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1 Analyzing uncertainty in critical nitrogen dilution curves

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13

14 Highlights

- 15 • We present a Bayesian method for estimating parameters of critical nitrogen dilution
16 curve
- 17 • It does not require the classification of nitrogen-limited against non-nitrogen-limited
18 data
- 19 • It can be easily implemented using freely-available software
- 20 • This method is useful for analyzing uncertainty in the fitted critical nitrogen curves
- 21 • It can take prior knowledge about parameter values into account.

22

23 Abstract

24 Nitrogen critical curves are frequently used to diagnose the N status of crops and grasslands.
25 They play an important role in plant modelling and are frequently used in fertilizer
26 management tools. During the last 20 years, a number of studies have been conducted for
27 comparing critical curves obtained in different conditions (e.g., different cultivars) and
28 understanding the origin of their difference. However, uncertainty in the determination of
29 coefficient of these curves is generally poorly analyzed in these studies, which increase the
30 risk of false conclusions, in particular on the existence of differences between species,
31 cultivars and cropping systems. Here, we present a Bayesian statistical model for estimating
32 parameters of critical nitrogen dilution curve from experimental data. Contrary to standard
33 methods commonly used for fitting critical nitrogen dilution curves, the proposed approach
34 allows one to fit these curves in only one step, i.e., directly from the original biomass and
35 nitrogen content measurements. Specifically, this method does not require the classification
36 of nitrogen-limited data against non-nitrogen-limited data and does not necessitate the
37 preliminary identification of critical nitrogen concentrations. Another advantage of the
38 proposed method is that it can be easily implemented using freely-available software. We
39 illustrate its practical interest using experimental data collected for winter wheat in France,
40 and for maize and rice in China. We show that this method is useful for analyzing uncertainty
41 in the fitted critical nitrogen curves and for comparing several curves obtained for different
42 crop species and cultivars. The proposed method is based on the specification of prior
43 probability distributions defining plausible ranges of values for the critical curve parameters,
44 and we show here that it is preferable to use prior distributions that are not very informative
45 if we want to limit their influence on the final result.

46 **Keywords:** Bayesian statistics, critical concentration, critical N curve, nitrogen, probabilistic
47 expert elicitation, uncertainty.

48

49 1. Introduction

50 Nitrogen (N) fertilization plays a major role in agricultural production but excess of N in agro-
51 ecosystems has negative impacts on water pollution (Zhao et al. 2007), and increases risk of
52 ammonia and N₂O emissions (Philibert et al. 2012; Ramanantenasoa et al. 2019). It is thus
53 essential to precisely manage N fertilization and to develop operational tools helping
54 farmers to determine optimal N fertilizer doses and times of application. A prerequisite for
55 the development of such tools is to estimate crop nitrogen requirements as accurately as
56 possible.

57 The concept of critical N concentration (N_C) is frequently used to diagnose the N status of
58 crops (Lemaire et al. 2008). The value of N_C represents the minimum N concentration that is
59 required for maximum biomass production. This concentration is usually computed as a
60 function of biomass using a simple mathematical model, often called critical N curve.

61 Although several variants of this model exist, the most common model is expressed as $N_C =$
62 $A_1 W^{-A_2}$ where N_C is the critical N concentration for biomass W , and where A_1 and A_2 are
63 two parameters that are estimated by fitting the model to a set of experimental data. Critical
64 N curves relating N_C to W have become popular since the late 1990s, and they have been
65 developed for a number of plant species, including winter wheat (Justes et al. 1994; Chen
66 and Zhu, 2013), oilseed rape (Colnenne et al., 1998), maize (Plénet and Lemaire, 2000),
67 ryegrass (Sandana et al. 2019), rice (Ata-Ul-Karim et al. 2017) among others.

68 It is essential to analyze uncertainty in fitted critical N curves in a rigorous manner. This is
69 important for assessing risk of N deficit or N excess and, also, for comparing critical curves
70 obtained in different conditions (e.g., sites, years, different cultivars and/or crop
71 managements) and understanding the origin of their difference. In some cases, two fitted
72 curves obtained in two different conditions are apparently different, but their difference
73 does not reflect a real difference due to the existence of a true effect of the factor studied,
74 but simply reflects errors in the estimated values of their parameters. In such cases,
75 concluding that there is a real difference and a real effect of the factor under consideration
76 will lead to a false conclusion. There is increasing concern that false findings may be very
77 frequent in research (Ioannidis, 2005). To limit risk of false discoveries, a rigorous analysis of
78 uncertainty is then crucial.

79 In practice, the parameters of critical N curves are estimated using a series of pairs of
80 biomass and plant N concentration measurements obtained at different dates during the
81 growing period for different N levels. Several methods have been proposed to estimate
82 parameters of critical curves from this type of data (Greenwood et al. 1990; Justes et al.,
83 1994; Chen and Zhu, 2013). All these methods require a classification of N-limited data vs.
84 non-N-limited data at each date of measurement. The two groups of data (N-limited vs. non-
85 N-limited) are then used to identify a so-called critical-N-concentration above which biomass
86 is assumed to reach its maximum value. A critical N curve is finally fitted to the series of
87 critical-N-concentration values obtained across the different dates of measurement.

88 Although this approach has been successful in fitting critical N curves in a great diversity of
89 contexts, it presents several limitations. This approach requires the definition of one
90 classification rule to distinguish N-limited vs. non-N-limited data and of a method to define
91 the N critical concentration from the two groups of data, and Chen and Zhu (2013) showed

92 that the fitted critical N curve can be sensitive to these choices. Another issue is that the
93 critical N curves are fitted to the selected critical N concentrations then considered as
94 perfectly known, ignoring their own uncertainties. Once the critical nitrogen concentrations
95 are estimated, the critical nitrogen curve is adjusted to their values without explicitly taking
96 into account their uncertainties. A consequence is that the confidence intervals of the
97 estimated parameters and of the fitted curves do not fully account for the uncertainties in
98 the selected critical N concentrations.

99 Here, we present a Bayesian statistical model for estimating parameters of critical nitrogen
100 dilution curve from experimental data. Contrary to standard methods commonly used for
101 fitting critical curves, the proposed approach allows one to fit these curves in only one step,
102 i.e., directly from the original biomass and nitrogen content measurements. Our approach is
103 illustrated with experimental data collected for wheat, maize and rice. We show that the
104 proposed method can be easily used to fit critical N curves, to analyze uncertainty, and to
105 compare the parameter values estimated for different species and cultivars.

106

107 2. Materials and Method

108 2.1. Data

109 2.1.1. Wheat

110 Data used in this study for wheat are those used by Justes et al. (1994). These data had been
111 extracted from a large experimental network with different year-location combinations in
112 France. In each experiment wheat crops were grown with at least four different levels of N
113 fertilizer supply and several plant samples were regularly harvested all along the crop
114 growth period until anthesis. Plant samples were analyzed to determine their aboveground
115 biomass (t ha^{-1}) and plant shoot N concentration (%) at each sampling date. A series of pairs
116 of N concentration and of biomass were thus obtained across the different N levels * dates
117 combinations (Appendix A) and included in a single dataset for the statistical analysis. The
118 dataset covers a large range of biomass values, from about 1 t ha^{-1} at the early stages of
119 plant growth to about 12 t ha^{-1} at plant anthesis. Crop were managed with ample P and K
120 supply, with irrigation when necessary for avoiding water stress, and with adequate plant
121 disease control. The total number of pairs of biomass and N content is equal to 73 (Table 1).

122 2.1.2. Maize

123 Four field experiments including each several N rates were conducted during the 2015 and
124 2016 growing seasons at Xinxiang (35.2°N , 113.8°E). The summer maize cultivars, N
125 application rates, sowing and harvesting dates, as well as soil characteristics, are
126 summarized in Appendix B. Soil samples were collected from 0 to 20 cm soil layer before
127 sowing summer maize crops. The samples were air-dried, sieved, and then used to measure.
128 All field experiments were arranged in a randomized complete block design with three
129 replicates. The size of each plot was 60m^2 in all the experiments. N fertilizer was applied

130 before sowing (50%) and at the jointing stage (50%). All plots received adequate quantities
131 of triple super-phosphate and potassium-chloride before sowing. Summer maize was
132 planted a density of 75,000 plants ha⁻¹ with a row spacing of 60 cm. The total number of
133 pairs of biomass (t ha⁻¹) and N content (%) is equal to 45 (Table 1).

134 2.1.3. Rice

135 Four multi-N rates (0 to 360 kg N ha⁻¹) field experiments using one Indica (Jingliangyou-534)
136 and one Japonica rice (Jiahua-1) cultivar were conducted during 2017 and 2018 rice growing
137 seasons in east China. Experiments were arranged with a randomized complete block design
138 having three repeats. The size of every plot was 5 m × 5 m with the inter-row spacing of 30
139 cm. The planting density in all the experiments was approximately 22.2×10⁴ plants ha⁻¹. Five
140 N supply rates (0, 90, 180, 270, and 360 kg N ha⁻¹ as urea) were applied. 40% N was distributed
141 before transplanting, 10% at active tillering, 20% at panicle initiation, and 30% at booting. In
142 all experiments, ample phosphate and potassium fertilizers were incorporated into the soil as
143 monocalcium phosphate (Ca(H₂PO₄)₂) and potassium chloride (KCl) before transplantation.
144 Experiments were carried out according to local recommendations along with adequate plant
145 pest and disease control measures to ensure optimal production. Plant samples were regularly
146 harvested all along the crop growth period until heading (pre-anthesis growth period) for
147 determination of plant dry mass and plant N concentration to provide a set of plant dry mass-
148 %N data across the different N supply rates at each sampling stage. The total number of pairs
149 of biomass (t ha⁻¹) and N content (%) is equal to 60 (Table 1).

150

151 Table 1. Number of dates of measurement (called 'dates' in the model), average number of
152 N levels per date, and number of data (pairs of biomass and N content observations) for
153 each dataset

Crop/Cultivar	Number of dates of measurement	Average number of N levels per date	Number of data
Rice/Japonica	12	5	60
Rice/Indica	12	5	60
Maize/ZD958	10	4.5	45
Maize/DH605	10	4.5	45
Winter wheat	16	4.6	73

154

155 2.2. Model

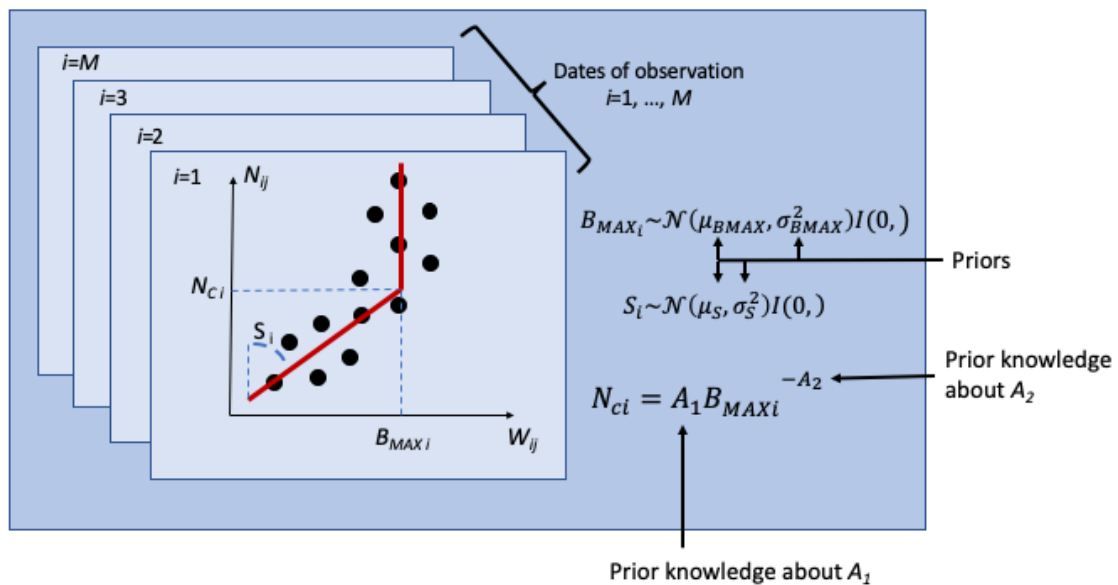
156 Our model is a Bayesian hierarchical model including three levels (Figure 1). The basic
157 principle of this model is to consider that the response of biomass to nitrogen content
158 follows a linear-plus-plateau function, as commonly considered in many studies (see for
159 example Chen and Zhu, 2013 and Zhao et al. 2018). The variability of the parameters of the
160 linear-plus-plateau function are described by probability distributions estimated from the
161 whole set of available data using a Bayesian method. The parameters of the critical nitrogen
162 dilution curve are then derived directly from the fitted probability distributions.

163 The first level of the model describes the biomass response to nitrogen content for a given
164 date of measurement based on a linear-plus-plateau function. Each date of measurement
165 corresponds to a specific crop growth stage in a given year at which biomass and N content

166 are measured for different N fertilizer levels. The second level of the model describes the
 167 variability of the parameters of the linear-plus-plateau function across observation dates
 168 using probability distributions. The critical nitrogen dilution curve is computed from these
 169 parameters. The third level describes prior knowledge about parameter values.

170

171 **Figure 1.** Graphical description of the three-level hierarchical Bayesian model. Level 1 describes the
 172 relationship between biomass and nitrogen content observations for each date of measurement (light blue).
 173 Level 2 describes the critical nitrogen dilution curve and the variability of biomass and nitrogen content
 174 between measurement dates using several probability distributions (dark blue). Level 3 describes prior
 175 knowledge about parameter values (outside part of the graphic). The indices i and j correspond to the dates of
 176 observation and the supplied N fertilizer rates, respectively. See text for details.



177

178 Level 1: Biomass response to nitrogen content

179 This part of the model describes the relationship between biomass (W_{ij} , $t \text{ ha}^{-1}$) and nitrogen
 180 content (N_{ij} , %) measurements in the i^{th} date of observation for the j^{th} nitrogen dose. We

181 assume that W_{ij} is distributed according to a Gaussian distribution whose mean value is
182 specified through a linear-plus-plateau function of the nitrogen content as follows:

183

$$184 \quad W_{ij} \sim \mathcal{N}(\mu_{ij}, \tau_b^2), \text{ with } \mu_{ij} = B_{MAX_i} + S_i(N_{ij} - N_{Ci}) \text{ if } N_{ij} < N_{Ci}$$

$$185 \quad \text{and } \mu_{ij} = B_{MAX_i} \text{ otherwise} \quad (1)$$

186

187 In Eq.(1), B_{MAX_i} is the maximum biomass in t ha^{-1} (non-N limited) in the i^{th} date (i.e., B_{MAX_i} is
188 equal to the mean value of W_{ij} when $N_{ij} \geq N_{Ci}$), S_i is the slope of the linear part of the
189 function (i.e., the increase rate of biomass per unit increase of nitrogen content, $\text{t ha}^{-1} \%N^{-1}$),
190 N_{Ci} is the critical nitrogen content for the i^{th} date (%), i.e., the value of nitrogen content (%)
191 above which B_{MAX_i} is reached, and τ_b^2 is the residual variance. We also assume that the
192 nitrogen content measurements (N_{ij}) is related to the critical nitrogen content (N_{Ci})
193 according to the distribution

194

$$195 \quad N_{ij} \sim \mathcal{N}(N_{Ci}, \tau_n^2), \quad (2)$$

196

197 where τ_n^2 is a variance determining how much the observed nitrogen contents N_{ij} can vary
198 around the critical nitrogen content N_{Ci} in the i^{th} date. In Eq.(2), nitrogen content
199 measurements are assumed to vary around the critical nitrogen with a variance equal to τ_n^2 .
200 A high (low) value τ_n^2 will reflect a strong (weak) variability of the measurements N_{ij} around
201 the critical nitrogen content N_{Ci} . Part of this variability reflects the different levels of applied
202 N considered in the field experiments and another part reflects measurement errors. With

203 Eq.(2), the values of N_{Ci} are constrained to remain in the same order of magnitude as the
 204 measured nitrogen contents. This prevents the model from producing N_{Ci} values
 205 inconsistent with observed values. However, Eq.(2) might not offer enough flexibility as it
 206 assumes that the mean value of N_{ij} is equal to N_{Ci} for every date i . For this reason, we
 207 consider a second model based on more flexible equation defined by:

$$208 \quad N_{ij} \sim \mathcal{N}(N_{Ci} + \theta_i, \tau_n^2), \quad (3)$$

209 where θ_i is the deviation between the mean value of N_{ij} and the critical nitrogen content
 210 N_{Ci} . Eq.(3) does not assume that the mean value of N_{ij} is equal to N_{Ci} for every
 211 measurement date. Indeed, with Eq.(3), the mean value of N_{ij} is not strictly equal to N_{Ci} but
 212 to $N_{Ci} + \theta_i$, and each measurement date is characterized by a specific value of θ_i . In the
 213 remaining part of the text, models 1 and 2 refer to models based on Eqs.(2) and (3),
 214 respectively.

215 **Level 2: Variability of biomass and nitrogen content between measurement dates**

216 We assume that the critical nitrogen content N_{Ci} is related to the maximum biomass B_{MAXi}
 217 (i.e., to the mean value of W_{ij} when $N_{ij} = N_{Ci}$) by a power function defined as

$$218 \quad N_{Ci} = A_1 B_{MAXi}^{-A_2} \quad (4)$$

219 where A_1 and A_2 are two parameters. The values of B_{MAXi} and of S_i are assumed to vary
 220 across dates according to two truncated Gaussian distributions defined by

$$221 \quad B_{MAXi} \sim \mathcal{N}(\mu_{BMAX}, \sigma_{BMAX}^2) I(0,) \text{ and } S_i \sim \mathcal{N}(\mu_S, \sigma_S^2) I(0,), \text{ where } I(a, b) \text{ is a truncation}$$

222 operator forcing values to fall within the range defined by a and b , $I(0,)$ thus indicating that

223 B_{MAXi} and S_i are forced to be positive. The use of a truncation is logical here as B_{MAXi}

224 represents a biomass (and is thus positive) and as the effect of nitrogen on biomass

225 (measured by S_i) is expected to be positive when $N_{ij} < N_{Ci}$. The distributions of B_{MAX_i} and
226 S_i determine the variability of the shape of the linear-plus-plateau function across
227 measurement dates. We assume that the values of θ_i in Eq.(3) vary across measurement
228 date as $\theta_i \sim \mathcal{N}(0, \tau_\theta^2)$. Here, a truncation is not required as there is no reason for θ_i to be
229 strictly positive.

230 **Level 3: Prior**

231 The model defined above included eight unknown quantities, namely $A_1, A_2, \mu_{BMAX}, \sigma_{BMAX}^2,$
232 $\mu_S, \sigma_S^2, \tau_n^2,$ and τ_b^2 . Prior knowledge on plausible values for these parameters are defined by
233 specifying prior probability distributions. Two types of priors are used successively here,
234 namely (i) weakly-informative priors and (ii) informative priors based on probabilistic expert
235 elicitation. These two types of priors are further denoted to as prior 1 and prior 2,
236 respectively.

237 The weakly-informative priors (priors 1) are designed to provide only little information about
238 the plausible values of the eight unknown quantities while reducing the chance to get
239 unrealistic values. These priors are defined by $\mu_{BMAX} \sim \mathcal{N}(6,10), \mu_S \sim \mathcal{N}(0,10),$
240 $A_1 \sim Unif(2,6), A_2 \sim Unif(0,0.5), 1/\sigma_{BMAX}^2 \sim Gamma(0.001,0.001), 1/$
241 $\sigma_B^2 \sim Gamma(0.001,0.001), 1/\tau_b^2 \sim Gamma(0.001,0.001), 1/\tau_n^2 \sim Gamma(0.001,0.001),$
242 $1/\tau_\theta^2 \sim Gamma(0.001,0.001).$

243 The informative priors (priors 2) are specified by expert elicitation. Probabilistic expert
244 elicitation consists of extracting an expert's knowledge about the likely values of some
245 unknown quantity of interest, and representing those beliefs with a probability distribution
246 (Morris et al., 2014; Chen et al., 2019). Here, one expert with a thorough and international
247 experience on critical N curves was elicited about the possible values of $A_1, A_2,$ and $\mu_{BMAX}.$

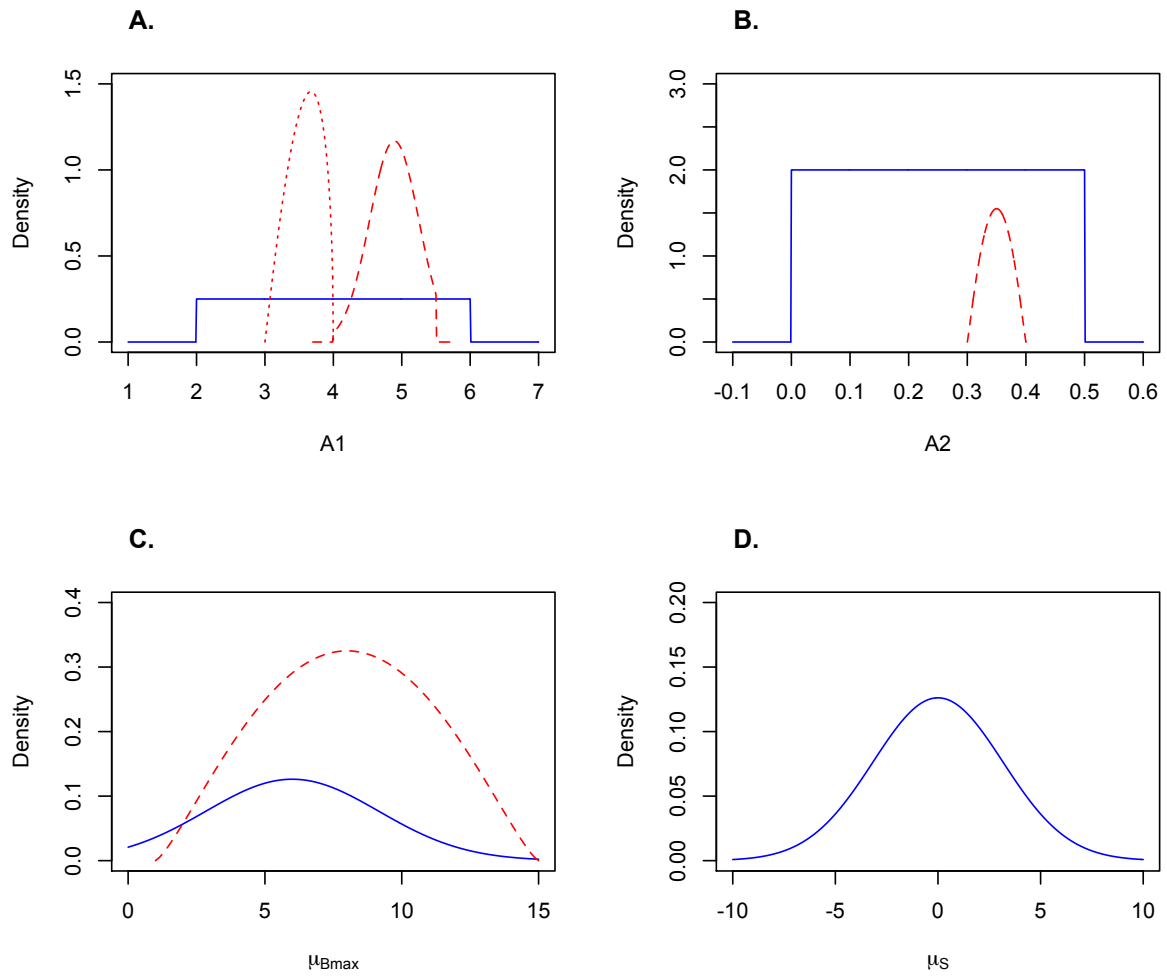
248 The elicitation was conducted following the procedure described in details by Chen et al.
249 (2019). As maize is a C4 crop, the expert chose to define two distributions for A_1 , one for
250 maize and one for the two C3 crop species considered (wheat and rice). For wheat and rice,
251 the elicited prior distributions defined by the expert are $\mu_{BMAX} \sim Beta(2.31, 2.31, 1, 15)$,
252 $A_1 \sim \mathcal{N}(4.89, 0.13)I(4, 5.5)$, $A_2 \sim Beta(2.12, 2.12, 0.3, 0.4)$. For maize, the prior for A_1 is
253 $A_1 \sim Beta(2.03, 1.5, 3, 4)$, but the other priors are unchanged. Note that the last two
254 parameters of the Beta distributions correspond to lower and upper bounds.

255 The two types of priors are shown in Figure 2 for the parameters of A_1 , A_2 , μ_{BMAX} , and μ_S .
256 Clearly, prior 2 covers narrower ranges of values than prior 1, in coherence with the fact that
257 prior 2 is designed to be more informative than prior 1. The difference between the two
258 types of prior is particularly strong for the two parameters of the critical N curve, i.e., A_1 and
259 A_2 (Figure 2AB). Noticeably, there is a marked difference between the priors of A_1 defined
260 by the expert for maize vs. wheat + rice. The prior defined for maize covers lower values
261 than the prior defined for wheat and rice (see the dotted vs. dashed lines in Figure 2A).

262

263

264 **Figure 2.** Priors distributions defined for the parameters A_1 (A), A_2 (B), μ_{BMAX} (C), and μ_S (D). Weakly-
 265 informative priors are represented by the continuous blue lines. Informative priors defined by expert elicitation
 266 for A_1 , A_2 , and μ_{BMAX} are indicated in red dashed lines or in red dotted lines. For A_1 , the informative prior is
 267 defined in dashed line for wheat and rice and in dotted line for maize. For A_2 and μ_{BMAX} , the informative priors
 268 are not differentiated among the three species by the expert and are all represented in dashed lines.



269

270

271

272 2.3. Posterior distributions

273 The posterior distributions of the model parameters are estimated with a Markov chain
274 Monte Carlo algorithm (MCMC) implemented with the R package rjags (Plummer, 2017)
275 using both types of priors, successively. The R code used to fit models 1 and 2 is presented in
276 Appendix D. With model 1 the convergence was achieved approximately after 10,000
277 iterations according to the Gelman-Rubin diagnosis. The first 10,000 iterations were
278 discarded and the MCMC algorithm was run for 40,000 additional iterations which were
279 then used to compute the median and 95% credibility intervals for several quantities of
280 interest, in particular A_1 , A_2 , $\mu_{B_{MAX}}$, μ_S , B_{MAX_i} and S_i for all observation dates. The median
281 values of B_{MAX_i} and S_i were used to fit a specific linear-plus-plateau function for each date
282 separately. We also computed the median and 95% credibility intervals of the critical
283 nitrogen dilution curve $N_C = A_1 B_{MAX}^{-A_2}$. With model 2 (based on Eq.3), the convergence
284 was achieved approximately after 10,000 to 50,000 iterations for the maize and wheat
285 datasets. However, with model 2, we were able to achieve convergence for rice, even with a
286 large number of iterations, probably due to the fact that model 2 was overparametrized for
287 rice. The results obtained with model 2 for maize and wheat were almost identical as those
288 obtained with model 1 (see appendix C). For this reason, we only present the results
289 obtained with model 1 in the next section. Nonetheless, values of A_1 and A_2 estimated with
290 model 2 can be found in Appendix C.

291

292 3. Results

293 3.1. Fitted critical N curves

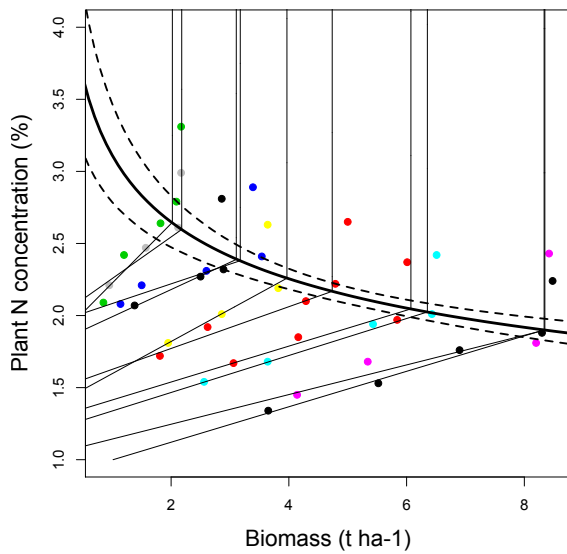
294 The fitted critical N curve and its 95% critical interval obtained for the maize cultivar DH605
295 with prior 1 are shown in Figure 3a. The width of the critical interval describes the level of
296 uncertainty in the fitted curve and directly reflects the distributions of the values of the
297 parameters A1 and A2 (Figure 3bc). Clearly, for the maize cultivar DH605, the level of
298 uncertainty in critical N depends on the biomass value. The width of the critical interval is
299 equal to about 0.5% of plant N concentration when the biomass is lower than 2 t ha⁻¹ and
300 becomes lower than 0.25% when the biomass is higher than 4 t ha⁻¹. The level of uncertainty
301 is thus lower for high compared to low biomass values. This decreasing trend in the level of
302 uncertainty is also observed for the second maize cultivar considered in this study (Appendix
303 A1), but not for wheat or rice (Appendix A2-A4). For the latter two crop species, the
304 uncertainty is small compared to maize, even for low biomass values, and its level does not
305 show any substantial increasing or decreasing trend. The uncertainty is especially low for
306 wheat for which the width of the 95% credibility interval is close to 0.1% over a wide range
307 of biomass values. For rice, the level of uncertainty is intermediate between maize and
308 wheat (Appendix A3-A4).

309

310

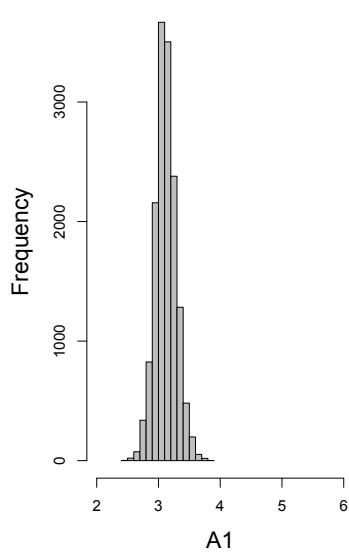
311 **Figure 3.** Fitted critical N curve obtained for the maize cultivar DH605 and its 95% credibility interval. In graphic
 312 3a, continuous and dashed thick lines represent the posterior median and the 95% credibility interval,
 313 respectively. The thin lines represent the linear-plus-plateau responses fitted for all combinations of
 314 measurement stage and year available in the dataset. Data collected for different stage*years are indicated by
 315 points of different colors. Posterior distributions of the parameters A1 and A2 (40,000 parameter values
 316 generated by MCMC) are presented in the histograms in graphics 3b and 3c, respectively. Results were
 317 obtained with prior 1. The ranges of the x-axis in b and c reflect the ranges of values covered by the prior
 318 distributions.

319 a.

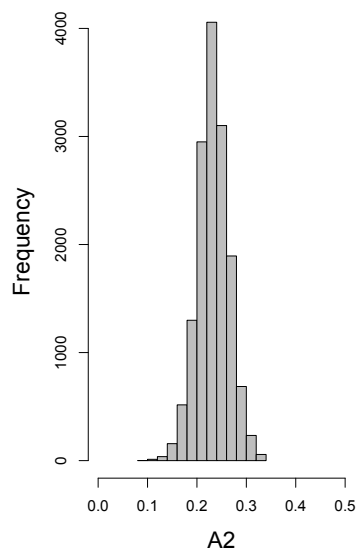


320

321 b.



c.



322

323

324 The whole set of fitted critical N curves obtained for the different crops and cultivars are
325 compared in Figure 4. With prior 1 (Figure 4A), the critical N curve obtained for wheat is
326 higher than those obtained for the other crop species when the biomass is lower than 4 t ha⁻¹
327 ¹, but it becomes lower than the critical N curve obtained for rice indica for higher values of
328 biomass. The critical curve of indica is higher than the curve of japonica but the difference is
329 very small for low biomass values (Figure 4A). The curves obtained for the two maize
330 cultivars are very similar and close to the curve of indica (Figure 4A).

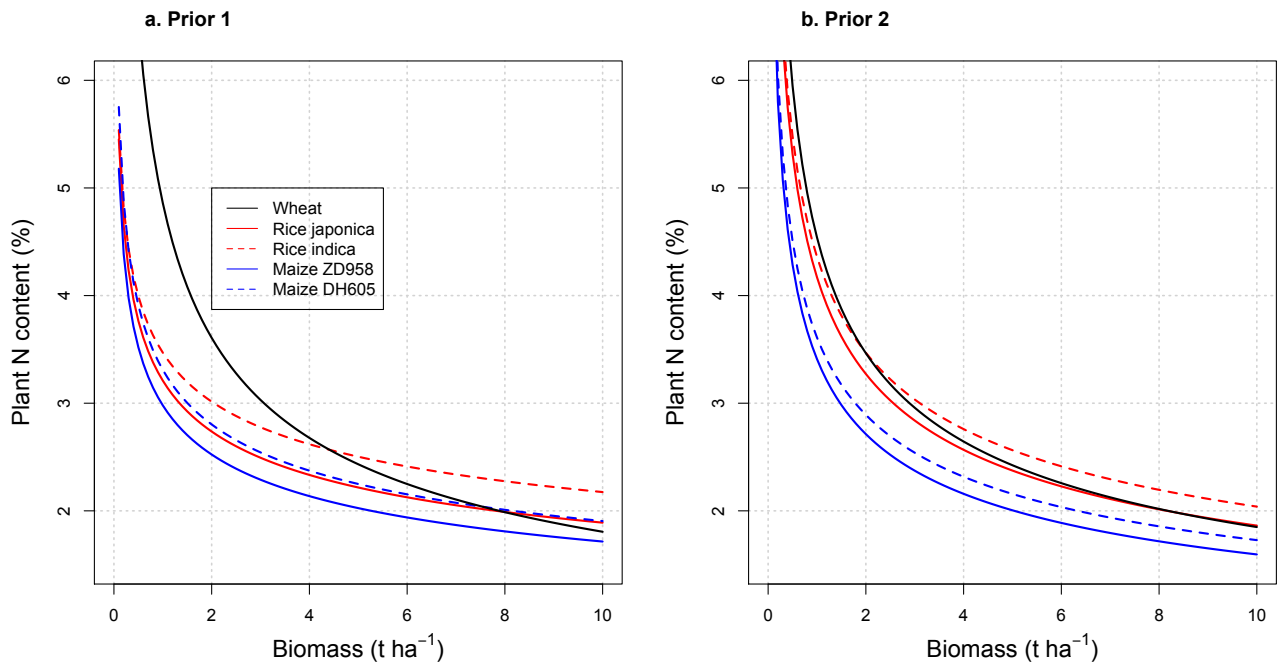
331 The curve obtained for wheat with prior 2 (Figure 4B) is very similar to the curve obtained
332 with prior 1. For wheat, the fitted critical N curve is thus insensitive to the choice of prior. On
333 the contrary, the curves obtained for rice indica and japonica are much higher with prior 2
334 compared to prior 1. With prior 2, the critical N curves of rice become very close to the
335 critical N curve of wheat (Figure 4B). For maize, compared to prior 1, the critical N curves
336 obtained with prior 2 tend to be slightly higher and closer to the curve obtained for wheat.

337 Overall, the differences between the critical N curves obtained for the different species and
338 cultivars are thus relatively small. These differences may simply reflect uncertainties in the
339 values of the parameters A1 and A2 characterizing the critical N curves. In order to conclude,
340 it is thus necessary to analyze the parameter values. This is done in the next section.

341

342

343 **Figure 4.** Fitted critical N curve obtained for wheat, maize (two cultivars), and rice (two cultivars). Each curve
344 corresponds to a posterior median obtained with prior 1 (A) or prior 2 (B).



345

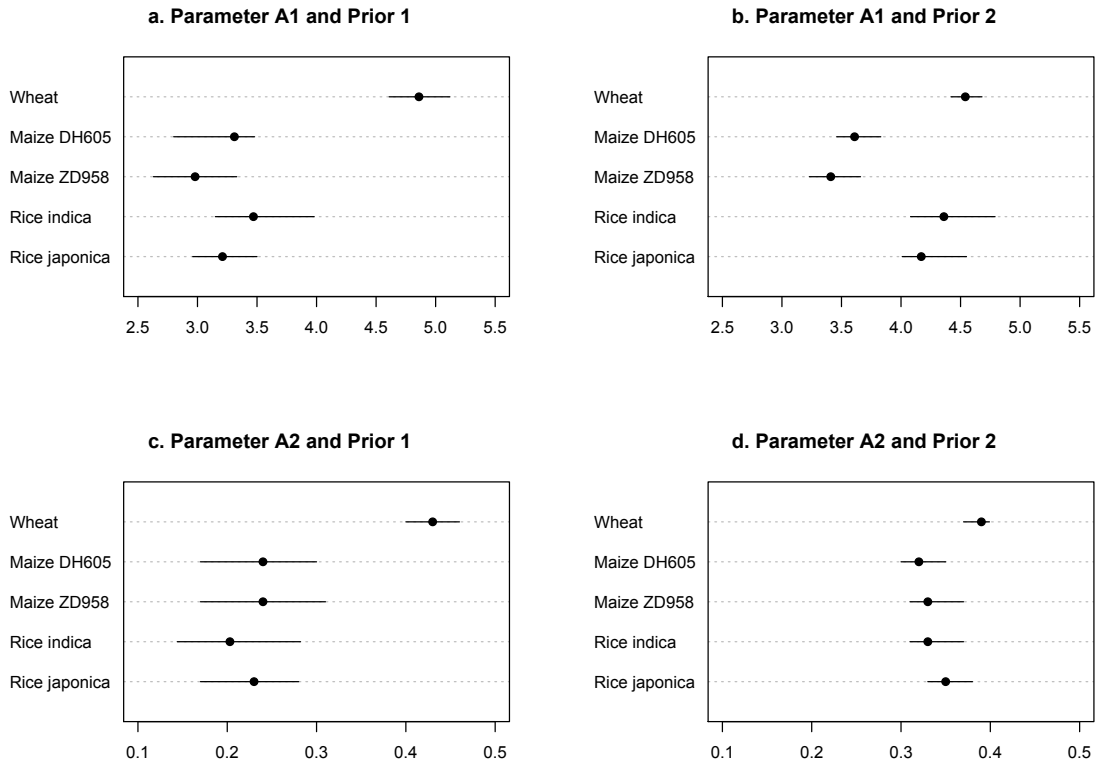
346

347 3.2. Estimated parameter values

348 Figure 5 shows the estimated parameter values obtained for the different crops and
349 cultivars. The posterior medians correspond to point estimates that can be used to draw
350 critical N curves, as shown in figures 3a and 4ab. The 95% credibility intervals presented in
351 Figure 5 cover 95% of the values sampled in the posterior distributions using MCMC. Thus,
352 the intervals shown in Figure 5 for maize DH605 cover 95% of the values of the histograms
353 presented in Figure 3bc. These intervals describe the levels of uncertainty in the values of
354 the parameters A1 and A2.

355

356 **Figure 5.** Estimated values (posterior medians) and 95% credibility intervals of parameters A1 (a, b, in %) and
357 A2 (c, d) with priors 1 (a, c) and 2 (b, d), for wheat, maize (two cultivars), rice indica, and rice japonica.



358

359

360

361 With prior 1 (Figure 5ac), the parameter values are significantly higher for wheat than for
362 the other crop species. For wheat, the posterior median is equal to 4.86 (95%CI=[4.61, 5.12])
363 for A1 and to 0.43 (95%CI=[0.40, 0.46]) for A2. In comparison, for maize and rice, the
364 posterior medians of A1 are always lower than 3.5 and those of A2 are always lower than
365 0.25. The uncertainty levels (reflected by the sizes of the credibility intervals) are
366 substantially higher for maize and rice than for wheat. This is because the number of
367 measurements used to fit the critical N curve is higher for wheat compared to maize and rice
368 (see also Appendix A). Because of their large credibility intervals, the parameter values
369 obtained for the two maize cultivars and for the two rice cultivars are not significantly
370 different.

371 The whole ensembles of parameter values drawn by MCMC from the posterior distributions
372 of A1 and A2 obtained with prior 1 are shown in Figure 6. These values are those used to
373 derived the posterior medians and credibility intervals presented in Figure 5ac. Parameter
374 values presented in Figure 6 show that A1 and A2 are positively correlated; high (low) values
375 of A1 tend to be associated with high (low) values of A2. Figure 6 also confirms that the
376 parameter values obtained for the two cultivars of maize strongly overlap, that those
377 obtained for the two rice cultivars partly overlap, and that the parameter values obtained
378 for wheat are much higher than those obtained for maize and rice.

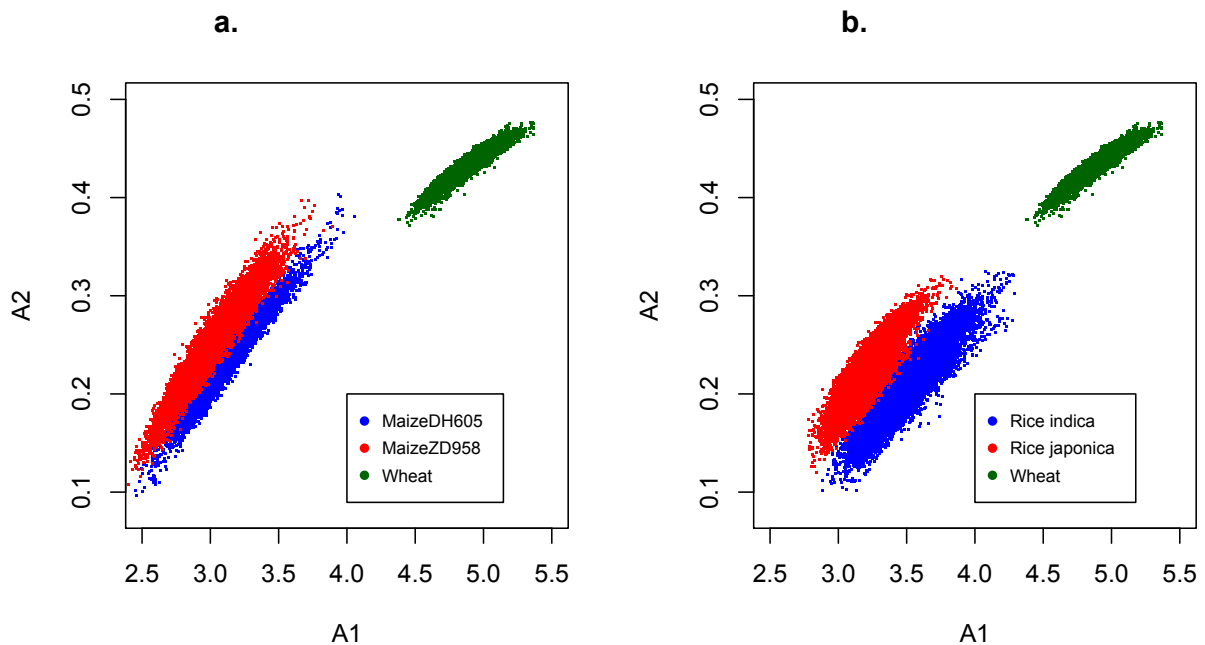
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382

383 **Figure 6.** Ensembles of parameter values drawn from the posterior distributions of A1 and A2 (obtained with
384 model 1 and prior 1). Maize vs. Wheat (a) and Rice vs. Wheat (b).



385

386

387 The use of prior 2 (informative priors) instead of prior 1 does not substantially impact the
388 parameter values estimated for wheat (Figure 5bd). For this crop, both priors lead to similar
389 values for A1 and A2. On the contrary, for rice, the estimated parameter values are much
390 higher with prior 2 than with prior 1. Consequently, the parameter values obtained for rice
391 with prior 2 are not significantly different from those obtained for wheat anymore. This is
392 because the informative priors (prior 2) defined for rice and wheat force the values of A1 to
393 be higher than 4 and the values of A2 to be higher than 0.3 (Figure 2ab). For wheat, prior 2
394 has no substantial impact because the posterior medians of A1 and A2 obtained with prior 1
395 were already higher than 4 and 0.3, respectively. For rice, the use of prior 2 has a strong
396 impact on the estimated parameter values because the posterior medians of A1 and A2
397 obtained with prior 1 were much lower than 4 and 0.3.

398 For maize, the use of prior 2 has also a strong impact on the estimated values of A2 (Figure
399 5d) but less on the values of A1. This is because the informative prior defined for A1 (prior 2)
400 is different for maize than for rice and maize (Figure 2a). For maize, the informative prior
401 defined for A1 forces the values of this parameter to fall within the range 3-4, i.e., close to
402 the posterior medians of A1 obtained with prior 1. The use of prior 2 instead of prior 1 has
403 thus a limited impact on A1 for maize.

404

405 4. Discussion

406 The proposed Bayesian method has several advantages. First, it does not require any
407 preliminary classification of N-limited data against non-N-limited data and does not
408 necessitate the preliminary identification of critical N concentration values. This is an
409 important advantage because it was shown that the critical N curve is sensitive to the
410 method used for estimating critical N concentration values (i.e., type of statistical test and
411 type I error level) and because there is no consensus on how these critical N concentration
412 values should be estimated (Greenwood et al. 1990; Justes et al., 1994; Chen and Zhu, 2013).
413 Our Bayesian approach can be implemented even with sparse data, i.e., when observations
414 are available for a limited number of fertilizer doses only. This is made possible because the
415 proposed model borrows strength from all dates of measurements and because parameters
416 are estimated by combining data with prior information.

417 Second, the proposed method can be easily implemented with free software to fit critical
418 nitrogen curves. The R code presented in appendix D can be easily run to estimate critical N
419 dilution curves using a dataset including only three columns; a column with the biomass
420 observations, a column with the associated nitrogen concentration observations, and a

421 column with the indices identifying the different dates of the dataset. This R code produces
422 chains of values for all parameters, including the two parameters defining the critical N
423 curve. The generated chains of values can be easily summarized by standard quantities such
424 as median, mean, and percentiles, and can be used to estimate the N critical curve and
425 compute its credibility interval. In our applications, 10,000 iterations were sufficient to reach
426 convergence in most cases and the computation time did not exceed 1 or 2 minutes using a
427 standard commercial computer.

428 Finally, another advantage of the proposed approach is that it facilitates the analysis of the
429 uncertainty of the fitted critical N curves. The proposed method is based on a Bayesian
430 hierarchical model whose parameters are estimated taking into account the number of
431 observation dates included in the data set, the number of data available per date and the
432 variability of observations between and within dates. The estimation results are expressed
433 by probability distributions from which the uncertainty of any quantity of interest can easily
434 be analyzed. In particular, our approach allows us to calculate the credibility intervals of the
435 N critical curves and their parameters. Our applications show that, because the dataset used
436 for wheat has been constituted from a large number of experiments network across France,
437 the uncertainty of critical N curve for wheat is relatively low. For maize and rice in China,
438 where the numbers of available data are smaller, the widths of the credibility intervals are
439 larger revealing a higher level of uncertainty.

440 From the probability distributions and credibility intervals computed by our method, it is
441 possible to compare different species of crops, cultivars or cropping systems, taking into
442 account uncertainties in parameter estimates. Since critical nitrogen curves are often
443 included in mechanistic crop models, the probability distributions provided by our method

444 could also be useful for performing uncertainty and sensitivity analyses with these models
445 (Wallach et al. 2019). The importance of rigorous uncertainty analysis is illustrated by some
446 of the results of our case studies where we found that parameter estimates for different
447 cultivars of the same species could not be considered statistically significant when
448 uncertainty is taken into account. Clearly, in our examples, the differences between the
449 point estimates of the critical N curve parameters obtained for the different cultivars are
450 small compared to the associated levels of uncertainty.

451 Like all Bayesian methods, our approach allows modellers to combine two sources of
452 information to estimate the parameters. More specifically, it combines prior information
453 based on expert knowledge and experimental data. Prior information is described using
454 probability distributions that summarize the initial state of knowledge on parameter values
455 before using the data. Here, we use two types of priors. The former are poorly informative
456 and are designed to provide little information on plausible values of model parameters. They
457 do not therefore strongly limit the values of the parameters. The second priors are more
458 informative and are specified by the probabilistic elicitation of an expert. This technique
459 allows to represent the experts' knowledge on the value of a parameter through a
460 probability distribution.

461 Probabilistic elicitation is useful when you want to rely on both experimental data and
462 expert knowledge for parameter estimation. The use of informative prior is useful when the
463 number of observations available is low and insufficient to accurately estimate parameter
464 values. However, this approach should be used with caution, as it can have a significant
465 effect on parameter estimates, especially when the size of the data set is small. In our
466 applications, the parameter estimates obtained for wheat are not substantially influenced by

467 the choice of prior because the size of the dataset is relatively large in this case. For wheat,
468 both priors lead to similar point estimates and credibility intervals. In contrast, for maize and
469 rice, the sizes of the data sets are smaller and, in both cases, the values of the estimated
470 parameters are sensitive to the choice of a prior; they take on larger values and their
471 credibility intervals are narrower when calculations are made with informative a priori.
472 When used, informative priors should therefore be defined by using qualified experts based
473 on relevant information.

474 We believe that our approach opens new perspectives for the estimation of critical nitrogen
475 dilution curves. Different variants of the model proposed here could be tested in the future
476 in order to better take into account possible correlations between measurements, to better
477 describe the a priori information available on the values of the parameters, or to handle
478 larger networks of experiments.

479

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483

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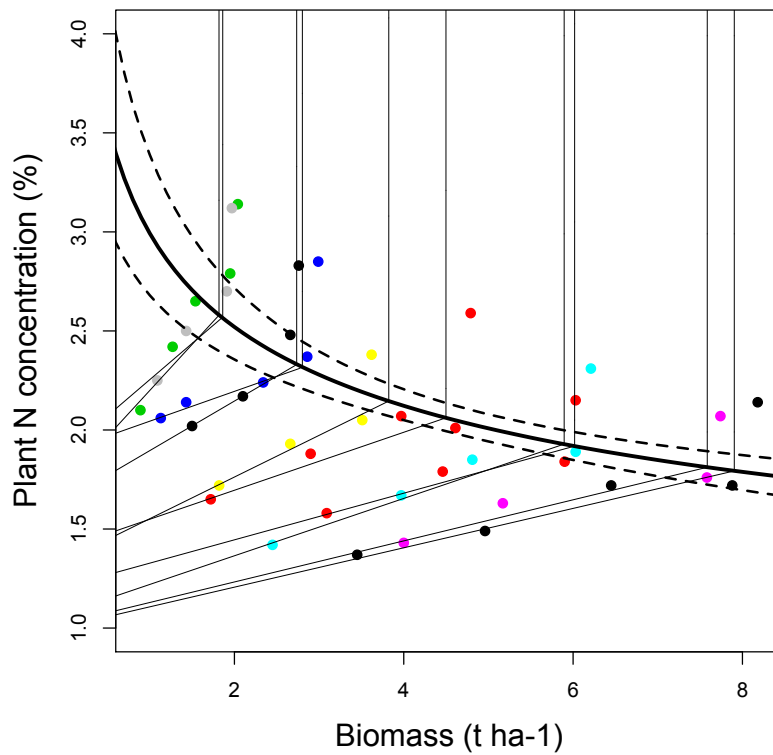
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527 Appendix A: Individual fitted critical N curves

528 In this appendix, we present the posterior median, the 95% credibility intervals and the
529 experimental data obtained for maize ZD958m (see main text for the other maize cultivar),
530 rice (Japonica and Indica) and wheat.

531

532 A1. Maize ZD958m



533

534

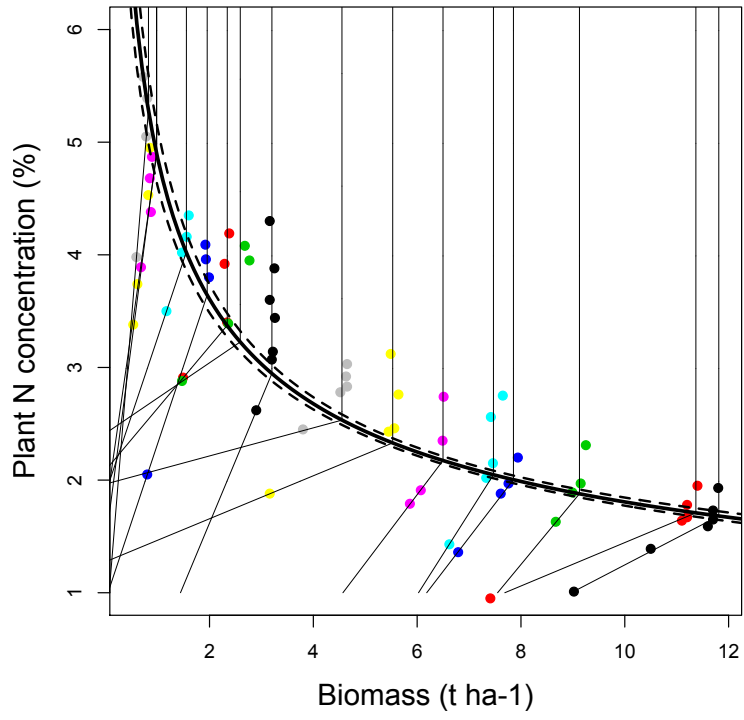
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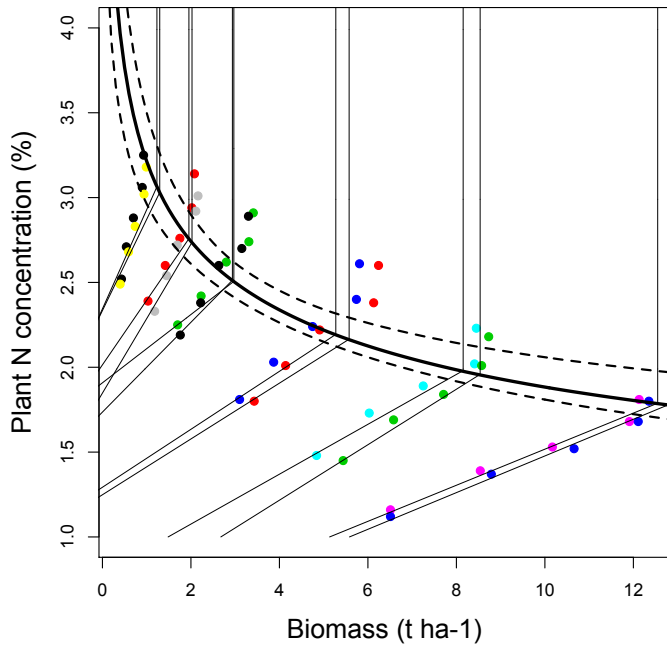
539 A2. Wheat



540

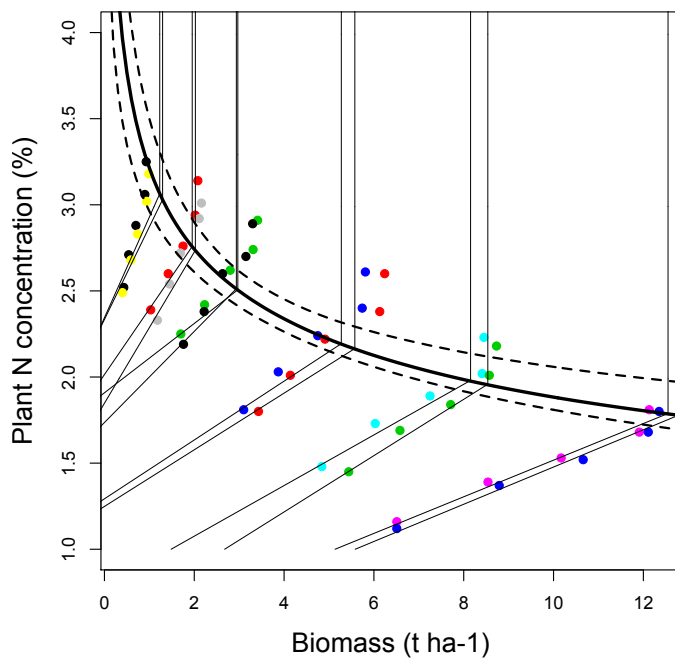
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542 A3. Rice Japonica



543

544 A4. Rice Indica



545

546

547

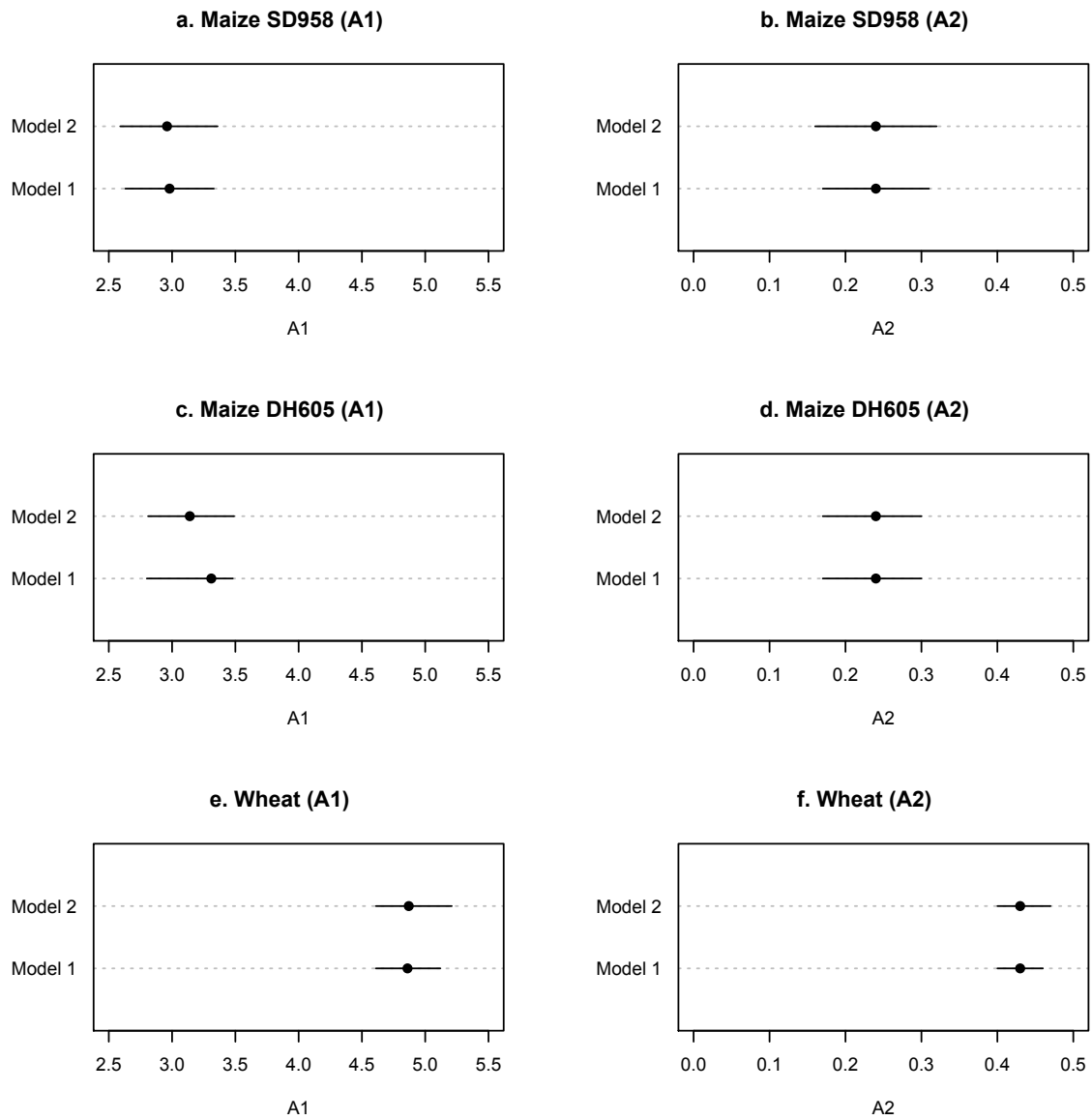
548 Appendix B: Characteristics of the maize experiments

549

Experiment No.	Sowing/Harvesting date	Soil characteristics	Cultivar	N(kg N ha ⁻¹)	Sampling stage
Experiment 1	8-Jun	Type: light loam soil	Zhengdan958	0 (N0)	Elongation stage
(2015 Xinxiang)	25-Sep	Organic matter: 12.26 g kg ⁻¹	(ZD958)	75 (N1)	Bell stage
		Total N: 0.74 g kg ⁻¹		150 (N2)	Tasseling stage
		Olsen-P: 35.67 mg kg ⁻¹		225 (N3)	Anthesis stage
		NH ₄ OAc-K ⁺ : 84 mg kg ⁻¹		300 (N4)	Silking stage
Experiment 2	8-Jun	Type: sandy light loam soil	Denghai605	0 (N0)	Elongation stage
(2015 Xinxiang)	25-Sep	Organic matter: 10.43 g kg ⁻¹	(DH605)	75 (N1)	Bell stage
		Total N: 0.61 g kg ⁻¹		150 (N2)	Tasseling stage
		Olsen-P: 33.94 mg kg ⁻¹		225 (N3)	Anthesis stage
		NH ₄ OAc-K ⁺ : 76 mg kg ⁻¹		300 (N4)	Silking stage
Experiment 3	6-Jun	Type: light loam soil	Zhengdan958	0 (N0)	Elongation stage
(2016 Xinxiang)	22-Sep	Organic matter: 14.2 g kg ⁻¹	(ZD958)	90 (N1)	Bell stage
		Total N: 0.83 g kg ⁻¹		180 (N2)	Tasseling stage
		Olsen-P: 44 mg kg ⁻¹		270 (N3)	Anthesis stage
		NH ₄ OAc-K ⁺ : 90 mg kg ⁻¹			Silking stage
Experiment 4	6-Jun	Type: light loam soil	Denghai605	0 (N0)	Elongation stage
(2016 Xinxiang)	22-Sep	Organic matter: 9.5 g kg ⁻¹	(DH605)	90 (N1)	Bell stage
		Total N: 0.57 g kg ⁻¹		180 (N2)	Tasseling stage
		Olsen-P: 23.51 mg kg ⁻¹		270 (N3)	Anthesis stage
		NH ₄ OAc-K ⁺ : 58.45 mg kg ⁻¹			Silking stage

550

551 Appendix C: Estimated values of A1 and A2 for maize and wheat
552 obtained with model 1 (based on Eq.(2)) and model 2 (based on
553 Eq.(3)).



554

555

556

557 Appendix D: R Code

558 **Model 1**

559 ####Data

560 # Q=total number of biomass observations

561 # K=number of dates

562 # W=column of data including biomass observations

563 # N=column of data including observations of nitrogen concentrations

564 # Date=column with the indices identifying the different dates of the dataset

565

566 ####Model parameters

567 # Nc=Critical nitrogen concentration

568 # Bmax=maximum biomass value in a specific date

569 # S=slope of the linear-plus-plateau function

570 # W=biomass increase per unit of nitrogen concentration

571 # A1 and A2 = parameters of the critical N curve

572 # tau_b and tau_n = 1/residual variances for biomass and nitrogen content observations

573 # Mu_Bmax,Prec_Bmax = parameters defining the between-date variability of Bmax

574 # Mu_S,Prec_S = parameters defining the between-date variability of S

575

576 Q<-length(Date)

577 K<-length(unique(Date))

578

579 modelstring= "

580 model {

581

582 for (i in 1:Q)

583 {

584 W[i]~dnorm(mu[i], tau_b)

```

585     N[i]~dnorm(Nc[Date[i]], tau_n)
586     mu[i]<-min(Bmax[Date[i]], Bmax[Date[i]]+S[Date[i]]*(N[i]-Nc[Date[i]]))
587 }
588
589 for (j in 1:K)
590 {
591     Nc[j]=A1*Bmax[j]^(-A2)
592     Bmax[j]~dnorm(Mu_Bmax,Prec_Bmax)T(0,)
593     S[j]~dnorm(Mu_S,Prec_S)T(0,)
594     }
595
596     #Weakly informative
597     Mu_Bmax~dnorm(6,0.1)
598     Mu_S~dnorm(0,0.1)
599     A1~dunif(2,6)
600     A2~dunif(0,0.5)
601
602     #Informative prior C3
603     #A1~dnorm(4.89,7.72)T(4,5.5)
604     #ZA2~dbeta(2.12,2.12)
605     #A2=(0.4-0.3)*ZA2+0.3
606     #ZMu_Bmax~dbeta(2.31,2.31)
607     #Mu_Bmax=(15-1)*ZMu_Bmax+1
608     #Mu_S~dnorm(0,0.1)
609
610     #Informative prior C4
611     #ZA1~dbeta(2.03,1.5)
612     #A1=(4-3)*ZA1+3
613     #ZA2~dbeta(2.12,2.12)
614     #A2=(0.4-0.3)*ZA2+0.3
615     #ZMu_Bmax~dbeta(2.31,2.31)
616     #Mu_Bmax=(15-1)*ZMu_Bmax+1
617     #Mu_S~dnorm(0,0.1)
618
619     Prec_Bmax~dgamma(0.001,0.001)
620     Prec_S~dgamma(0.001,0.001)
621     tau_b~dgamma(0.001,0.001)
622     tau_n~dgamma(0.001,0.001)
623
624 }
625 "
626 writeLines(modelstring, con="model.txt")
627
628 model<-jags.model('model.txt', data=list('W'=W, 'N'=N, 'Date'=Date, 'Q'=Q, 'K'=K),
629     n.chains=3, n.adapt=10000)
630
631

```

632 **Model 2**

```
633 modelstring= "  
634 model {  
635  
636   for (i in 1:Q)  
637   {  
638     W[i]~dnorm(mu[i], tau_b)  
639     N[i]~dnorm(Nc[Date[i]]+Theta[Date[i]], tau_n)  
640     mu[i]<-min(Bmax[Date[i]], Bmax[Date[i]]+S[Date[i]]*(N[i]-Nc[Date[i]]))  
641   }  
642  
643   for (j in 1:K)  
644   {  
645     Nc[j]=A1*Bmax[j]^(-A2)  
646     Bmax[j]~dnorm(Mu_Bmax, Prec_Bmax)T(0,)  
647     S[j]~dnorm(Mu_S, Prec_S)T(0,)  
648     Theta[j]~dnorm(0, tau_t)  
649     }  
650  
651     #Weakly informative  
652     Mu_Bmax~dnorm(6,0.1)  
653     Mu_S~dnorm(0,0.1)  
654     A1~dunif(2,6)  
655     A2~dunif(0,0.5)  
656  
657     #Informative prior C3  
658     #A1~dnorm(4.89,7.72)T(4,5.5)  
659     #ZA2~dbeta(2.12,2.12)  
660     #A2=(0.4-0.3)*ZA2+0.3  
661     #ZMu_Bmax~dbeta(2.31,2.31)  
662     #Mu_Bmax=(15-1)*ZMu_Bmax+1  
663     #Mu_S~dnorm(0,0.1)  
664  
665     #Informative prior C4  
666     #ZA1~dbeta(2.03,1.5)  
667     #A1=(4-3)*ZA1+3  
668     #ZA2~dbeta(2.12,2.12)  
669     #A2=(0.4-0.3)*ZA2+0.3  
670     #ZMu_Bmax~dbeta(2.31,2.31)  
671     #Mu_Bmax=(15-1)*ZMu_Bmax+1  
672     #Mu_S~dnorm(0,0.1)  
673  
674     Prec_Bmax~dgamma(0.001,0.001)  
675     Prec_S~dgamma(0.001,0.001)  
676     tau_b~dgamma(0.001,0.001)  
677     tau_n~dgamma(0.001,0.001)
```

```
678         tau_t~dgamma(0.001,0.001)
679     }
680     "
681     writeLines(modelstring, con="model.txt")
682     model<-jags.model('model.txt', data=list('W'=W, 'N'=N, 'Date'=Date, 'Q'=Q, 'K'=K),
683         n.chains=3, n.adapt=10000)
684
685
```