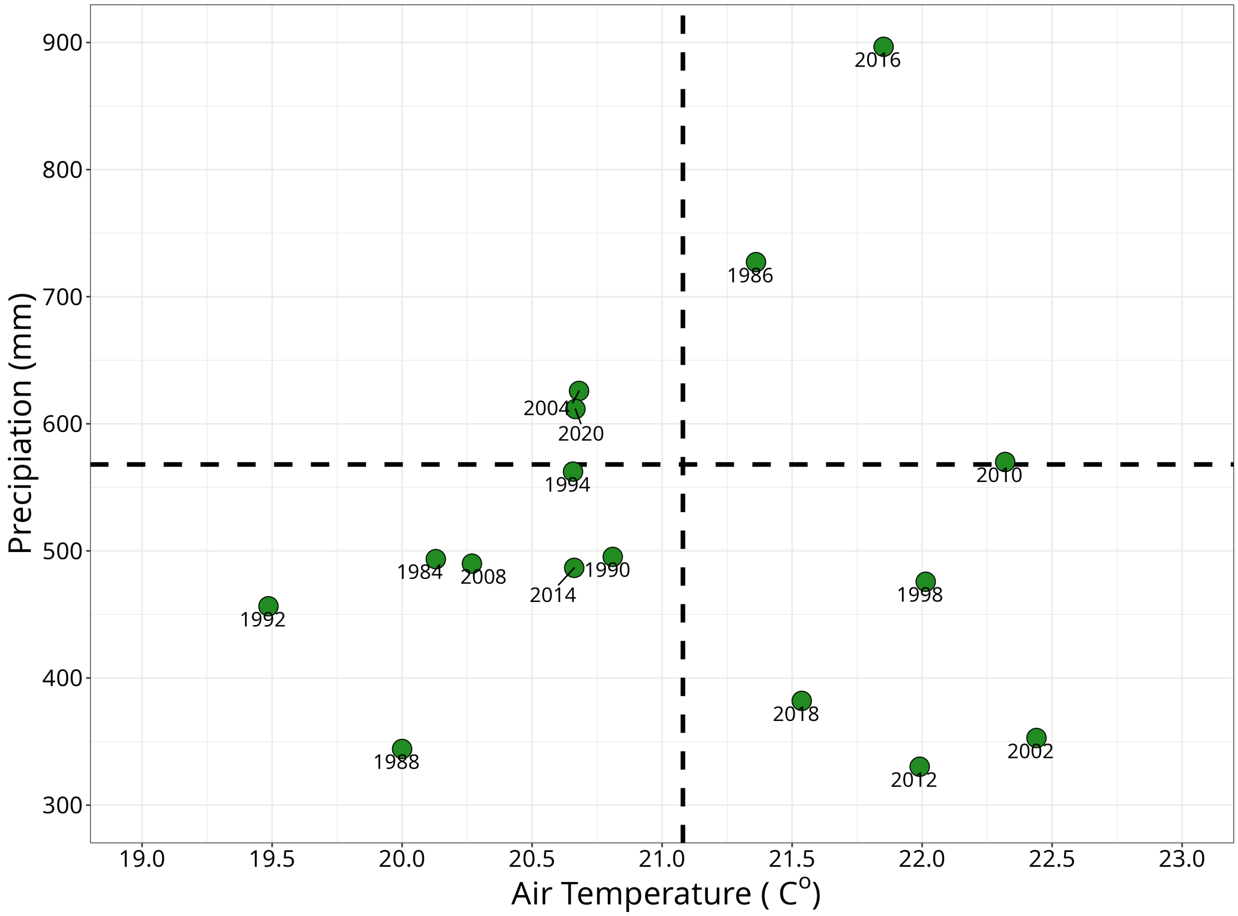

Figure 5.1. Variation of precipitation (mm) and mean air temperature (Celsius) spanning from April-to-September, reflecting the soybean cropping seasons, from Kansas River Valley Experiment Field, Topeka, KS (US). Vertical and horizontal dashed lines represent the historical mean of precipitation (568 mm) and air temperature (21.1 oC).

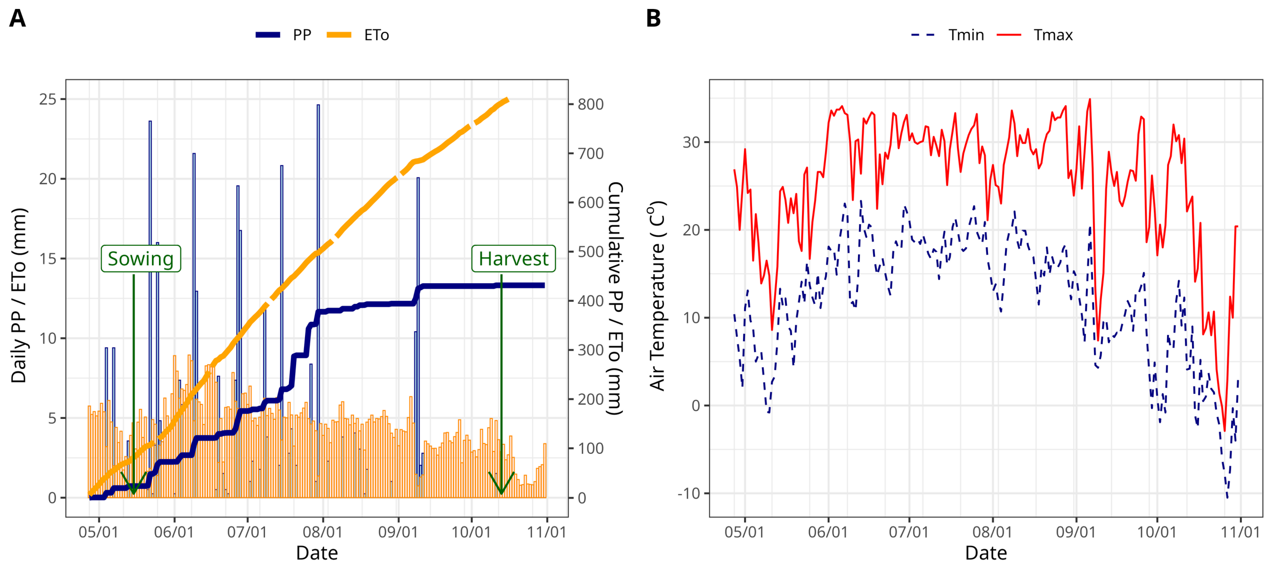

Figure 5.2. A: Daily and cumulative precipitation (PP) and reference evapotranspiration (ETo); B: daily minimum and maximum air temperature for the 2020 cropping season at case study II, Scandia, KS.

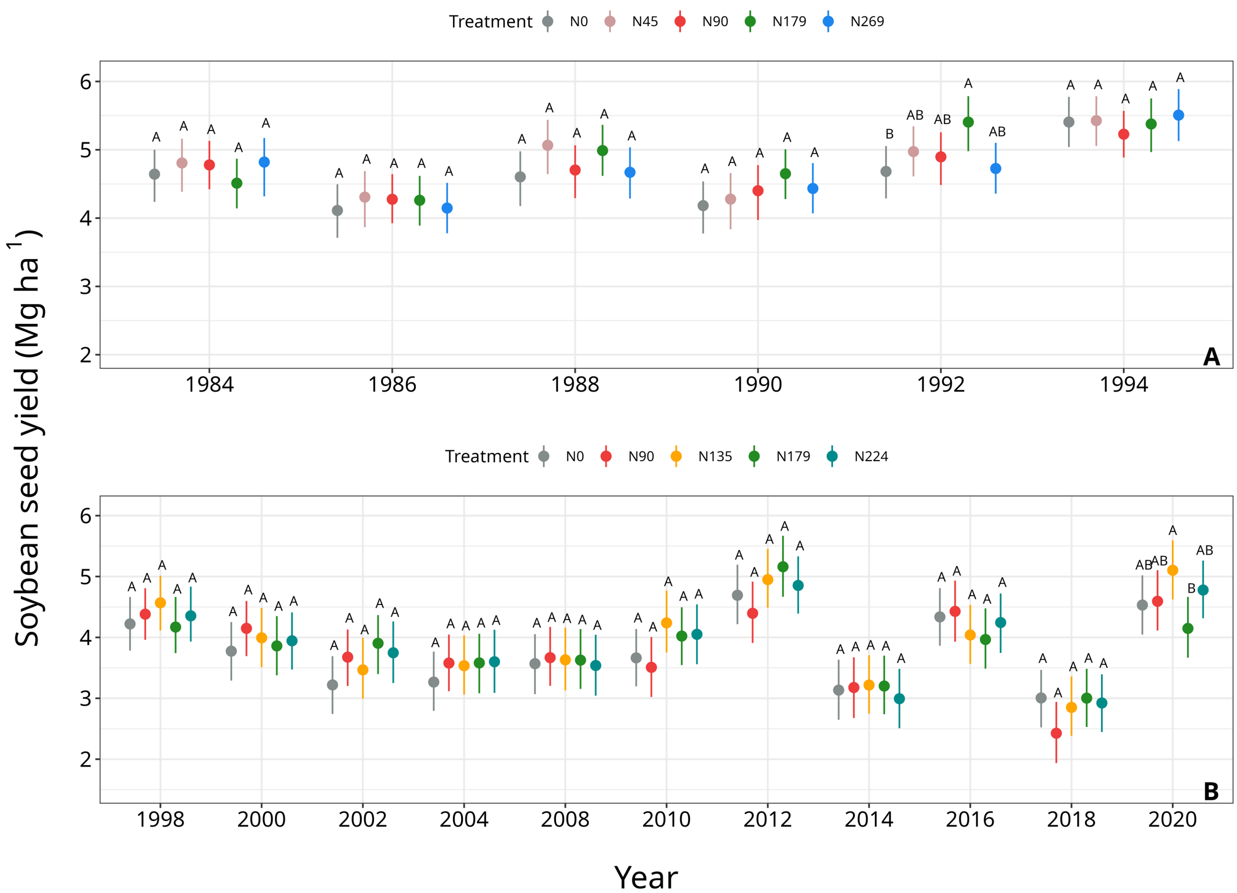

Figure 5.3. Soybean seed yield depending on different N rates on the previous maize crops over the years for the two periods under study (A: 1983-1994, and B: 1997-2020) in the case study I, Kansas River Valley Experiment Field, Topeka, Kansas. Whiskers represent the 95%-credible intervals (from Bayesian posterior distributions). For A and B, within each year, same letters indicate no significant differences between treatments.

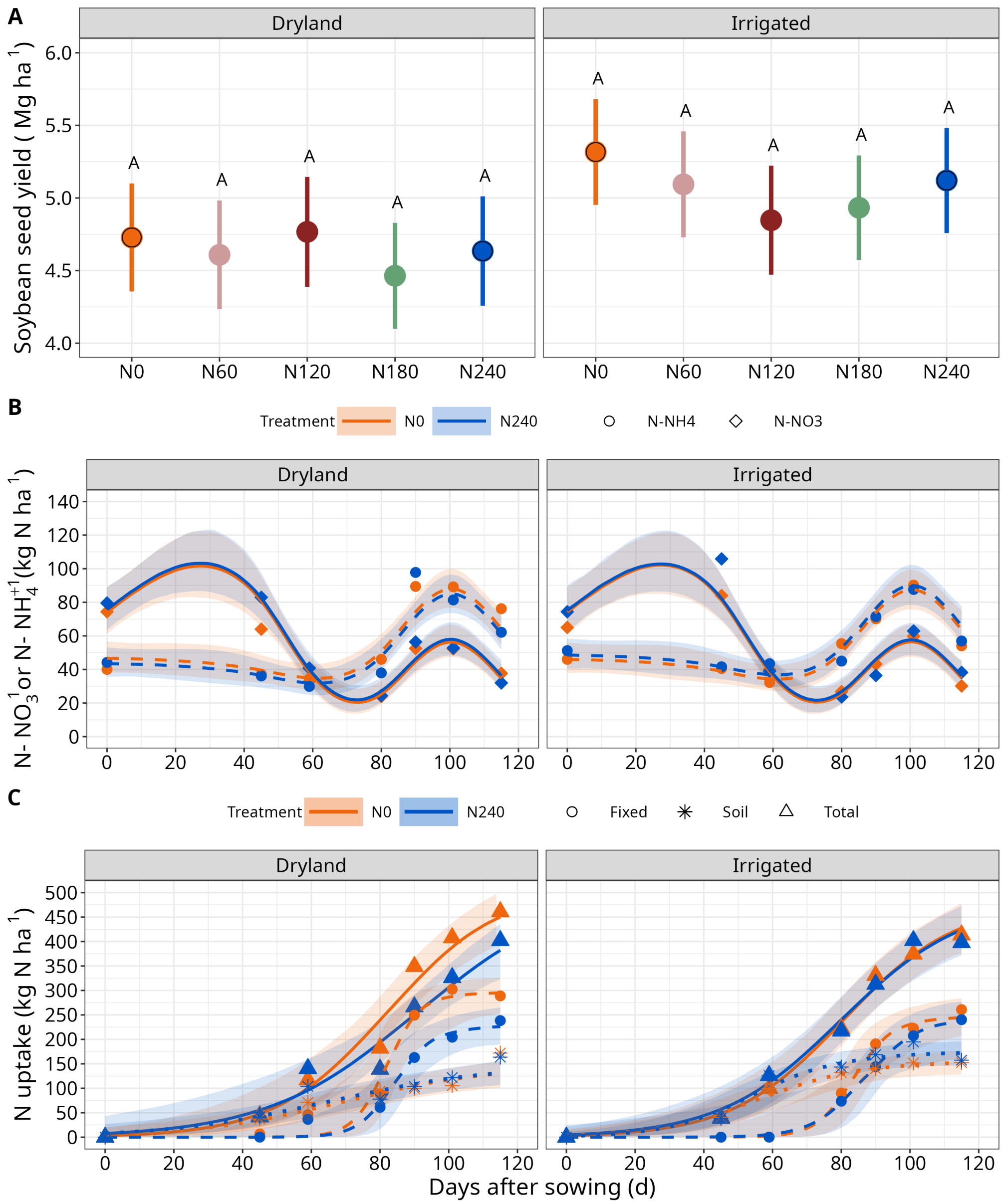

Figure 5.4. (A) Soybean seed yields for the five N rates on the previous maize crop at the case study II (North Central Kansas Experimental Research Station, Scandia, Kansas), 2020 cropping season. (B) Seasonal dynamics of soil N availability as NO_3^--N and NH_4^+-N, and (C) total N uptake and its fixed-N and soil-N uptake components for N0 and N240 in the previous maize. In A, whiskers represent the 95%-credible intervals (from Bayesian posterior distributions), for which same letters indicate no significant differences between treatments within the same irrigation phase. In B and C, ribbons around the curves indicate the 95%-credible intervals for the process models.

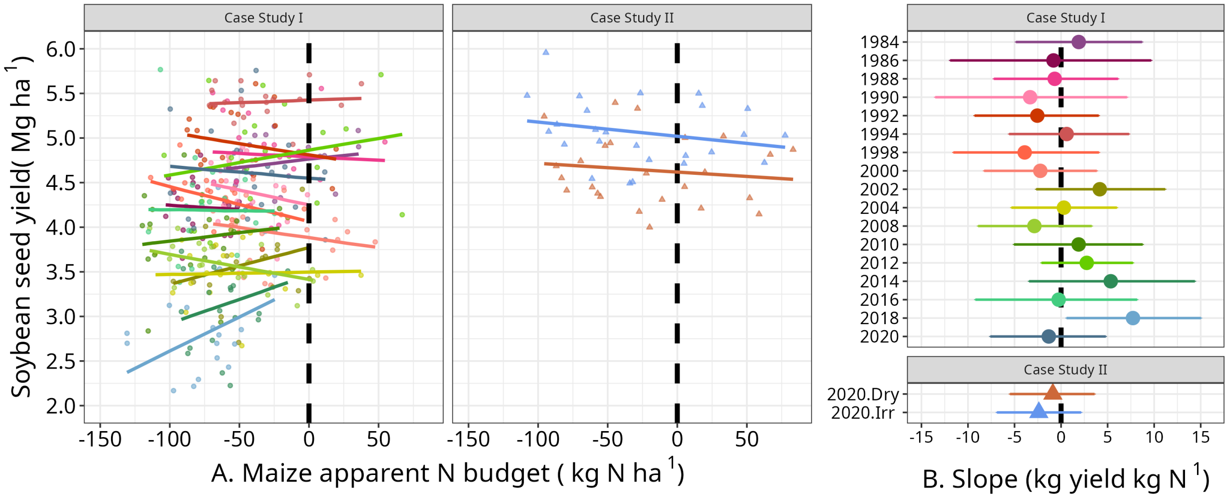

Figure 5.5. A, Soybean seed yield as a function of apparent N budget in previous maize crops for the case study I (Kansas River Valley Experiment Field, Topeka, Kansas), and case study II (North Central Kansas Experimental Research Station, Scandia, Kansas). In B, whiskers represent the 95%-credible intervals (from Bayesian posterior distributions) for the slopes (not significant when including zero).

Chapter 6: Revisiting linear regression to test agreement in continuous predicted-observed datasets

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Abstract

In agricultural research and related disciplines, using a scatter plot and a regression line to visually and quantitatively assess agreement between model predictions and observed values is an extensively adopted approach, even more within the simulation modeling community. However, linear model fit, use, and interpretation are still controversial in the literature. The overall goal of this research is to evaluate the usefulness of a symmetric regression line to test agreement on predicted-observed datasets. The specific aims of this study are to: i) discuss the selection of a regression model to fit a line to the predicted-observed scatter, and ii) provide a geometric interpretation of the regression line, decomposing the prediction error into lack of accuracy and lack of precision components, via utilization of illustrative field crop datasets. This study tested and contrasted three alternative linear regression models (Ordinary Least Squares -OLS-, Major Axis -MA-, and Standardized Major Axis -SMA-) in terms of assumptions, loss functions, parameters estimates, and model interpretation for the predicted-observed case. When the uncertainty of predictions and observations are unknown, the SMA represents the most appropriate approach to fit a symmetric-line describing the bivariate predicted-observed scatter. The SMA-line serves as a reference to estimate a weighed difference between predictions and

observations. Moreover, this symmetric regression can assist in the decomposition of the square error into additive components related to both lack of accuracy and precision. In summary, the SMA regression tackles the axis orientation problem of the traditional OLS (y vs. x or x or y) and allows to identify error sources that are meaningful to the user. This work offers a novel and simple perspective about the use of linear regression to assess simulation models performance. In order to assist potential users, we also provide a tutorial to compute the proposed assessment of agreement using R-software.

6.1. Introduction

Accurate and precise predictions are the ideal outcome of any simulation model. Accuracy refers to the closeness between predicted (P) and observed (O), linked to systematic error or bias. Precision relates to dispersion, or proximity between data points, connected to random variability. Simulations could be both accurate and precise, accurate but imprecise, precise but inaccurate, or inaccurate and imprecise (Figure 6.1). The level of agreement is conditional to these two concepts, essential for assessing models' performance (Gauch et al., 2003; Tedeschi, 2006).

A broad set of scoring rules were designed to capture different aspects of agreement (Duveiller et al., 2016; Tedeschi, 2006). Perhaps, the mean square error (MSE) and its square root (RMSE) are the most popular in academia (Gneiting, 2011). The coefficients of correlation (r) and determination (R^2) are also widely used for model evaluation, but provide limited information about agreement (Yang et al., 2014). Alternatively, the concordance correlation coefficient (CCC) (Lin, 1989) is another popular normalized metric to evaluate both accuracy and precision at the same time. Although a myriad of additional agreement indices have been developed (Gupta et al., 2009; Moriasi et al., 2007; Willmott et al., 2012, among others), the visual assessment with a scatter plot and a regression line is still widely used in agricultural and related research areas (Piñeiro et al., 2008). A scatter plot presents the advantage of showing data distribution and dispersion patterns (Loague and Green, 1991; Willmott, 1981). Similarly, although there are objections to use linear regression (Harrison, 1990; Kobayashi and Salam, 2000), it is still commonly used to test a null hypothesis of agreement, with the H0: intercept = 0 and slope = 1 (Analla, 1998; Smith and Rose, 1995; Yang et al., 2014).

The ordinary least squares (OLS) is perhaps the most widely adopted model for linear regression. However, for the P-O case, a lack of accord persists related to the scatter's orientation (Piñeiro et al., 2008), dependent and independent variables (Analla, 1998). To the present, there are three prominent positions in the literature. The first supports the PO orientation by considering O as reference (error-free), so using O as the regressor variable and P as the dependent (y) (Willmott, 1981; Yang et al., 2014). A second approach supports the OP orientation, arguing that only O contains natural variability whereas P comes mostly from deterministic models (Mayer and Butler, 1993; Tedeschi, 2006) and considering that PO orientation distorts the interpretation of the relationship (Piñeiro et al., 2008). The third position supports that the orientation does not matter (Mitchell, 1997) since both P and O contain random error, arguing that not acknowledging the uncertainty on predictions (i.e., deterministic) does not imply a null uncertainty (St-Pierre, 2016).

Alternatively, bivariate regression models are characterized by their symmetry, that is, invariant to the axis orientation (Draper and Smith, 1998; Smith, 2009). Representing this group, the major axis (MA) and standardized MA (SMA) regressions are dimension-reduction techniques producing one-dimensional summaries of the scatter (Jolliffe, 2002; Warton and

Weber, 2002), broadly used in biology for testing proportionality (isometry vs. allometry) between random variables (Warton et al., 2006). Therefore, a symmetric regression model may represent a suitable alternative for the P-O case.

Disaggregating the prediction error is also a major concern for model evaluation that deserves attention (Gauch et al., 2003; Kobayashi and Salam, 2000; Wallach and Thorburn, 2017). Revisiting the concept of symmetry and the decomposition of the error using bivariate regression models, new methods have been developed to compare satellite images that could be applied for the P-O case (Ji and Gallo, 2006; Duveiller et al., 2016).

The main objective of this study is to discuss the usefulness of a symmetric regression line to test agreement on continuous P-O datasets. Our specific goals are to: i) discuss the selection of the regression model, and ii) propose a geometric interpretation of the square error producing both lack of accuracy and precision. Lastly, we offer a tutorial in R Software (R Core Team, 2021) for this analysis publicly available at: https://doi.org/10.7910/DVN/EJS4M0 (Correndo et al., 2021c).

6.2. Theoretical framework

6.2.1. The general error-in-variables model.

Either to predict or to observe a quantity (e.g. crop yield) are both techniques producing values with uncertainty, whether it is acknowledged or not (St-Pierre, 2016). To compare how equivalent two techniques are we could define a general model (Francq and Govaerts, 2014), which is referred in the literature as “error-in-variables” model (Moran, 1971), measurement error models (Fuller, 1987), or Model-II regression (Legendre and Legendre, 1998). For illustrative purposes, we first use the conventional axis-denomination: x as horizontal, and y as vertical. We also assume no correct orientation since either P or O can be used either as x or y.

Given the i^{th} subject from a sample of size n (i = 1, …, n), we may assume that measurable data (y_i and x_i) represent unobservable, "true or latent", data (Y_i and X_i) plus their corresponding errors (Eq. 6.1). The error terms ε_i and μ_i are assumed to be independent and normally distributed (Gaussian), with variances σ_ε^2 and σ_μ^2. Finally, we may also assume the true variables are connected by a linear relationship, where α (intercept) and β (slope) represent the parameters of the linear model.

$$\begin{aligned} y_i &= Y_i + \varepsilon_i, \\ x_i &= X_i + \mu_i, \\ Y_i &= \alpha + \beta X_i. \end{aligned} \qquad \textbf{(6.1)}$$

Assuming normal and independent residuals (Warton et al., 2006), we can obtain maximum-likelihood estimators $\hat{\beta}$ and $\hat{\alpha}$, approximating the underlying model (Eq. (6.1)) with Eq. (6.2).

$$\hat{y}_i = \hat{\alpha} + \hat{\beta} x_i. \qquad \textbf{(6.2)}$$

6.2.2. The specific regression models

6.2.2.1. Residuals and loss functions

The well-known OLS regression is often referred to as Model-I regression (Legendre and Legendre, 1998). Model-I is an special case of the general model, assuming null error for one of the variables (ε_i or μ_i equal to zero) (McArdle, 2003; Sokal and Rohlf, 1995; Warton et al., 2006). Thus, OLS regression has two non-reciprocal solutions. The first is the traditional

OLS regression, OLSv (y vs. x), assuming normality of "vertical" residuals ($\varepsilon_i \sim N\left(0, \sigma_\varepsilon^2\right)$) with lack of error in x_i ($x_i = X_i$, $\sigma_\mu^2 = 0$). The second, OLSh (x vs. y), also known as inverse regression (Tan and Iglewicz, 1999), assuming normality of "horizontal" residuals ($\mu_i \sim N\left(0, \sigma_\mu^2\right)$) with lack of error in y_i ($y_i = Y_i$, $\sigma_\varepsilon^2 = 0$).

In contrast, symmetric regressions such as MA and SMA assume there is error in both x and y (Warton et al., 2006), with a bivariate-normal distribution and independent errors

$$\begin{pmatrix} \varepsilon_i \\ \mu_i \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma_\varepsilon^2 & 0 \\ 0 & \sigma_\mu^2 \end{pmatrix}\right).$$

Each model applies a different definition of "line-of-best-fit" based on the residuals. This definition is known as the "loss-function", a mathematical expression that we seek to minimize when estimating the regression parameters (Table 6.1). For example, minimizing the square vertical ($\hat{\varepsilon}_i$; Eq. (6.3)) (Figure 6.2A) or horizontal residuals ($\hat{\mu}_i$, Eq. (6.4)) (Figure 6.2B), OLSv and OLSh provide the lines-of-best-fit for the "prediction" of the dependent variable as the minimize the error about it (Legendre and Legendre, 1998).

Alternatively, both MA and SMA provide a single line (symmetric) defining the relationship regardless of which variable is x or y. The MA regression minimizes $\hat{d}_i$ (Eq. **(6.5)**), as the sum square of the Euclidean distances (h_i) (Figure 6.2C). For this reason, MA is also known as orthogonal regression (Carroll and Ruppert, 1996; Fuller, 1987). The SMA model considers instead the cross-product of differences ($\hat{z}_i$) in terms of both x and y, Eq. (6.6) (Figure 6.2D). Due to its residuals-geometry, SMA is also known as the least-triangles regression (Teissier, 1948; Barker et al. 1988), among other names (Warton et al., 2006).

6.2.2.2. Estimating the regression slope

For the general model Eq. **(6.1)**, the maximum-likelihood slope-estimator ($\hat{\beta}$) is always Eq. **(7)** regardless of the specific model (McArdle, 1988; Smith, 2009; Tan and Iglewicz, 1999).

$$\hat{\beta}=\frac{s_y^2-\lambda s_x^2+\sqrt{\left(s_y^2-\lambda s_x^2\right)^2+4\lambda s_{xy}^2}}{2 s_{xy}}. \qquad \textbf{(6.7)}$$

where s_x^2 and s_y^2 are the sample variances, s_{xy}^2 the sample covariance between $\boldsymbol{x}$ and $\boldsymbol{y}$, and s_{xy} is the sum of the product of the difference between x and its mean and y and its mean. For any regression model, s_x^2, s_y^2, s_{xy}, and s_{xy}^2 do not change, since they are properties of the data. However, Eq. (7) implies that specific models present different slope-formulas (Table 6.2), and an intercept-estimators ($\hat{\alpha}$) conditional to the previous estimation of $\hat{\beta}$ (Supplementary material: Chapter 6). The single distinction among the models is λ Eq. (6.8), the quotient of uncertainties between variables, also known as the variance or precision ratio (Carroll and Ruppert, 1996; Smith, 2009).

$$\lambda=\frac{\sigma_\varepsilon^2}{\sigma_\mu^2}. \qquad \textbf{(6.8)}$$

For the P-O case, the uncertainty in O_i can be obtained from replications, while the uncertainty in P_i is rarely acknowledged by simulation models, however, eventually obtainable via resampling methods (*e.g.*, Monte-Carlo simulations) (St-Pierre, 2016) or multi-model ensembles (Makowski, 2017). Nonetheless, the most likely scenario if facing unmeasured or non-measurable variances to estimate λ, for which the strategy is assuming λ equal to a specific value (McArdle, 1988). This is the main distinction among the candidate models (Table 6.2). Still, the question is, to what degree are these models robust to wrong values of the precision ratio λ? (McArdle, 2003).

The two asymmetric OLS-models represent the extreme cases where either y_i or x_i are assumed exact (error-free). With OLSv we assume that variance $\sigma_{\mu}^2=0$, so $\lambda \to \infty$ and the $\hat{\beta}_{OLSv}$ estimator is Eq. (6.9). With OLSh we assume that $\sigma_{\varepsilon}^2=0$, so $\lambda \to 0$ and the $\hat{\beta}_{OLSh}$ estimator is Eq. (6.10). All other solutions lie in between, included MA and SMA (Francq and Govaerts, 2014; McArdle, 2003; Smith, 2009).

With the MA regression we assume that both variables have been obtained with the same uncertainty, so $\sigma_{\varepsilon}^2=\sigma_{\mu}^2$ and $\lambda=1$ (McArdle, 1988). Thus, the $\hat{\beta}_{MA}$ estimator is Eq. (6.11). Lastly, with SMA regression we assume that variances σ_{ε}^2 and σ_{μ}^2 are proportional to the sample variances s_x^2 and s_y^2, respectively, so $\lambda=s_y^2/s_x^2$. Thus, the $\hat{\beta}_{SMA}$ estimator is Eq. (6.12), which is simply the ratio between the standard deviations. Since $\hat{\beta}_{SMA}$ represents the geometric mean between the two extreme OLS solutions (OLSv and OLSh), SMA is also known as the geometric mean regression and considered a fair compromise solution (Sprent and Dolby, 1980; Barker et al., 1988; McArdle, 1988; Francq and Govaerts, 2014).

6.2.3. Selection of the regression model

If the scientific question involves a prediction line, still the error should be partitioned asymmetrically about the response variable (Smith, 2009; Warton et al., 2006). However, the question for the P-O case involves a descriptive line instead of a prediction line. In that respect, other methods can be considered as better “summary lines” as compared to OLS, which does not satisfy symmetry (Isobe et al., 1990).

By minimizing the error in both directions (Figure 6.2C, 6.2D), both MA and SMA are more suitable models than OLS to obtain a summary line. The best option is the more robust model to wrong values of λ (McArdle, 2003). In this sense, the SMA assumes a value of λ based on the available data ($\lambda = s_y^2 / s_x^2$), while MA simply assumes equal P_i and O_i uncertainties. In fact, the use of MA has been proven as substantially riskier (greater bias and variance on estimations) as compared to SMA (McArdle, 1988; Francq and Govaerts, 2014). Therefore, when λ is unknown, the SMA regression should be preferred to other alternatives (Francq and Govaerts, 2014; McArdle, 1988).

6.2.4. Testing regression parameters?

The classical use of a regression line to test P-O agreement has its basis on the interpretation of $\hat{\beta}$, to test proportional or multiplicative bias (H_0: $\hat{\beta} = 1$; H_1:$\hat{\beta} \neq 1$), and $\hat{\alpha}$ to detect a systematic additive bias (H_0: $\hat{\alpha} = 0$; H_1:$\hat{\alpha} \neq 0$). However, a major drawback has been outlined for the *t-test* for $\hat{\beta}$ against a specific value (*e.g.*, 1): it is ambiguous. In other words, the more dispersion in the cloud of points (less precise), the greater its error and the harder to reject the null hypotheses (Harrison, 1990; Lin, 1989; Mitchell, 1997; Reckhow et al., 1990). Similarly, the smaller the error, the more chances of rejection even with a regression-line similar to the 1:1-line (Lin, 1989).

6.2.5. Error decomposition using linear regression

Evaluating the performance of a regression line forced to $\hat{\beta}$ = 1 and $\hat{\alpha}$ = 0 has been suggested as a straightforward alternative to test agreement (Analla, 1998), which is equivalent to estimate the *MSE* (or *RMSE*) symmetrically accounting for the error with respect to the 1:1

line. In the same line, we argue that instead of pursuing a comparison of regression parameters that suffers from ambiguity, we could use the SMA line-of-best-fit for a geometrical comparison against the 1:1 line. This approach uses the SMA line to: i) decomposing the square error into unsystematic (lack of precision) and systematic (lack of accuracy) components, and ii) producing related precision and accuracy metrics.

6.2.5.1. Error decomposition with SMA-line

It has been suggested to use SMA regression for decomposing the total sum of squares (*TSS*) (Table 6.3; Figure 6.3A) into two additive components (Ji and Gallo, 2006): i) the sum of unsystematic differences (SUD_{SMA}), and ii) the sum of systematic differences (SSD_{SMA}).

The first term, SUD_{SMA}, is equivalent to the error about the SMA-line. For the P-O case, it is the sum of product of differences between the SMA-line and both P_i and O_i simultaneously (Table 6.3). Geometrically, the SUD_{SMA} represents the sum of "triangle-rectangles" formed between the data points and the SMA-line (Figure 6.3B). The second term, SSD_{SMA}, can be expressed as the sum of square differences between the SMA-line and the 1:1-line (Table 6.3). Geometrically, the SSD_{SMA} represents the sum of the area of squares formed between the SMA-line and the 1:1 line (Figure 6.3C). Finally, the $TSS = SUD_{SMA} + SSD_{SMA}$. Intuitively, as the SMA-line approaches the 1:1 line, the lack of accuracy will approach zero ($SSD_{SMA} \rightarrow 0$), and most of the error will be on the unsystematic (lack of precision) component ($SUD_{SMA} \rightarrow TSS$).

To express the decomposition in terms of the *MSE* (Table 6.3) we can simply divide the SUD_{SMA} and SSD_{SMA} by the sample size (n), which results in two measures that we can define as the Mean Lack of Precision (*MLP*), and the Mean Lack of Accuracy (*MLA*), respectively. Moreover, *MLP* and *MLA* can be transformed to original units as their square roots (*RMLP* and

RMLA). Finally, considering their relative contribution to the *MSE*, we can also express them as the Percentage Lack of Precision (*PLP*) and the Percentage Lack of Accuracy (*PLA*) (Table 6.3).

6.2.5.2. Error decomposition with OLS- and MA-line

To the extent of our knowledge, Willmott (1981) was the first proposing a direct error decomposition using a regression line. Using the OLS regression of P vs. O, he suggested the utilization of two error indices as additive components of the MSE: i) the unsystematic mean square error (MSE_U), related to imprecision, and ii) the systematic mean square error (MSE_S), related to inaccuracy. Thus, MSE_U and MSE_S are the analogous of our MLP and MLA, respectively. Similarly, in terms of the TSS, if multiplied by the sample size (n), MSE_U and MSE_S are equivalent to the sum of unsystematic (SUD_{OLS}) and systematic differences (SSD_{OLS}), respectively.

Geometrically, SUD_{OLS} represents the sum of the areas of n squares obtained from the difference between the actual P_i and the value given by the OLS-line ($\widehat{P}_i$) (Supplementary Table 6.1; Supplementary Figure 6.1A); while SSD_{OLS} represents the sum of the areas of n squares obtained from the difference between the OLS-line and the 1:1 line (where $P_i = O_i$) . Thus, unsystematic and systematic proportions of the error can be simply estimated as ratios of the components to the TSS [or to the MSE, as expressed by Willmott et al. (1981)].

Although Willmott's decomposition is a straightforward strategy often used for model evaluation (Wallach et al., 2019), its major flaw is related to the use of OLS regression as the core model. Hence, it transfers the asymmetry issue (Figure 6.2) to the decomposition, as results are not irrespective to the axis orientation. Specifically, Willmott (1981) supports the use of the PO orientation. As thoroughly explained in Sections 2.1, 2.2, and 2.3, this decision implies neglecting the error in the O axis, which ultimately modifies the error decomposition into the systematic and unsystematic components. Therefore, unless the user is completely confident in the uncertainty of O values being insignificant, we are skeptical about the reliability of the Willmott's MSE_U and MSE_S components. Instead, as the SMA model is likely to provide a more reliable summary regression line (Section 2.3), it is also presumptive to produce a more trustworthy error decomposition (Supplementary Table 6.1).

For example, the illustrative dataset displayed on Figure 6.2 has a *TSS* equal to 38.25 (MSE = 3.825). Following Willmott's decomposition, the unsystematic error would be SUD_{OLS} equal to 21.53 (MSE_U = 2.153, $MSE_{U\%}$ = 56%), while the systematic error SSD_{OLS} equal to 16.72 (MSE_S = 1.672, $MSE_{S\%}$= 44%). However, applying the SMA decomposition, the unsystematic error is SUD_{SMA} equal to 30.87 (*MLP* = 3.087, *PLP* = 81%), while the systematic error is SSD_{SMA} equal to 7.38 (MLA = 0.738, *PLA* = 19%). Thus, although both approaches produce precision (MSE_U, *MLP*) and accuracy (MSE_S, *MLA*) components additive to the MSE, omitting (OLS) or not (SMA) of the uncertainty in O values generates a different partitioning of the error. In such case, we prefer to proceed with the model that implements a safeguard by considering uncertainty in both axis when defining the line-of-best-fit (SMA).

Similarly, an error decomposition using the MA regression has been proposed by Duveiller et al. (2016), who tested agreement between satellite images. However, we recommend users to be cautious with its implementation as the strategy presents some major drawbacks (Supplementary Table 6.1; Supplementary Figure 6.1B). Related calculations are publicly available at https://dataverse.harvard.edu/dataset.xhtml?persistentId=doi:10.7910/DVN/EJS4M0 (Correndo et al., 2021c).

6.2.5.3. Equivalence with other error decompositions

A similar error decomposition was proposed by Kobayashi and Salam (2000), who decomposed the *MSE* into: i) the square bias, as $(\bar{O}-\bar{P})^2$, ii) the square difference between standard deviations, as $(s_O - s_P)^2$ and iii) the lack of correlation weighted by standard deviations, $2 s_O s_P (1-r)$. Our inaccuracy term (*MLA*) is equivalent to the sum of the square bias (additive bias) and the square difference between the standard deviations (proportional bias) (Table 6.3). Sharing the same interpretation (random error), our lack of precision term (*MLP*) is equivalent to the Kobayashi's lack of correlation (Table 6.3). While Kobayashi and Salam (2000) assumes $(s_O - s_P)^2$ as part of the random variability, we consider it as part of the lack of accuracy component. Note that the classical mean bias error (MBE, Table 6.5) is equivalent to the square bias component expressed in the original units of the variable of interest. However, MBE it is only related to additive bias, missing the proportional bias component.

Regarding the relative contribution of the error components, our decomposition also matches with the Theil's partial inequality components (Smith and Rose, 1995). Theil's decomposition segregates the *TSS* into three terms: i) a proportion associated with the square bias (additive), ii) a proportion associated with inconsistency (proportional bias), and iii) the unexplained variance. The proportion that *MLA* explains from *MSE* (*PLA*) is equal to the sum of the first two Theil's components (square bias and inconsistency), while the proportion that the *MLP* explains from *MSE* (*PLP*) is equal to the Theil's unexplained variance term. While Smith and Rose (1995) relate the inconsistency term to the slope of OLS regression using OP orientation, we instead relate it to the SMA regression line.

Although these decompositions produce the same results as ours, we offer alternative interpretations. A demonstration of the equivalence between the decomposition strategies is provided at Correndo et al. (2021c) .

6.3. Applied examples

6.3.1. Illustrative dataset

The hypothetical dataset used to illustrate Figures 6.2 and 6.3 has been intentionally set to n = 10; $\boldsymbol{x}$ = 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0; and y = 4.0, 5.5, 2.5, 4.5, 8.0, 5.0, 6.0, 10.0, 7.5, 8.5. At Figure 6.2, variables are in-purpose named as x and y, so either of them could correspond to P or O. The OLSv approach (Figure 6.2A) results in a regression line $\hat{y}_{OLSv}$ = 2.47 + 0.57x; while using OLSh (Figure 6.2B), the regression line is $\hat{y}_{OLSh}$ = -0.52 + 1.02x. Moreover, while the OLSv slope is significantly different from 1 ($\hat{\beta}_{OLSv}$-$CI_{95\%}$ = 0.40 – 0.73), the OLSh is not ($\hat{\beta}_{OLSh}$-$CI_{95\%}$ = 0.79 – 1.46), exposing the OLS asymmetry not only for the slope estimations but also for their confidence intervals. This emphasizes OLS could result in a different degree of ambiguity for testing the slope depending on the scatter orientation, as OLSv and OLSh may produce opposite results when testing isometry (H_0: $\hat{\beta}$ = 1).

In contrast, the use of MA or SMA results in symmetric (algebraically invertible) lines. Thus, when switching axes, y *vs.* x and x *vs.* y produce identical lines (Figure 6.2C, 6.2D). Thus, $\hat{y}_{MA}$ = 1.62 + 0.70x and $\hat{y}_{SMA}$ = 1.19 + 0.76x, both slopes significantly different from 1 ($\hat{\beta}_{MA}$-$CI_{95\%}$ = 0.50 – 0.93; $\hat{\beta}_{SMA}$-$CI_{95\%}$ = 0.61 – 0.95). The error decomposition of the same dataset showed in Figure 6.3 indicates that from the *MSE* (3.82), the unsystematic component, the *MLP* (3.24) represents 84.68%, while the systematic component, the *MLA* (0.58) represents 15.32% of total error. Expressed in original units, *RMLP* = 1.80 and *RMLA* = 0.76.

6.3.2. APSIM datasets

Four datasets as collections of point forecasts from multiple locations belonging to simulation modules at different stages of their calibration process of APSIM model (Holzworth et al., 2018) were selected to represent contrasting scenarios of agreement between P and O (Table 6.4). The first example is a set of simulations of wheat grain N (g m^{-2}) with both high accuracy and high precision (Figure 6.4A). The second example corresponds to simulations of barley grain number (thousand of counts m^{-2}) with high accuracy but medium to low precision (Figure 6.4B). The third and the fourth datasets were intentionally selected from models still under development and thus, their level agreement is distant from ideal. However, these examples serve to purpose of illustrating different sources of prediction error. The third dataset is a collection of sorghum grain number (thousand of counts m^{-2}) simulations with low accuracy and medium precision (Figure 6.4C). Lastly, the fourth example is a set of simulations of above-ground dry-matter on chickpea (kg ha^{-1}) with low accuracy and medium precision (Figure 6.4D).

The assessment of agreement was carried out via the SMA regression and complemented with selected metrics of agreement (Table 6.5). The selected metrics were intended to measure precision (r, R^2, MLP, RMLP, and PLP), accuracy (MBE, MLA, PLA), or both (MSE, RMSE, CCC). The concordance correlation coefficient (CCC) (Lin, 1989) is a normalized metric that summarizes in a single score the precision (r) weighed by an accuracy coefficient (*Xa*) (Table 6.5). It evaluates the degree to which data pairs fall on the 1:1 line, and it is broadly used to assess agreement (Carrasco et al., 2013). A CCC = 1 denotes a perfect agreement, CCC = 0 means no agreement, and CCC = −1 corresponds to a perfect disagreement (P = − O).

For the first example (Figure 6.4A; Table 6.6A), results show a SMA line very close to the 1:1 line, with both intercept and slope non-significantly different the former from zero and the latter from 1. Regarding the error metrics, the correlation reflects the high precision (r = 0.92), while concordance (CCC = 0.91) reveals a low penalization due to lack of accuracy. The relative contribution to MSE (2.78) shows that most of the error is due to lack of precision (PLP = 94.8%) and 5% is due to lack of accuracy (PLA).

Similarly, the second example (Figure 6.4B; Table 6.6B) shows a SMA line very close to the 1:1 line, with an intercept non-significantly different from zero, and a slope non-significantly different from 1. However, the error metrics show a comparatively lower precision (r = 0.67). Since the sample is also very accurate (SMA line not different from 1:1), a CCC = 0.67 reflects the almost null penalization of r due to lack of accuracy. Thus, the relative contribution to the MSE (=15.89) shows that most of the error is due to lack of precision (PLP = 98.9%) and just about 1% is due to lack of accuracy (PLA).

The third example (Figure 6.4C; Table 6.6C) shows a SMA line different from the 1:1 line, with an intercept greater than zero and a slope lower than 1 (evidence of proportional bias). In this case, the precision is slightly greater (r = 0.74) than for the second example, but the lack of accuracy results in a penalization of the concordance (CCC = 0.62). The contribution to the MSE (37.99), shows that the lack of agreement is due to both lack of precision (PLP = 55.5%) and accuracy (PLA = 44.5%) in similar levels.

Lastly, the example of simulated of dry-matter on chickpea, with low accuracy and medium precision (Figure 4D; Table 6D), shows a SMA line also different from the 1:1 line with an intercept significantly lower than zero and a slope significantly higher than 1. In this case, the level of precision results similar (r = 0.67) to the second example; however, the CCC (=0.28) shows a significant penalization due to the lack of accuracy. Indeed, the relative contributions to the MSE (=1.83 × 105) exhibits that most of the error obeys to a lack of accuracy (PLA = 81.3%) rather than a lack of precision (PLP = 18.7%).

6.4. Discussion

This article provides a novel perspective on using linear regression to test agreement between P and O values. Previous research in ecology has primarily discussed the axis-orientation, however, constrained to the OLS regression (Piñeiro et al., 2008). In this study, we have integrated concepts from methodological research developed at other disciplines including but not limited to: biometry (Jolicoeur, 1990; Warton et al., 2006), astronomy (Isobe et al., 1990), chemistry (Francq and Govaerts, 2014), anthropology (Smith, 2009), remote sensing (Duveiller et al., 2016; Ji and Gallo, 2006) and statistics (Carroll and Ruppert, 1996; Draper and Smith, 1998; Jolliffe, 2002; Tan and Iglewicz, 1999).

Supported on theory and examples, we have illustrated the adequacy of SMA regression as a simple linear model to test predictive ability. Whereas the traditional OLS is the most appropriate model to answer a prediction question (Legendre and Legendre, 1998; Smith, 2009), for the P-O case, we instead seek a descriptive-line of the scatter. As long as P and O variances are available, more sophisticated solutions like defining equivalence intervals are worth to be explored (St-Pierre, 2016; Tan and Iglewicz, 1999). The SMA resulted in the less biased descriptive line-of-best-fit, but in spite of advantages some caution should be considered such as with small sample sizes ($n < 20$), and presence of outliers (Miller Jr., 1986) or moderate to low correlations ($r < 0.60$) that could distort parameter estimates (Jolicoeur, 1990). Lastly, with issues of obtaining a reliable estimate for $\hat{\beta}_{SMA}$, it has been proposed that SMA should be calculated conditional to a significant correlation (Ricker, 1984), testing the assumption of a linear relationship between the variables (McArdle, 1988).The second major novelty relates to the recommendation of how to use the regression line. Beyond the traditional slope and intercept tests, we suggest to use the regression to decompose the square error producing two meaningful metrics: lack of precision and lack of accuracy. This offers the advantage of a lack of accuracy component defined not only as a difference in terms of the means (classical definition of bias, James et al. (2013)) but also as a deficiency of the model on reproducing the distribution pattern of O values (Kobayashi and Salam, 2000; Smith and Rose, 1995), which relates to proportional bias (i.e., slopes ≠ 1). We have illustrated this with the sorghum dataset (Figure 6.4C, Table 6.6C), a case with very similar Pi and Oi means (MBE = 0.72; square bias = 0.52); however, still with an evident proportional bias (with over- and under-estimations). In this case, the proposed lack of accuracy (MLA, PLA) components identified this inconsistency whereas the traditional definition of bias (MBE) could not.

If users and modelers are interested in using normalized error metrics to complement the evaluation, we also recommend to use indices or coefficients that cover both accuracy and precision. The single use of r and R^2 does not provide a complete assessment of the agreement (Lin et al., 2002; Yang et al., 2014) since a very inaccurate model (data points far from the 1:1 line) could still result in high r and R^2 values (Krause et al., 2005). We have illustrated this with the barley (Figure 6.4B; Table 6.6B) and chickpea datasets (Figure 6.4D; Table 6.6D). Although sharing similar r and R^2, the agreement is clearly lower for the chickpea case because it presents lack of accuracy. Therefore, other normalized metrics that also provide a notion of accuracy (bias) ought to be considered. Lin's CCC could be an appropriate complement, as it can be decomposed into a precision (r) and accuracy (χa) (Table 5) and its scoring rule is easy to interpret. When no additive and/or proportional bias is present, Xa= 0, and CCC will take the value of r. Additionally, CCC offers the possibility of statistical inference if we assume that CCC is a sample estimator of a population parameter (ρ_{CCC}) (Lin et al., 2002). In this sense, the CCC and its components could be considered as a normalized metric that provide similar information to the use of MSE and its accuracy and precision components.

Here we encourage the use of a symmetric regression line (SMA) that is geometrically linked to the most widely used prediction error metric in academia, the MSE (Gneiting, 2011). Although previous research presented equivalent MSE decompositions using pure formulae (Smith and Rose, 1995; Kobayashi and Salam, 2000), the use of the SMA-line adds a geometric and visually appealing interpretation of the lack of accuracy and precision components of the MSE. A normalized and complementary metric for the evaluation of agreement could be the CCC, as it also considers both accuracy and precision components. Nonetheless, a myriad of additional scoring rules not considered in this work have been developed for model evaluation, crucial for model improvement (Wallach et al., 2019). Before this overwhelming world of model evaluation criteria, modelers and users might feel submerged under "The Paradox of Choice" (Schwartz, 2004) and then simply choose the most popular metric (e.g. R^2, RMSE). Therefore, we consider that further research on comparing the behavior of scoring rules, evaluating pros and cons, should be pursued to offer users accessible guidelines (narrow down the number of choices) on the best indicators (which could vary on a case-by-case basis) to assess the performance of prediction models.

6.5. Conclusions

This manuscript explains the underlying theory, formulae, and illustrative examples to guide the selection of a linear regression model for testing agreement in continuous P-O datasets.

We argue the need for a symmetric regression with an interpretation invariant to the axis orientation highlighting the adequacy of the SMA model over other alternatives. Beyond the classical hypothesis testing of the regression-line, our SMA-based approach offers a simple error decomposition producing metrics related to lack of accuracy and precision.

Table 6.1. Loss functions of alternative regression models. OLSv: vertical ordinary least squares, OLSh: horizontal ordinary least squares, MA: Major Axis; SMA: Standardized Major Axis.

Regression model	Loss function	
OLSv	$\sum_{1}^{n} \hat{\varepsilon}_i = \sum_{1}^{n} \left(y_i - \hat{y}_i \right)^2.$	**(6.3)**
OLSh	$\sum_{1}^{n} \hat{\mu}_i = \sum_{1}^{n} \left(x_i - \hat{x}_i \right)^2.$	**(6.4)**
MA	$\sum_{i=1}^{n} \hat{d}_i = \sum_{i=1}^{n} h_i^2 = \sum_{i=1}^{n} \left(x_i - \hat{x}_{0i} \right)^2 + \left(y_i - \hat{y}_{0i} \right)^2.$	**(6.5)**
SMA	$\sum_{i=1}^{n} \hat{z}_i = \sum_{i=1}^{n} \left(\lvert x_i - \hat{x}_i \rvert \right) \left(\lvert y_i - \hat{y}_i \rvert \right).$	**(6.6)**

Table 6.2. Maximum likelihood estimators for alternative regression lines. OLSv: vertical ordinary least squares, OLSh: horizontal ordinary least squares, MA: Major Axis; SMA: Standardized Major Axis.

Regression model	**Assumed precision ratio (λ)**	**Slope formula**	
OLSv	$\lambda \to \infty$	$\hat{\beta}_{OLSv} = \frac{s_{xy}}{s_x^2}.$	**(6.9)**
OLSh	$\lambda \to 0$	$\hat{\beta}_{OLSh} = \frac{s_y^2}{s_{xy}}.$	**(6.10)**
MA	$\lambda = 1$	$\hat{\beta}_{MA} = \frac{s_y^2 - s_x^2 + \sqrt{\left(s_y^2 - s_x^2\right)^2 + 4 s_{xy}^2}}{2 s_{xy}}.$	**(6.11)**
SMA	$\lambda = s_y^2 / s_x^2$	$\hat{\beta}_{SMA} = \frac{s_y}{s_x}.$	**(6.12)**

Table 6.3. Decomposition of the square error into: i) sum of unsystematic differences (SUDSMA) and sum of systematic differences (SSDSMA) expressed as the sum of squares; ii) mean lack of precision (MLP) and mean lack of accuracy (MLA) expressed as square difference [equivalent to square bias -SB- and square difference between standard deviations -SDSD- (Kobayashi and Salam, 2000)]; iii) root transformed to original units (lack of precision –RMLP-, lack of accuracy –RMLA-); or iv) percentage lack of precision (PLP) and percentage lack of accuracy (PLA), which can eventually be further decomposed into percentage additive bias (PAB) and percentage proportional bias (PPB).

Expre-ssions	**Total**	**Lack of Precision**	**Lack of Accuracy**
Sum	$TSS=\sum_{i=1}^{n}\left(O_i-P_i\right)^2$	$SUD_{SMA}=\sum_{i=1}^{n}\left(\left\|P_i-\widehat{P}_i\right\|\right)\left(\left\|O_i-\widehat{O}_i\right\|\right)$	$SSD_{SMA}=\sum_{i=1}^{n}\left(O_i-\widehat{P}_i\right)^2 \equiv \sum_{i=1}^{n}\left(P_i-\widehat{O}_i\right)^2$
Mean	$MSE=\frac{TSS}{n}$	$MLP=\frac{SUD_{SMA}}{n} \equiv 2s_O s_P(1-r)$	$MLA=\frac{SSD_{SMA}}{n} \equiv SB+SDSD=\left(\bar{O}-\bar{P}\right)^2+\left(s_O-s_P\right)^2$
Root Mean	$RMSE=\sqrt{MSE}$	$RMLP=\sqrt{MLP}$	$RMLA=\sqrt{MLA}$
%	-	$PLP(\%)=100\frac{MLP}{MSE}$	$PLA(\%)=100\frac{MLA}{MSE}$ $PAB(\%)=100\frac{\left(\bar{O}-\bar{P}\right)^2}{MSE}$ $PPB(\%)=100\frac{\left(s_O-s_P\right)^2}{MSE}$

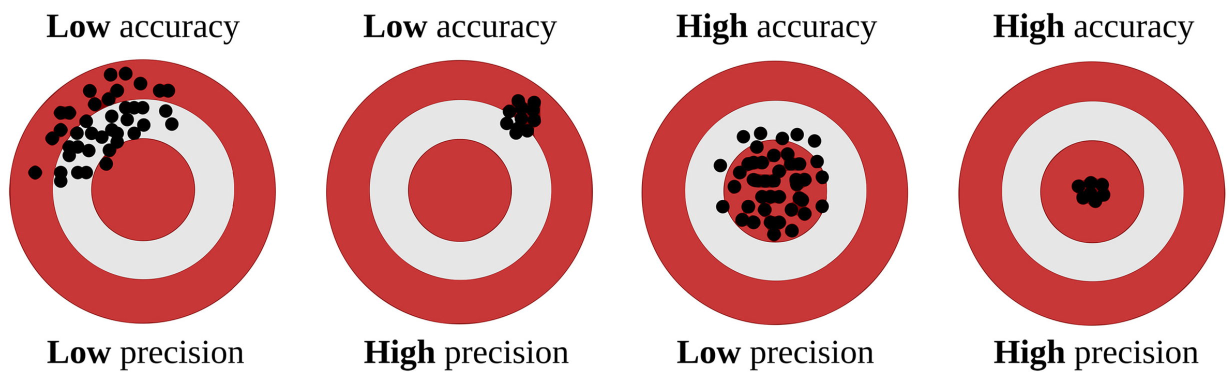

Figure 6.1. Hypothetical combinations of accuracy and precision. Adapted from Tedeschi (2006).

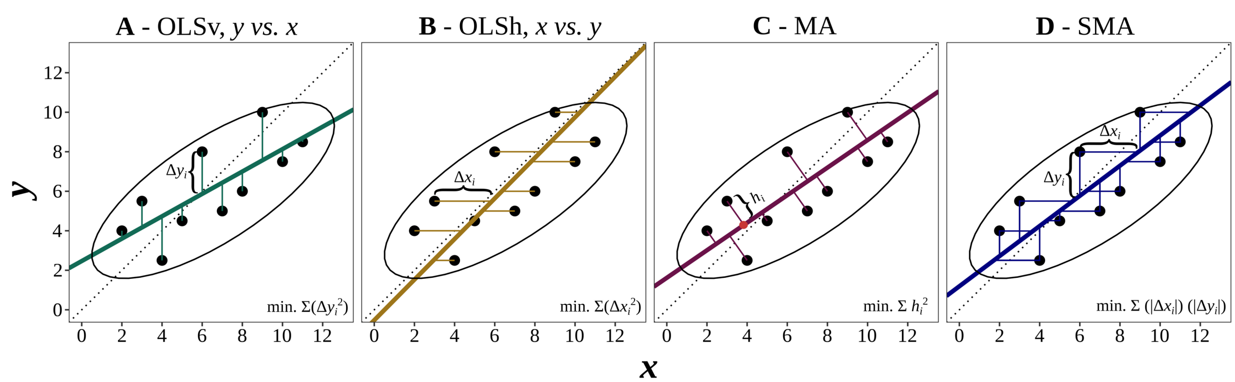

Figure 6.2. Illustration of error partitioning by asymmetric (A, B) and symmetric (C, D) regression models for the same dataset (*x = 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0; y = 4.0, 5.5, 2.5, 4.5, 8.0, 5.0, 6.0, 10.0, 7.5, 8.5*). A: Ordinary Least Squares vertical (OLSv, *y* vs. *x*, $\hat{y}_i = 2.47 + 0.57\,x_i$); B: Ordinary Least Squares vertical (OLSh, *x* vs. *y*, $\hat{y}_i = -0.53 + 1.03\,x_i$); C: Major Axis regression (MA, $\hat{y}_i = 1.62 + 0.70\,x_i$); D: Standardized Major Axis regression (SMA, $\hat{y}_i = 1.19 + 0.76\,x_i$). In C, the red dot over the MA-line represents the coordinates $(\hat{x}_{0i};\hat{y}_{0i})$ described in Eq. (5) (Table 1). Ellipses represent the 95% confidence ellipses to the joint bivariate normal distributions fitted on the data.

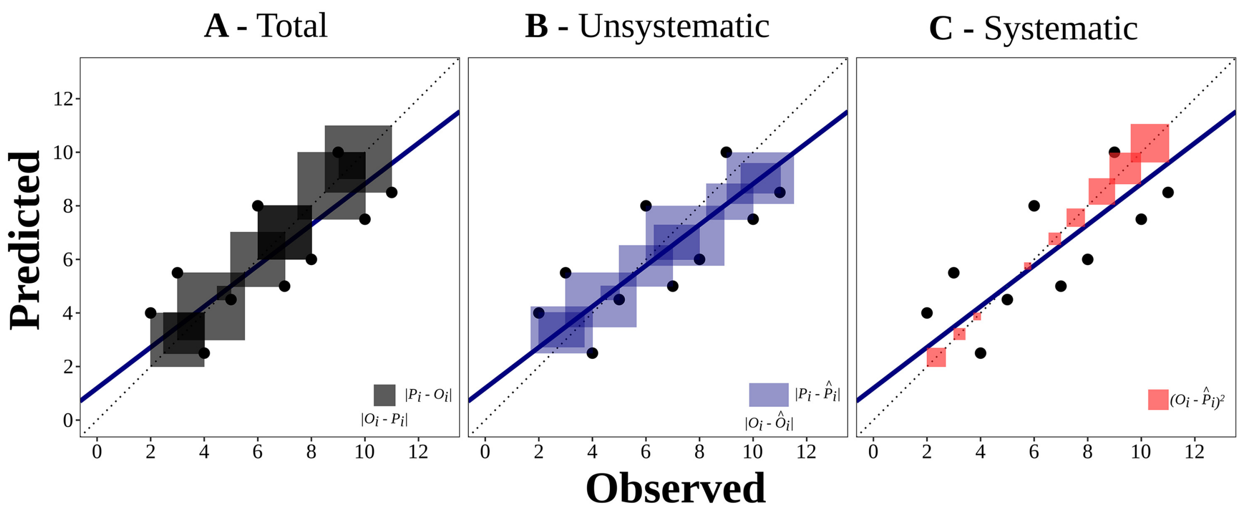

Figure 6.3. Decomposition of the total sum of square differences (A) into the unsystematic (B, lack of precision) and the systematic differences (C, lack of accuracy) using standardized major axis regression (SMA). For this example, *TSS* = 38.25 (*MSE* = 3.82), SUD_{SMA} = 32.39 (*MLP* = 3.24, *PLP* = 84.68%), SSD_{SMA} = 5.86 (*MLA* = 0.59, *PLA* = 15.32%).

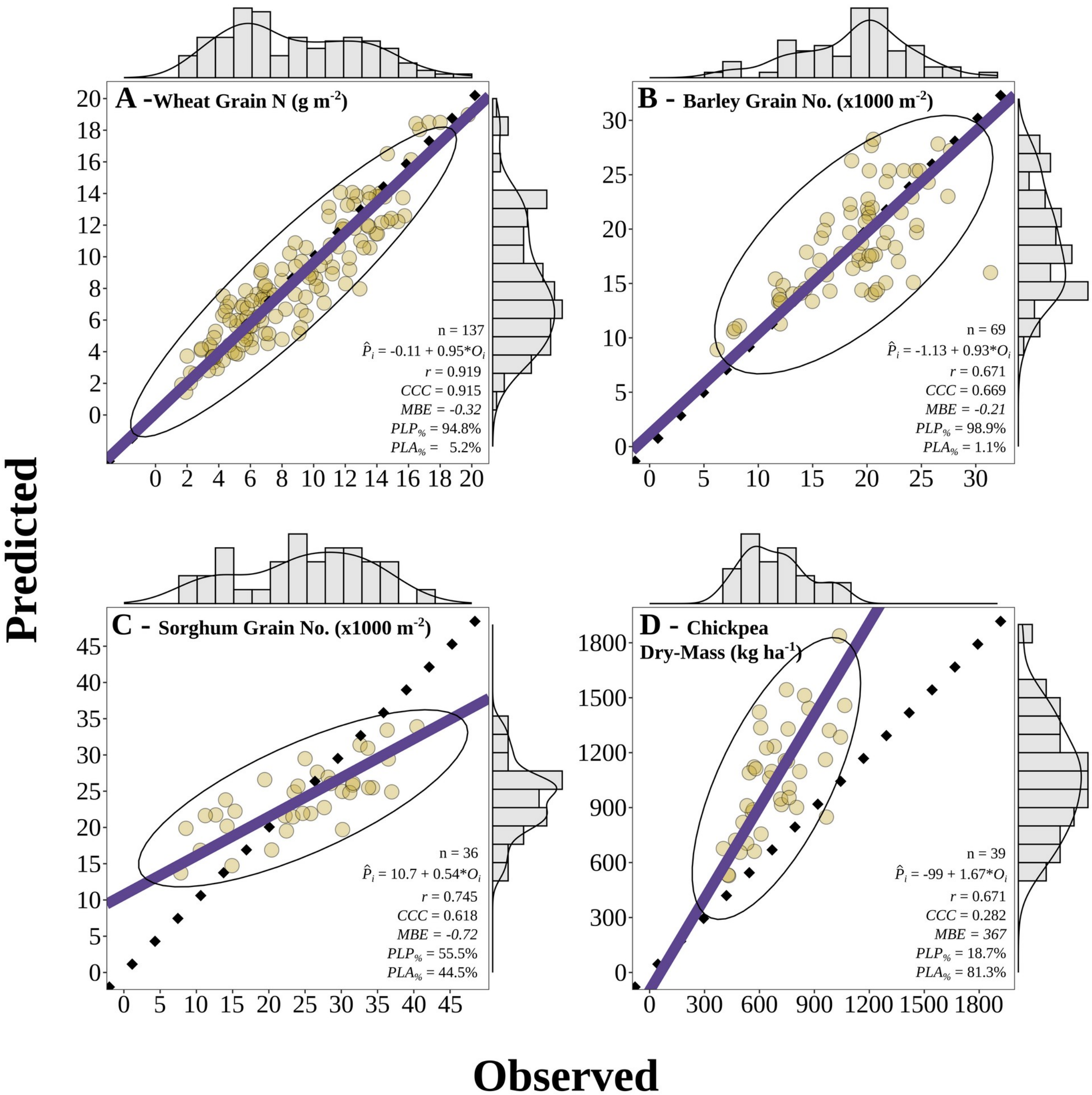

Figure 6.4. Real datasets from APSIM crop simulation model (Holzworth et al., 2018) showing contrasting scenarios of predicted-observed agreement. A: high accuracy and precision. B: high accuracy and low precision. C: medium accuracy and medium precision. D: low accuracy and medium precision. Ellipses represent the 95% confidence ellipses to the joint bivariate normal distributions fitted on the data.

Chapter 7: Conclusions

The first objective of this dissertation was *to assess the contribution of soil, weather, and crop management factors on the prediction of maize productivity without external N application.* In Chapter 2, we documented that crop management factors such as previous crop and irrigation in combination with soil organic matter contributed to explain half of the variability of maize yield without N fertilization, while the inclusion of variables linked to weather improved the prediction performance. From a practical standpoint, a prediction framework including only spring weather variables (March-May) resulted in a similar performance than a framework including weather during the entire season. Refined prediction frameworks for Y0 could provide new insights on N responsiveness and result in a step-forward towards more collaborative and regional-scale N recommendation guidelines.

The second objective of this dissertation was *to identify the main drivers of both, expected values and uncertainties, of key components describing the process models for maize yield response to N fertilization.* In that regards, one of the main conclusions of Chapter 3 is that the expected values of N response components and, although more challenging, their related uncertainties are both susceptible to be modeled. Crop management factors largely affected the prediction of the expected yield without N fertilizer, but just slightly impacted (<5%) the uncertainty of the response (and their components) of yield to N fertilizer. Weather variables were, undoubtedly, the most relevant factors and roughly contributing to 80% of the explained variance to predict the uncertainties on the yield to N response process (and their components). Soil factors showed a limited but consistent contribution to explain both N response as well as their uncertainties.

The third objective of this dissertation was *to summarize the impact of water and N management practices in maize grain quality*. The meta-analysis conducted in Chapter 4 revealed that N fertilization not only increases yields but also has a positive impact on the grain protein concentration, however, both starch and oil remained relatively constant under contrasting N fertilization levels. Conversely, water stress resulted in an inconsistent effect on all the evaluated grain quality components, possibly due to changes in the moment, severity, and extent of the stress. A last major takeaway of this chapter is related to the possibility for maintaining or increasing oil concentration while improving protein, representing an exceptional opportunity for producing high quality and energy maize grain crops.

The fourth objective of this dissertation was *to study the residual effects of N management in maize on the following soybean crop.* For this purpose, in Chapter 5, we evaluated data from two case studies: (i) I, long-term (1983-2020), and (ii) II, detailed soil-plant characterization (2019-2020). Overall, soybean yields were marginally or not affected by the previous crop, maize N management. The estimated apparent N budgets from the preceding maize crop ranged from ca. -100 to +50 kg N ha^{-1}, soil residual N contents during the following soybean season were not affected by maize N management. Similarly, the N fixation was not or slightly impacted, with no compromise to soybean N uptake or seed productivity. Still, the long-term impact of soil N mining or soil N surplus on the contribution of N fixation to crop N demand remains on the spotlight for future research steps.

The fifth objective of this dissertation was *to evaluate statistical techniques for the assessment of agreement between predictions and observations*. Thus, in Chapter 6, we offered a novel and simple perspective about the use of linear regression to evaluate the performance of modeled (predicted) versus observed (measured) plant traits. Three alternative linear regression models (Ordinary Least Squares -OLS-, Major Axis -MA-, and Standardized Major Axis -SMA-) were compared in terms of their assumptions, loss functions, parameters' estimates, and on the interpretation for the predicted-observed case. When the uncertainty of predictions and observations are unknown, the SMA is the most adequate approach to fit a symmetric-regression line describing the scatter, which produces a reference line to estimate a weighed difference between predictions and observations. Furthermore, modelers can use this symmetric line to decompose the mean square error into additive components associated with the lack of both accuracy and precision of the model outcomes, allowing to identify error components.

This dissertation highlights the advantages of deploying cutting edge data analysis techniques for addressing research gaps on the N economy in maize-soybean farming systems. Machine learning, meta-analysis, and Bayesian statistics bring new horizons for improving forecast models as well as their interpretability. Machine learning methods bring the possibility of handling massive amounts of data while identifying complex association patterns to produce accurate forecasts; meta-analysis techniques offer a great opportunity to summarize results from multiple studies considering their degree of error; and Bayesian frameworks integrate existing knowledge with data to produce inference where the uncertainties and probabilities are on the spotlight.

The main limitations faced in our projects were related to (i) the lack of available metadata to explore more specific questions and, (ii) the limited interpretability of machine learning models. For instance, in Chapters 2 and 3, the lack of soil N supply indicators clearly constrained the assessment of soil features and their importance for the predicted frameworks. Similarly, in Chapter 4, the lack of studies evaluating the interaction between N and water stress (even more critically in combination) have limited the inference on potential co-limitations impacting maize grain quality components. Unfortunately, achieving unbalanced meta-databases is usual when performing literature reviews. As for the interpretability issue, the increasing computational power and development of new algorithms are essential to overcome this limitation. In this regards, cross-scales- and meta-learning models coupled with plant-soil system simulations represent a new era in agricultural science.

Forthcoming projects on N economy in maize and soybean farming systems should address the following challenges: (i) expand, provide incentives, and discuss standards in collaborative research in order to achieve more balanced multidimensional databases, (ii) further deploy machine learning tools such as the multi-ensembles models in order to improve predictive performance, (iii) invest on the development of cross-borders N guidelines based on process rather than on political borders, (iv) further assess the role of N management strategies on the nutritional value of maize grains and soybean seeds, (v) design, conduct, and analyze surveys to visualize stakeholders' perspectives regarding both the current as well as the under-development N decision-support tools, and (vi) invest more resources to maximize extension effectiveness, redesigning the outreach approaches when necessary.

The future generation of predictive models in agriculture must be able to capture complex GxExM interactions as well as to emulate how farmers deal with uncertainties in the real world. Therefore, forthcoming improvements on the decision support tools for N management into maize-soybean rotations should be ideally conceived under probabilistic frameworks, with risk management at the center of attention. Most of current models omit the evaluation of climatic and economic risks that the producers face in a regular basis. In contrast, farmers are basically obliged to manage their land adapting decisions to fit the spatio-temporal variation in their fields. Under this context, the awareness about uncertainties (and their drivers) should become one of the pillars of the dynamic N recommendations, which is crucial to convey wise information to stakeholders. Undoubtedly, we must move from static to dynamic, from *ex-post* to *ex-ante*, crop models in order to design optimized GxM adaptation strategies under future climates.

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