Supplementary material

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

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Supp. Table 2.1.

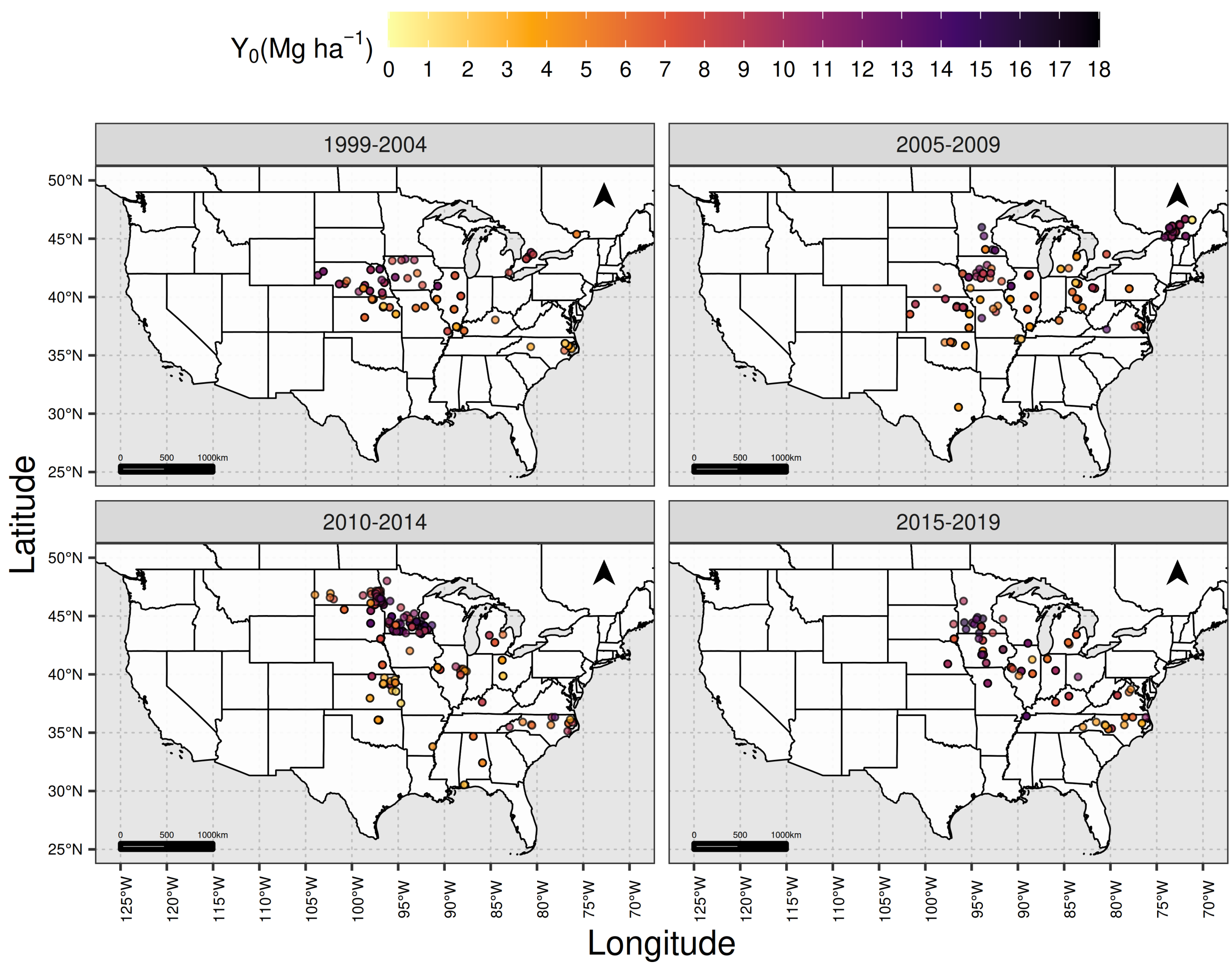
Data references, number of Y_0 (site-years), states and years covered by each source.

Source	Reference	Y_0 (site-years)	State/s	Year/s
1	Archontoulis (pers. comm.)	6 (6)	IA	2017-2018
2	Asebedo (2015)	5 (5)	KS	2012-2014
3	Barker (2011)	2 (2)	IA	2009-2010
4	Berg (2016)	14 (2)	SD	2014-2015
5	Cook et al. (2010)	5 (2)	PA	2007-2008
6	Correndo and Ciampitti (pers. comm.)	2 (1)	KS	2019
7	Corteva Agrisciences (pers. comm.)	130 (35)	IA, IL, IN, MN, MO, NE, SD, TN, WI	2011-2019
8	Coulter (pers. comm.)	11 (11)	MN	2015
9	Crozier et al. (2014)	4 (4)	NC	2010-2012
10	Edmonds et al. (2013)	4 (4)	OK	2005-2007
11	Ferdinand et al. (2003)	4 (2)	KS	2003
12	Foster 2014	5 (5)	KS	2012-2013
13	Franzluebbers (2018); Franzluebbers et al. (2018)	27 (27)	NC, VA	2014-2016
14	Gehl et al. (2005)	10 (10)	KS	2001-2002
15	Gordon (2003)	1 (1)	KS	2003
16	Henry et al. (2010)	8 (4)	OH	2007-2008
17	Hoben et al. (2011)	7 (7)	MI	2007-2008
18	Holland and Schepers (2010)	3 (3)	NE	2002-2004
19	Holou et al (2011)	2 (2)	MO	2008-2009
20	Janssen et al. (2006; 2011)	11 (8)	KS	2006-2010
21	Kelley and Moyer (2007; 2009)	18 (3)	KS	2005-2009
22	Kent et al. (2012)	8 (4)	MN	2011-2012
23	Lamond et al. (2001)	2 (2)	KS	2000-2001
24	Lindsey et al. (2015)	16 (4)	OH	2013-2014
25	Ma et al. (2005)	3 (3)	CAN	2000-2002
26	Maddux (2008)	3 (3)	KS	2006-2008
27	Mahama et al. (2016)	4 (4)	KS	2013-2014
28	Miller (2014)	32 (4)	OK	2013-2014
29	Miller et al. (2017)	4 (4)	OK	2013-2014
30	Mueller et al. (2013)	13 (13)	KS	2010-2011
31	Nafziger (pers. comm.)	140 (70)	IL	1999-2008
32	Rajkovich et al. (2017)	6 (6)	NC	2014-2015
33	Reese et al. (2014)	12 (4)	SD	2014-2015
34	Roberts et al. (2016)	2 (2)	AR	2011-2012
35	Rudnick et al. (2016)	9 (3)	NE	2012-2014
36	Ruf-Pachta et al. (2013)	4 (2)	KS	2005-2006
37	Ruiz-Diaz (2007)	6 (2)	IA	2005-2006
38	Ruiz-Diaz et al. (2008)	30 (30)	IA	2004-2006
39	Santoro (2015)	14 (3)	KY	2015-2016
40	Schwab and Murdock (2005)	4 (4)	KY	2003-2004
41	Shahandeh et al. (2011)	6 (3)	TX	2005-2007
42	Sharma (2014); Sharma et al. (2015, 2016a, 2016b)	51 (51)	ND	2011-2013
43	Shepard et al. (2011)	8 (8)	IL, OH	2006-2007
44	Sindelar et al. (2013; 2015)	36 (6)	MN	2009-2012

Source	Reference	Y_0 (site-years)	State/s	Year/s
45	Sistani et al. (2017)	2 (2)	KY	2007-2008
46	Stamper (2009)	8 (3)	KS	2007-2009
47	Steinke (pers. comm.)	18 (18)	MI	2011-2018
48	Torino et al. (2014)	10 (8)	AL	2010-2012
49	Tremblay (pers. comm.)	92 (92)	CAN	2000-20009
50	Tremblay et al. (2012)	46 (46)	IL, KS, MO, NE, OH, OK, VA, CAN	2006-2009
51	Tucker (2010)	10 (10)	KS	2006-2009
52	Walker et al. (2018)	14 (14)	MN	2014
53	Walsh et al. (2012)	9 (9)	OK	2005-2007
54	Wheeler (2014)	8 (8)	IL	2013
55	Williams et al. (2007a; 2007b)	25 (25)	NC	2000-2004
56	Williams et al. (2010)	6 (6)	MO	2000-2001
57	Wortmann et al. (2011)	32 (32)	NE	2002-2004
58	Yost et al. (2012; 2013; 2014)	58 (28)	MN	2009-2012
59	Zhu et al. (2015)	1 (1)	PA	2009

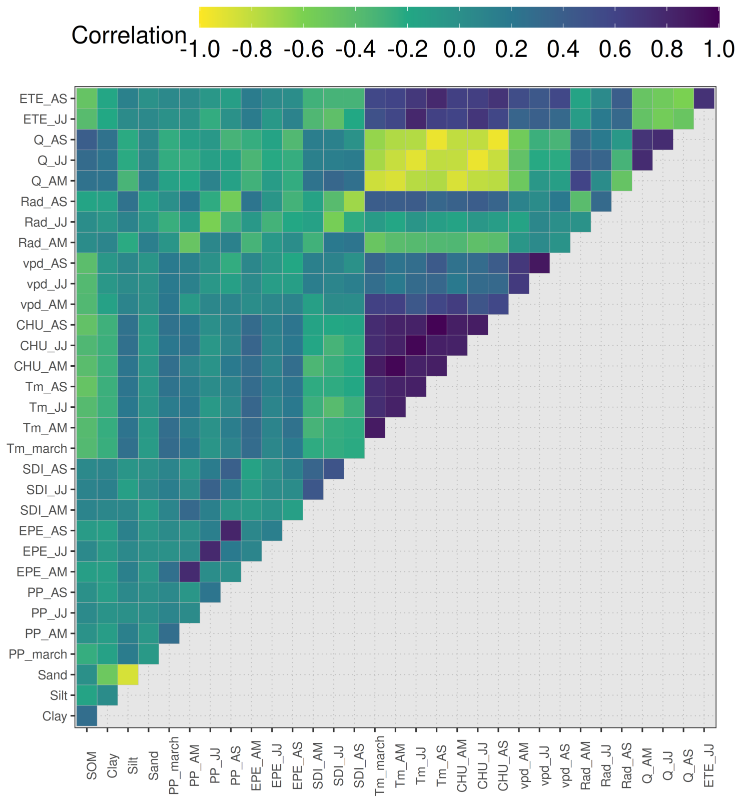
Supp. Figure 2.1.

Spatio-temporal distribution of maize nitrogen trials used for the analysis.



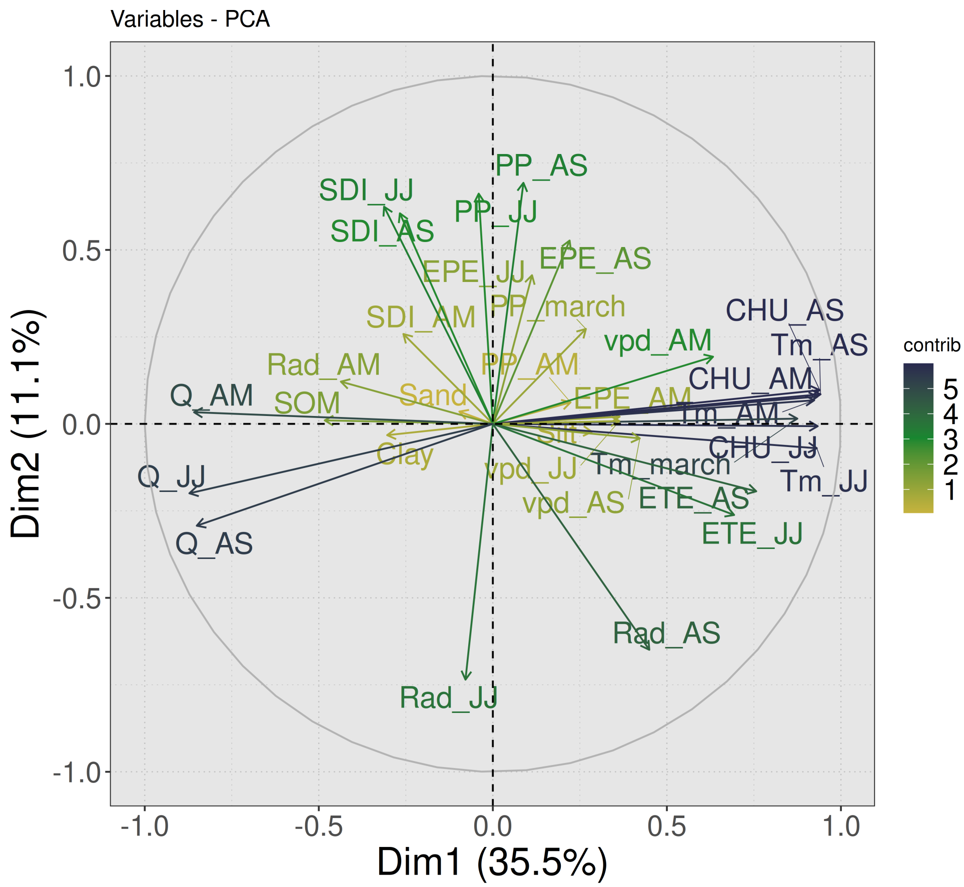
Supp. Figure 2.2.

Correlation matrix for continuous features used for the full model for maize yield prediction under N omission (Y_0, Mg ha^{-1}).



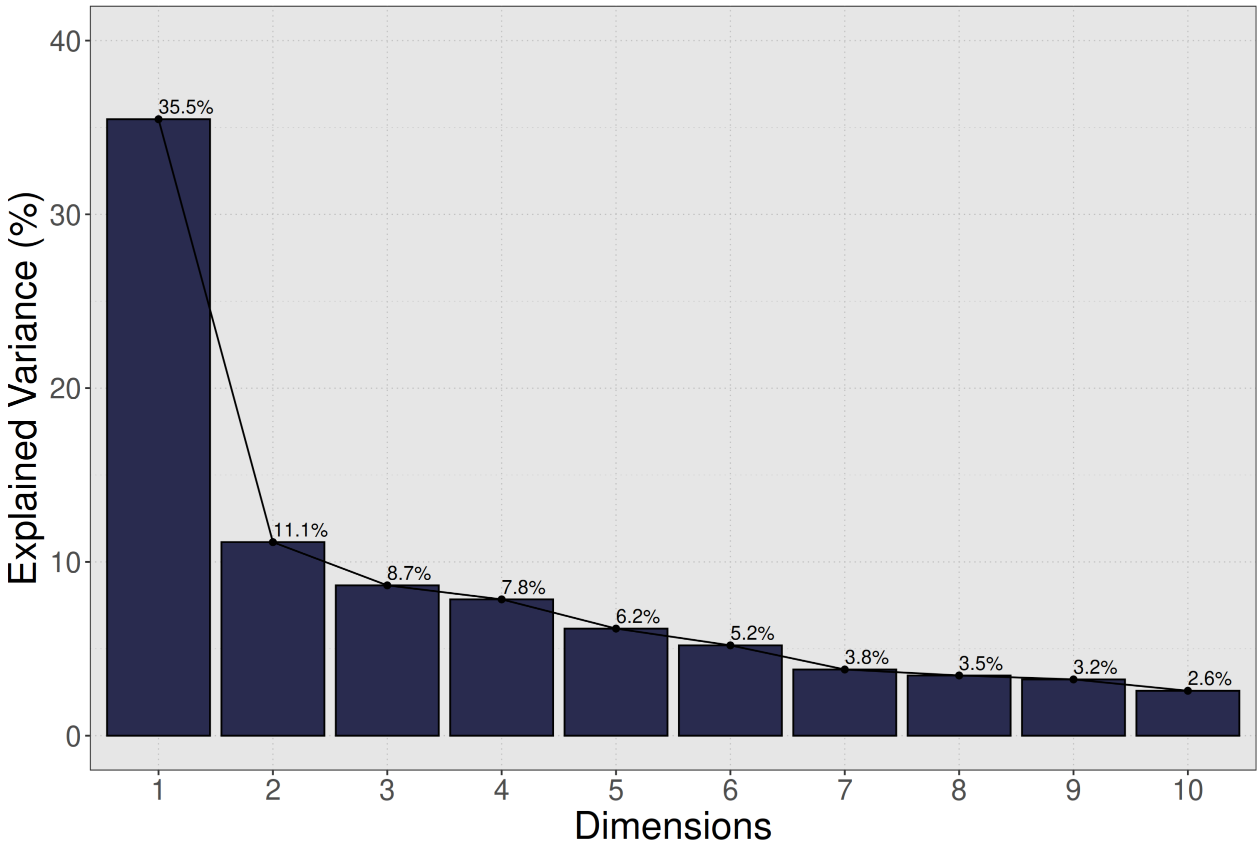
Supp. Figure 2.3A.

Biplot of principal components analysis for continuous features used for the full model for maize yield prediction under N omission (Y_0, Mg ha^{-1}).



Supp. Figure 2.3B.

Contribution of dimensions to the principal components analysis for continuous features used for the full model for maize yield prediction under N omission (Y_0, Mg ha^{-1}).



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Supplementary material

Chapter 3: Unraveling uncertainty drivers of the maize yield response to nitrogen:

A Bayesian and machine learning approach

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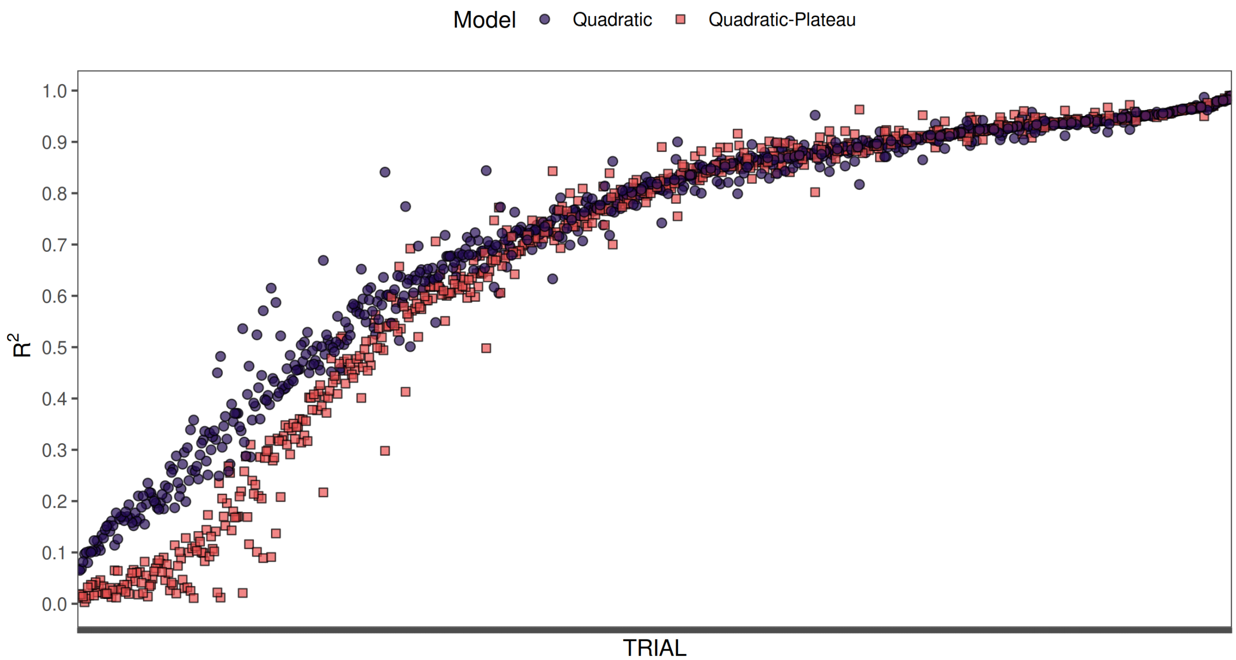
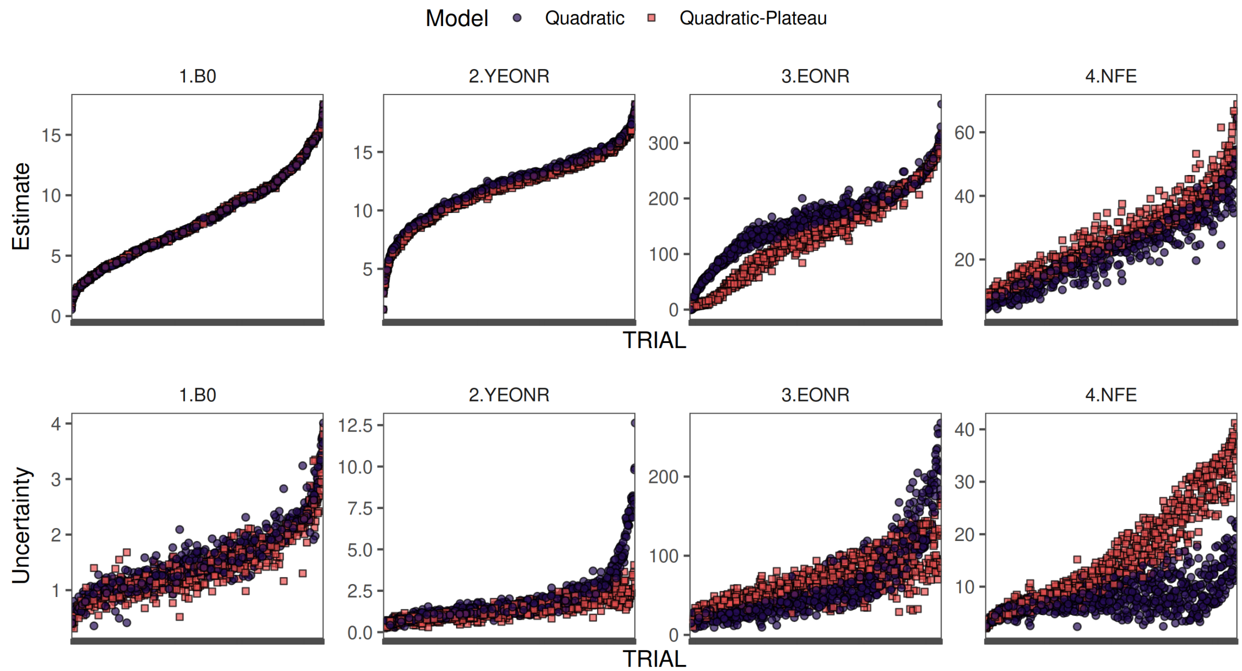
Supp. Figure 3.1.

Comparison of performance (R^2 median from posterior samples) obtained with quadratic and quadratic-plateau models for the 730 maize N response curves under study.



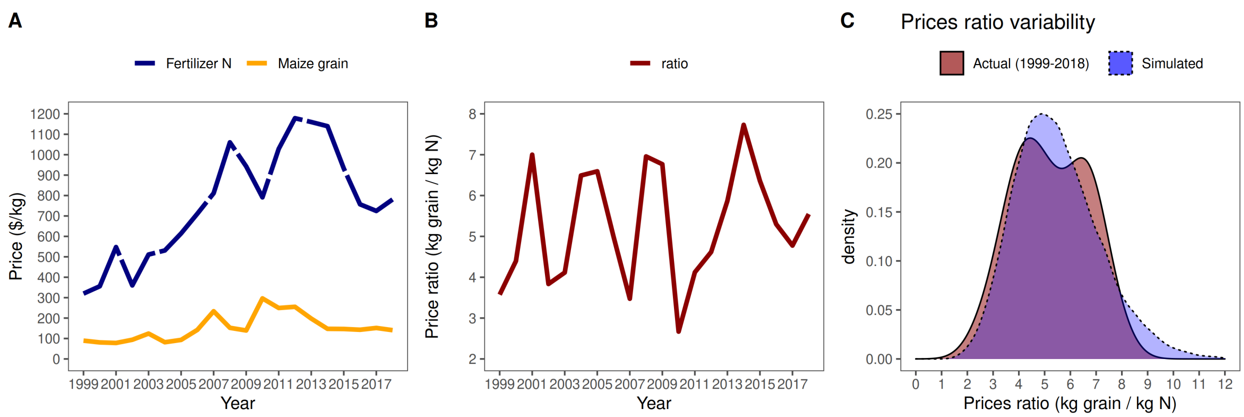
Supp. Figure 3.2.

Comparison of maize N response descriptors of interest (B0, YEONR, EONR, NFE) obtained with quadratic and Quadratic-Plateau models for the 730 maize N response curves under study.



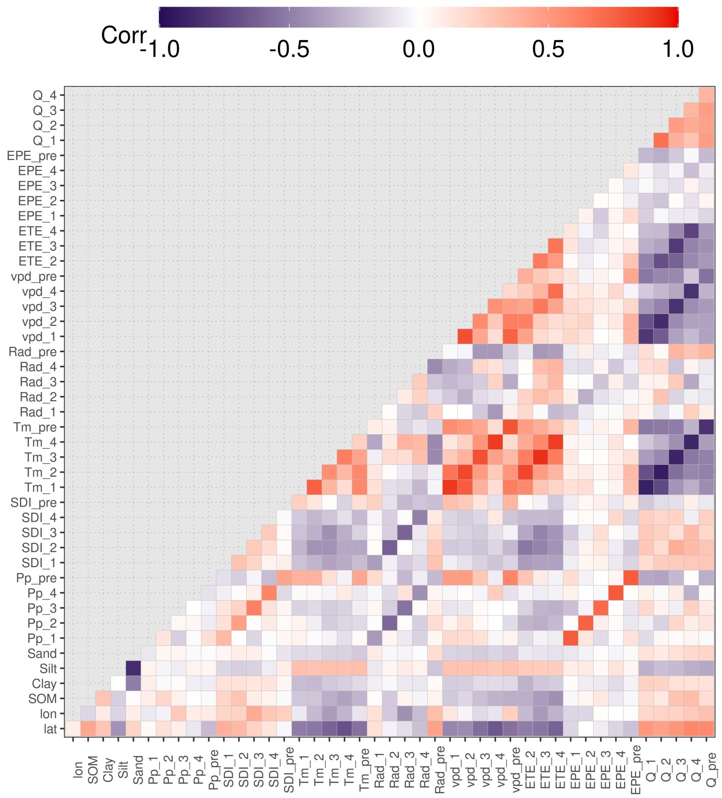
Supp. Figure 3.3.

Historical (1999-2018) maize grain and fertilizer N prices (A), prices ratios (B), and actual and simulated probability distributions of prices ratios (C). Simulated prices ratio distribution was used as a prior in the Bayesian analysis framework, representing a stochastic component associated with prices variability when performing the EONR calculations.



Supp. Figure 3.4.

Correlation matrix showing the linear association among the continous covariates used for predicting the components (B0, YEONR, EONR, NFE) of maize yield response to N.



Supp. Table 3.1.

Data references, number of curves (site-years), states and years covered by each source.

Source	Reference	Curves (site-years)	State/s	Year/s
1	Asebedo (2015)	4 (4)	KS	2012-2014
2	Berg (2016)	14 (2)	SD	2014-2015
3	Correndo and Ciampitti (pers. comm.)	4 (2)	KS	2019, 2020
4	Corteva Agrisciences (pers. comm.)	109 (19)	IA, IL, IN, MN, MO, NE, SD, TN, WI	2011-2019
5	Coulter (pers. comm.)	10 (10)	MN	2015
6	Crozier et al. (2014)	3 (3)	NC	2010-2012
7	Foster 2014	5 (5)	KS	2012-2013
8	Gordon (2003)	1 (1)	KS	2003
9	Hoben et al. (2011)	7 (7)	MI	2007-2008
10	Holland and Schepers (2010)	3 (3)	NE	2002-2004
11	Janssen et al. (2011)	4 (4)	KS	2006-2010
12	Lindsey et al. (2015)	16 (4)	OH	2013-2014
13	Miller et al. (2017)	4 (4)	OK	2013-2014
14	Nafziger (pers. comm.)	134 (68)	IL	1999-2008
15	Rajkovich et al. (2017)	4 (4)	NC	2014-2015
16	Rudnick et al. (2016)	9 (3)	NE	2012-2014
17	Ruiz-Diaz (2007)	6 (2)	IA	2005-2006
18	Ruiz-Diaz et al. (2008)	30 (30)	IA	2004-2006
19	Shahandeh et al. (2011)	5 (3)	TX	2005-2007
20	Sharma (2014); Sharma et al. (2015, 2016a, 2016b)	48 (48)	ND	2011-2013
21	Shepard et al. (2011)	8 (8)	IL, OH	2006-2007
22	Sindelar et al. (2013; 2015)	30 (6)	MN	2009-2012
23	Steinke (pers. comm.)	17 (15)	MI	2011-2018
24	Torino et al. (2014)	10 (8)	AL	2010-2012
25	Tremblay (pers. comm.)	79 (79)	CAN	2000-20009
26	Tremblay et al. (2012)	41 (41)	IL, KS, MO, NE, OH, OK, VA, CAN	2006-2009
27	Tucker (2010)	9 (9)	KS	2006-2009
28	Walker et al. (2018)	14 (14)	MN	2014
29	Wheeler (2014)	7 (7)	IL	2013
30	Wortmann et al. (2011)	32 (32)	NE	2002-2004
31	Yost et al. (2012; 2013; 2014)	58 (32)	MN	2009-2012
32	Zhu et al. (2015)	1 (1)	PA	2009

Supp. Table 3.2.

Details of metrics (scoring rules) used for the assessment of agreement between predicted and observed values of B0, YEONR, EONR, and NFE. P_i: predicted value for the i^{th} trial; O_i: observed value at the i^{th} trial; n: size of the learning sample.

#	Scoring rule	Details	Formula
1	RMSE	Root mean square error	$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)^2}$
2	RRMSE	Relative RMSE	$\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)^2}}{\overline{O}}$
3	MBE	Mean bias error	$\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i) = \overline{P} - \overline{O}$
4	ME	Nash-Sutcliffe model efficiency	$1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(O_i - \overline{O})^2}$
5	KGE	Kling-Gupta model efficiency	$1 - \sqrt{(r-1)^2 + (\frac{s_P}{s_O} - 1)^2 + (\frac{\overline{P}}{\overline{O}} - 1)^2}$
6	CCC	Concordance correlation coefficient	$\frac{2s_{PO}}{s_P^2 + s_O^2 + (\overline{O} - \overline{P})^2}$
7	R^2	Coefficient of determination	$\frac{s_{PO}^2}{s_P^2 s_O^2}$

where,

$$s_P = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - \overline{P})^2}$$

$$s_O = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(O_i - \overline{O})^2}$$

$$s_{PO} = \frac{1}{n}\sum_{i=1}^{n}(P_i - \overline{P})(O_i - \overline{O})$$

and

$$r = \frac{s_{PO}}{s_P s_O}$$

.

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Supplementary Material

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

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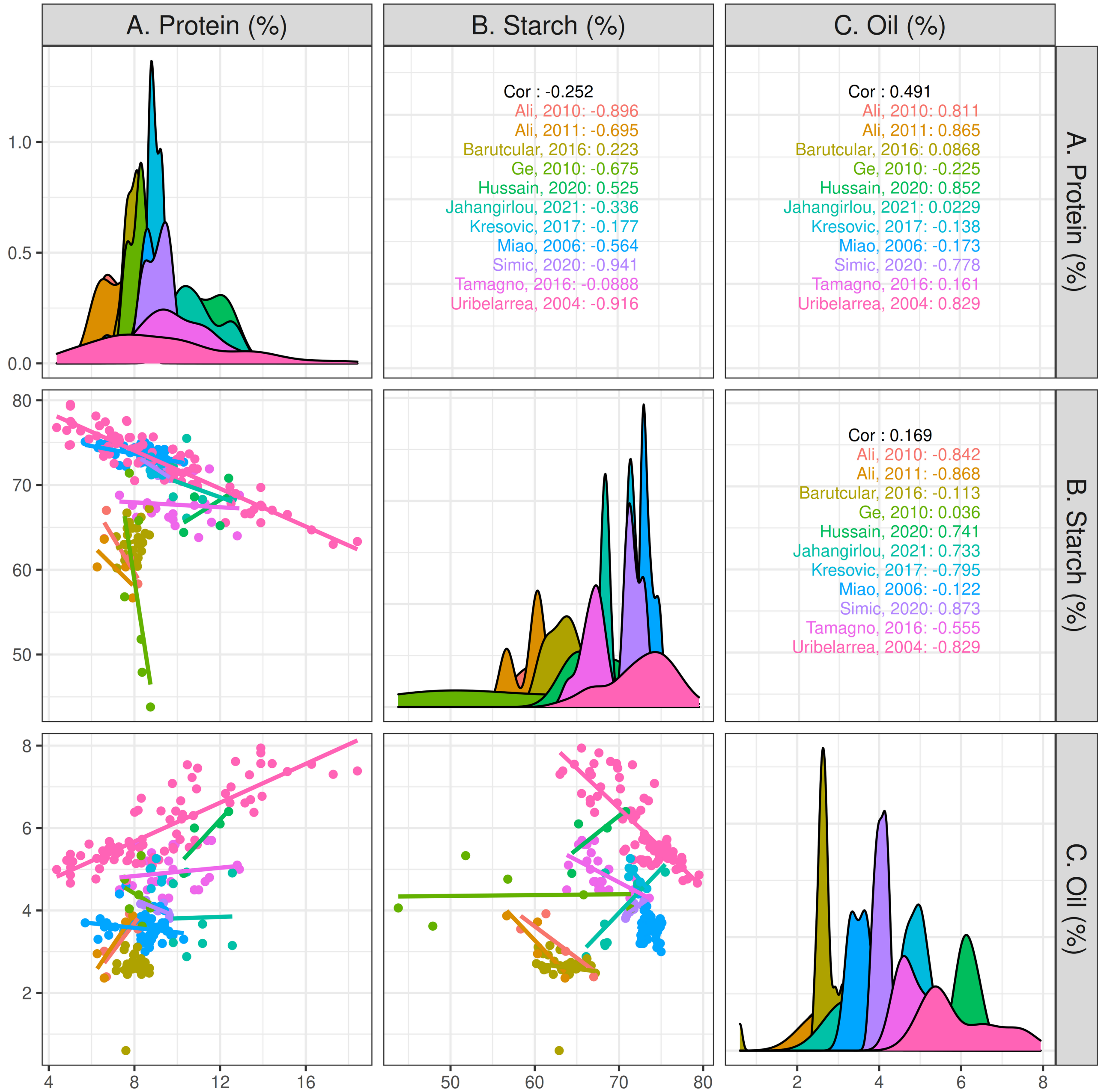

Supplementary Figure 4.1. Correlation matrix between protein concentration (%), starch concentration (%), and oil concentration (%) split by study quantifying the three variables (n = 239) (**Table 4.1**).

Supplementary Figure 4.2. By-study summary of effect sizes (%) of nitrogen fertilization on maize grain quality components (A – Protein, B – Starch, and C – Oil) considering the rate level (Low -<70 kg N ha^{-1}-, Med - 71-150 kg N ha^{-1}-, and High ->150 kg N ha^{-1}-). Within each variable, symbols represent the mean effect, shape size represents the weight, and whiskers their respective 95% confidence intervals (CI, whiskers), which were transformed from lnRR into percentage (exp(lnRR)-1*100), as the protein, starch or oil concentration variation in N fertilized compared to their respective control (0 kg N ha^{-1}).

Supplementary Material

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

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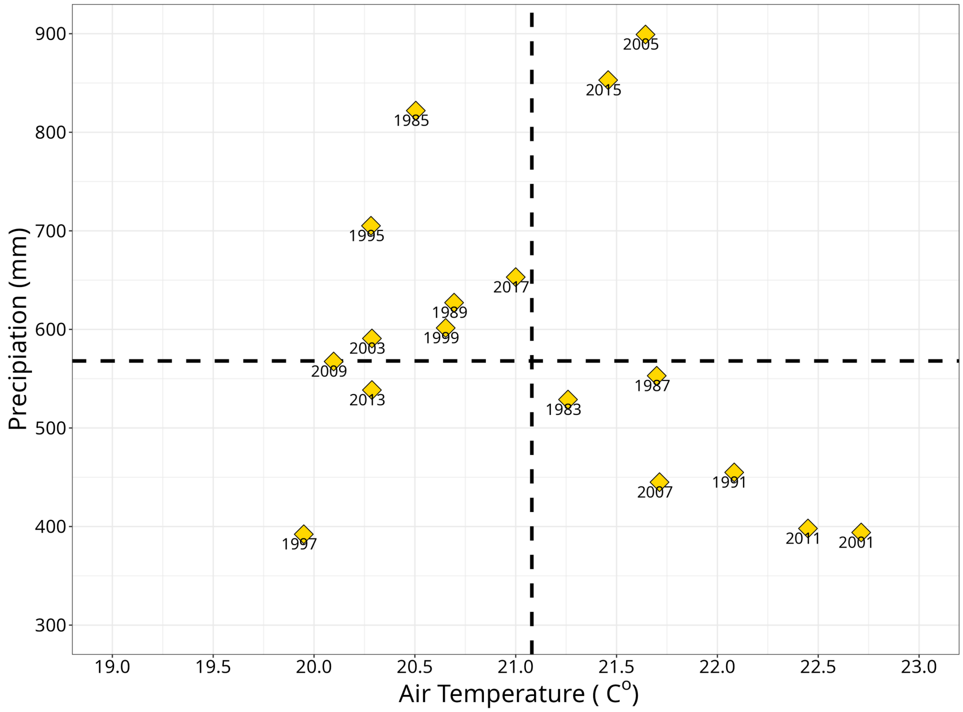
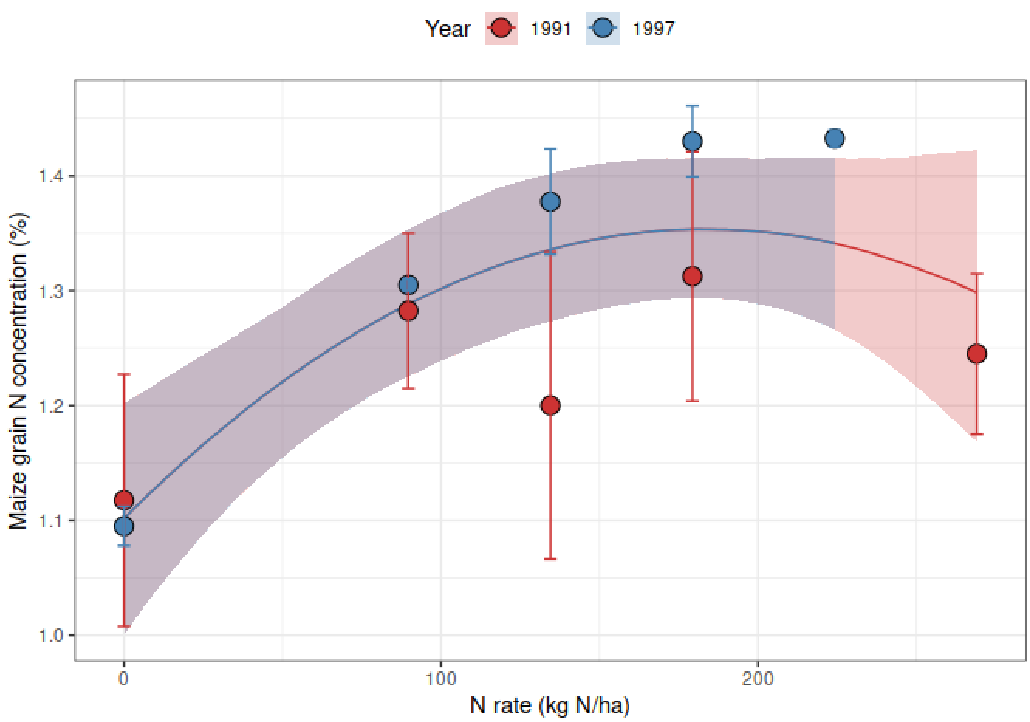
Supplementary Table 5.1. General soil and crop management practices at the long-term maize-soybean rotation nutrition trial. Kansas River Valley Experiment Field, Topeka, KS.

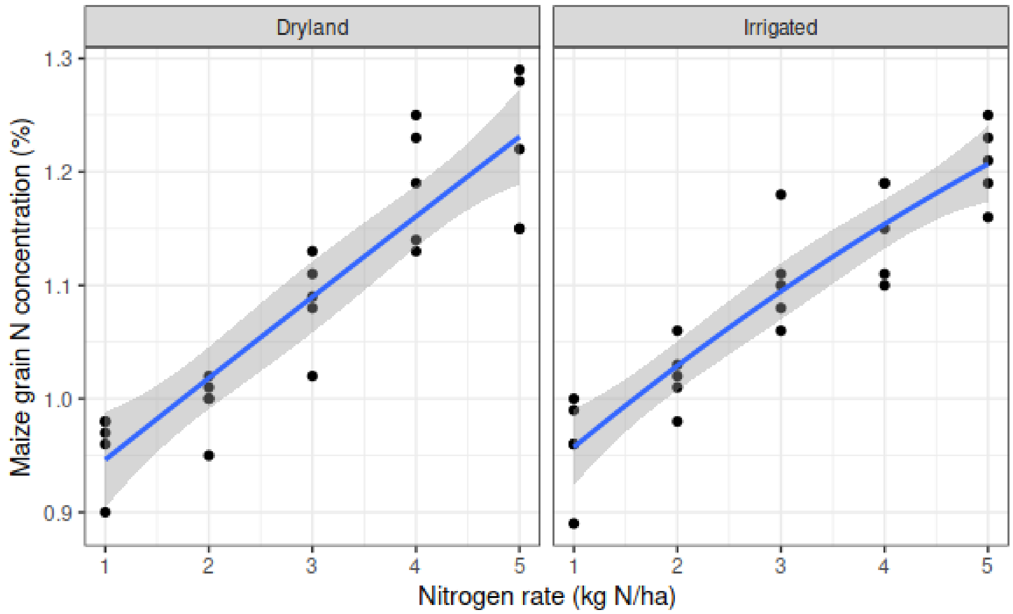
Crop	Year	Hybrid or Variety	Seed rate (seeds m^{-2})	Sowing date	Harvest date	Irrigation (mm)
Maize	1983	BoJac 603	6.2	04-21	09-09	243
	1985	Pioneer 3377	6.2	04-16	09-04	149
	1987	Pioneer 3377	6.2	04-22	09-02	228
	1989	Pioneer 3377	6.4	04-18	09-18	418
	1991	Jacques 7820	6.2	04-09	09-05	287
	1993	Jacques 7820	6.2	04-22	09-17	0
	1995	Mycogen 7250	6.2	04-06	09-25	153
	1997	DeKalb DKC626	6.2	-	-	92
	1999	DeKalb DKC626	7.1	04-13	-	108
	2001	Golden Harvest H2547	7.1	04-20	10-02	162
	2003	Pioneer 33R77	7.1	04-11	09-16	235
	2005	DeKalb DKC63-81	7.1	04-18	10-07	96
	2007	Asgrow RX785	7	04-23	09-06	106
	2009	DeKalb DKC63-42		05-06	-	25
	2011	DeKalb DKC63-49	6.8	04-18	09-06	180
	2013	Pioneer 1151	7.1	04-30	09-24	244
	2015	Pioneer 1105	7.6	04-14	09-10	164
	2017	Pioneer 1257	7.5	04-25	09-20	204
	2019	Pioneer 1197	7.8	04-22	09-16	110



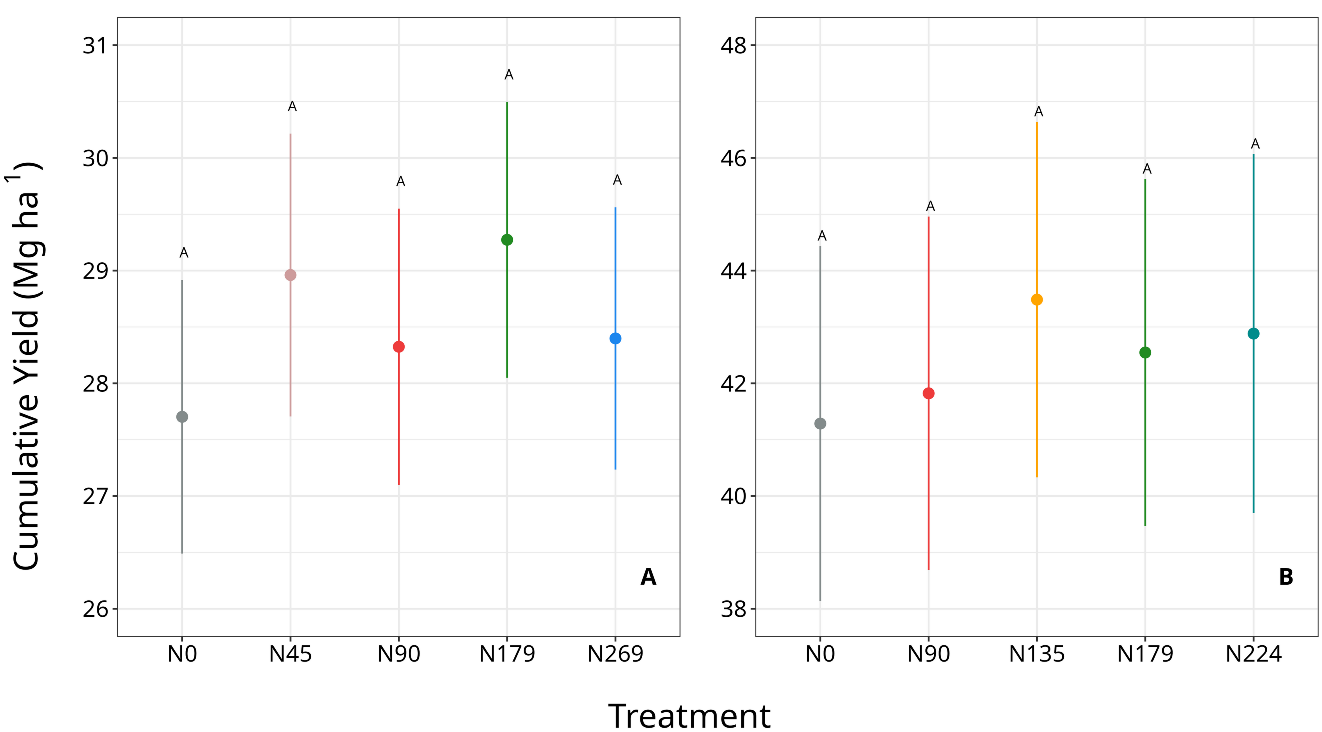
Supplementary Figure 5.1. Weather classification of maize cropping seasons over time. Case study I, Kansas River Valley Field Experiment.



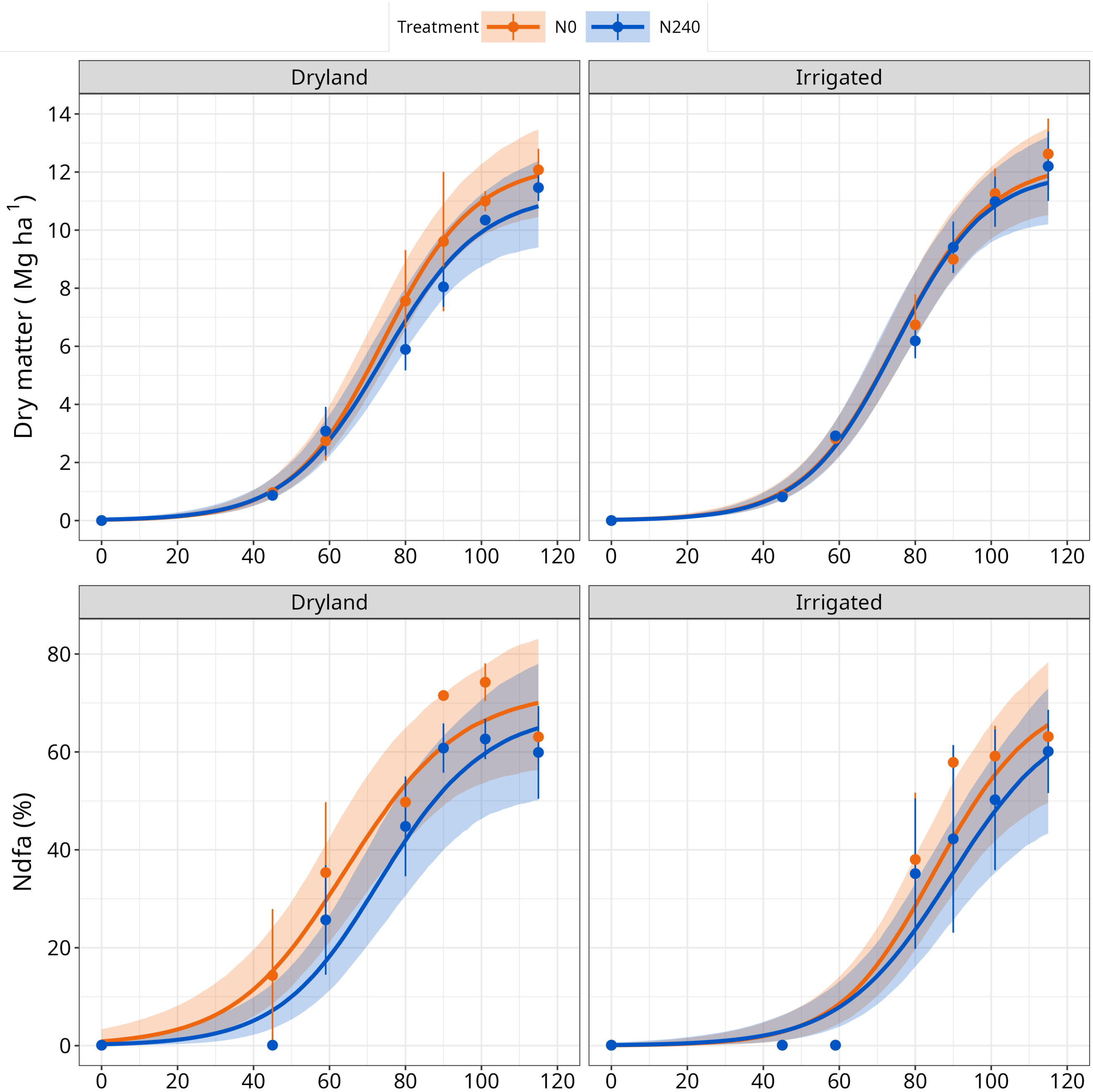
Supplementary Figure 5.2A. Model of maize grain N concentration as a function of N rate based on 1991 and 1997 measurements. Case study II.



Supplementary Figure 5.2B. Model of maize grain N concentration as a function of N rate. Case study II. 2019 cropping season.



Supplementary Figure 5.3. Accumulated soybean seed production (Mg ha^{-1}) 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).



Supplementary Figure 5.4. Soybean dry matter accumulation (Mg ha^{-1}) and nitrogen derived from atmosphere (Ndfa, %) during the 2020 cropping season. Case study II. Scandia, KS.

Supplementary Material

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

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Supplementary material for Section 6.2. Theoretical framework.

1. Symmetry in the error-in-variables model.

The parameter (slope and intercept) estimators for the general model Eq. **(1)** can be expressed Eq. **(2)** (y vs. x) and as X_i as a function of Y_i, Eq. **(3)**, where γ and ϕ represent the intercept and slope, respectively.

$$\begin{aligned} y_i &= Y_i + \varepsilon_i, \\ x_i &= X_i + \mu_i, \\ Y_i &= \alpha + \beta X_i. \end{aligned} \qquad \textbf{(1)}$$

$$\hat{y}_i = \hat{\alpha} + \hat{\beta} x_i, \qquad \textbf{(2)}$$

$$\hat{x}_i = \hat{\gamma} + \hat{\phi} y_i. \qquad \textbf{(3)}$$

This distinction is particularly relevant for the OLS regression where the orientation matters. If we select a model that is asymmetric (OLS) and project Eq. **(2)** and Eq. **(3)** in the same axis-orientation (y as vertical, x as horizontal), they will produce two different regression lines (**Figure 6.2A-B**). In contrast, if the selected model is symmetric, lines derived from Eq. **(2)** and Eq. **(3)** will be coincident and algebraically invertible (*i.e.*, reciprocal slopes, $\hat{\beta} = 1/\hat{\phi}$), which is the case of MA and SMA models.

2. Estimating the intercept

For all the regression models here, the estimation of the intercept ($\hat{\alpha}$) is simply reduced to **Eq. (4)**, which is ultimately dependent on the previous estimation of the slope ($\hat{\beta}$) (Warton et al., 2006). This simplification takes advantage of these regression lines passing through the centroid of the data given by the variable means coordinates ($\bar{x}$, $\bar{y}$).

$$\hat{\alpha} = \bar{y} - \hat{\beta}\,\bar{x}. \qquad \textbf{(4)}$$

3. Background of error decomposition using linear regression

This section is intended to offer a comparison, up to our knowledge, of the three main approaches in the literature to decompose error using linear regression. As we provided evidence in the article, SMA offers results closer to optimal as compared to the alternative approaches.

3.1. Error decomposition with OLS-line

Willmott (1981) proposed the utilization of two error indices as additive components of the MSE. In order to provide a geometric interpretation of the components proposed by Willmott (1981), we multiply *MSE* by the sample size (*n*) and express the decomposition in terms of the total sum of squares (*TSS*). Using OLS regression of P vs. O, Willmott proposed following TSS components (**Supplementary Table 1**): i) the sum of unsystematic differences (*SUD*), related to imprecision, and ii) the sum of systematic differences (*SSD*), related to inaccuracy.

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 Figure 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 $P_i = O_i$) (not shown). Willmott (1981) proposed the sum of SUD_{OLS} plus SSD_{OLS} as equal to *TSS*. Therefore, unsystematic and systematic proportions of the error can be simply estimated as ratios of the components to the TSS. This represents a very simple and straightforward approach. For example, the illustrative dataset displayed on **Supplementary Figure 1A** has a *TSS* = 38.25, being SUD_{OLS} = 21.53, SSD_{OLS} = 16.72(See **Correndo et al. (2021) for demonstration**). Nonetheless, the use of a symmetric regression model such as the SMA (instead of OLS) to estimate the line-of-best-fit would result in a more reliable summary-line and thus error decomposition, as demonstrated below.

3.2. Error decomposition with MA-line

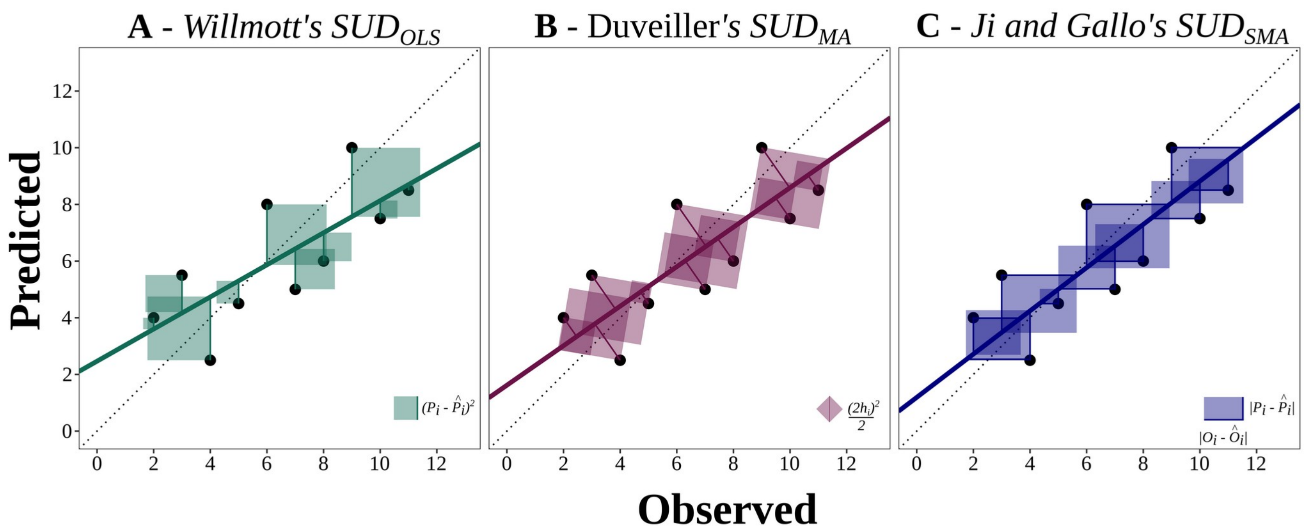
Duveiller et al. (2016) proposed an alternative method to decompose the square error but using a symmetric regression. Their approach consists in using the MA residuals (h_i) to obtain the unsystematic error component. Authors estimate the MA-line (and its residuals) by deriving the first principal component and its eigenvalues from the variance-covariance matrix (See Supplementary material of Duveiller et al. (2016)). The residuals of the MA line, h_i (**Supplementary Figure 1C**), can be considered the radius of a square. Based on this, authors propose the sum of unsystematic differences (SUD_{MA}) equal to the sum of $2h_i^2$. Geometrically, SUD_{MA} was designed to represent the sum of (rotated) squares area, which diagonal ($2h_i$) is perpendicular to the MA line (**Supplementary Figure 1B**). However, , since SUD_{MA} is based on a different data-projection (rotated axis, *x'y'*), this approach offers an independent estimation of the unsystematic component. Unfortunately, this implies that SUD_{MA} cannot be considered as an additive component of the sum of squares -*TSS*- (based on the original *xy*-projection), which is our intention -See **Correndo et al. (2021) for demonstration-**. Consequently, Duveiller et al. (2016) have not specified a formula for the computation of the systematic error component.

3.3. Error decomposition with SMA-line

The third alternative for error decomposition uses SMA regression, referred by authors as geometric mean functional relationship (Ji and Gallo, 2006). Authors proposed the sum of unsystematic differences (SUD_{SMA}) as equal to the loss function minimized by the SMA-line **(Supplementary Table 1)**. This corresponds to the sum of product of differences between the SMA-line and both P_i and O_i values simultaneously. Geometrically, the SUD_{SMA} represents the sum of "triangle-rectangles" formed from the difference between the data points (P_i, O_i) and the SMA-line (**Supplementary Figure 1C**). Authors assumed that $SSD_{SMA} = TSS - SUD_{SMA}$ but have not specified the formula for it. However, it is possible to specify SSD_{SMA} as the sum of square differences between the SMA-line and the 1:1-line (**Supplementary Table 1**). This can be done in two equivalent forms: i) as the sum of square differences between the SMA-line-values for observed ($\hat{O}_i$) and the 1:1-line-values (where $O_i = P_i$); or ii) as the sum of square differences between the SMA-line-values for predicted ($\hat{P}_i$) and the 1:1 line-values (where $P_i = O_i$). Geometrically, the SSD_{SMA} represents the sum of the area of *n* squares formed between the SMA-line and the 1:1 line (**Supplementary Figure 1C**). Thus, it can be proven that the sum of SUD_{SMA} (n rectangles) + SSD_{SMA} (n squares) = TSS (n squares). Results then intuitive that 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 ($SUD_{SMA} \rightarrow TSS$).

Supplementary Table 6.1. Error decomposition using alternative regression lines. For Willmott (1981), $\widehat{P}_i$ represents the fitted value of P obtained from the OLS regression of P vs. O.

Error Components	**OLS**	**MA**	**SMA**
	Willmott (1981)	*Duveiller et al. (2016)*	*Adapted from Ji and Gallo (2006)*
Total Sum of Squares (TSS)	$\sum_{i=1}^{n} (O_i - P_i)^2$		
Sum of Unsystematic Differences (SUD) *-lack of precision-*	$\sum_{i=1}^{n} (P_i - \widehat{P}_i)^2$	$\sum_{i=1}^{n} 2h_i^2$	$\sum_{i=1}^{n} \lvert P_i - \widehat{P}_i \rvert \lvert O_i - \widehat{O}_i \rvert$
Sum of Systematic Differences (SSD) *-lack of accuracy-*	$\sum_{i=1}^{n} (O_i - \widehat{P}_i)^2$	-	$\sum_{i=1}^{n} (O_i - \widehat{P}_i)^2, \equiv \sum_{i=1}^{n} (P_i - \widehat{O}_i)^2.$
Notes	$TSS = SUD_{OLS} + SSD_{OLS}$	No SSD term	$TSS = SUD_{SMA} + SSD_{SMA}$



Supplementary Figure 6.1. Geometric representation of the sum of unsystematic differences proposed by Willmott (1981) (A, SUD_{OLS}), Duveiller et al. (2016) (B, SUD_{MA}), and Ji and Gallo (2006) (C, SUD_{SMA}), using asymmetric (A) and symmetric regression lines (B, C). SUD_{OLS} = 21.53; SUD_{MA} = 30.87, SUD_{SMA} = 32.39.

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