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► **To cite this version:**

David Makowski, Ben Zhao, Syed Tahir Ata-Ul-Karim, Gilles Lemaire. Analyzing uncertainty in critical nitrogen dilution curves. *European Journal of Agronomy*, 2020, 118, pp.126076. 10.1016/j.eja.2020.126076 . hal-03117535

**HAL Id: hal-03117535**

**<https://hal.science/hal-03117535v1>**

Submitted on 14 Nov 2023

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# 1 Analyzing uncertainty in critical nitrogen dilution curves

2 David Makowski <sup>1,2,\*</sup>, Ben Zhao<sup>3</sup>, Syed Tahir Ata-UI-Karim<sup>4</sup>, Gilles Lemaire<sup>5</sup>

3 1. University Paris-Saclay, INRAE, AgroParisTech, UMR 211 78850 Thiverval-Grignon France

4 2. CIREN, 45bis Avenue de la Belle Gabrielle, 94130 Nogent-sur-Marne France

5 3. Key Laboratory of Crop Water Use and Regulation, Ministry of Agriculture, Farmland Irrigation  
6 Research Institute, Chinese Academy of Agricultural Sciences, 380 Hongli road, Xinxiang, Henan  
7 453003, PR China

8 4. Key Laboratory of Soil Environment and Pollution Remediation, Institute of Soil Science, Chinese  
9 Academy of Sciences, 71 East Beijing Road, Nanjing, Jiangsu 210008, P. R. China

10 5. Honorary Director of Research INRAE (retired), Lusignan, 86500, France.

11 \* Corresponding author

12 [david.makowski@inrae.fr](mailto:david.makowski@inrae.fr)

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 N<sub>2</sub>O 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 ( $\text{t ha}^{-1}$ ) 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  $1 \text{ t ha}^{-1}$  at the early stages of  
119 plant growth to about  $12 \text{ t ha}^{-1}$  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 ( $35.2^{\circ}\text{N}$ ,  $113.8^{\circ}\text{E}$ ). 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  $60\text{m}^2$  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<sup>-1</sup> with a row spacing of 60 cm. The total number of  
133 pairs of biomass (t ha<sup>-1</sup>) 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<sup>-1</sup>) 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 22.2×10<sup>4</sup> plants ha<sup>-1</sup>. Five  
140 N supply rates (0, 90, 180, 270, and 360 kg N ha<sup>-1</sup> 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(H<sub>2</sub>PO<sub>4</sub>)<sub>2</sub>) 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<sup>-1</sup>) 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

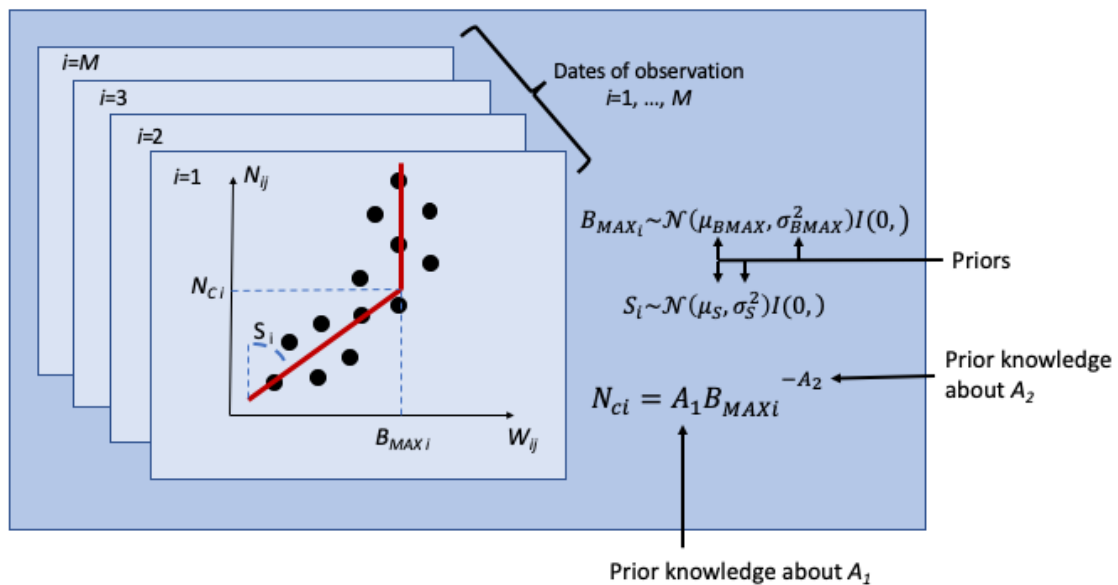
156 Our model is a Bayesian hierarchical model including three levels (Figure 1). The basic  
157 principle of this model is to consider that the response of biomass to nitrogen content  
158 follows a linear-plus-plateau function, as commonly considered in many studies (see for  
159 example Chen and 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 ha<sup>-1</sup>) and nitrogen  
 180 content ( $N_{ij}$ , %) measurements in the  $i^{\text{th}}$  date of observation for the  $j^{\text{th}}$  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  $\text{t ha}^{-1}$  (non-N limited) in the  $i^{\text{th}}$  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  $i^{\text{th}}$  date (%), i.e., the value of nitrogen content (%)  
191 above which  $B_{MAX_i}$  is reached, and  $\tau_b^2$  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  $\tau_n^2$  is a variance determining how much the observed nitrogen contents  $N_{ij}$  can vary  
198 around the critical nitrogen content  $N_{Ci}$  in the  $i^{\text{th}}$  date. In Eq.(2), nitrogen content  
199 measurements are assumed to vary around the critical nitrogen with a variance equal to  $\tau_n^2$ .  
200 A high (low) value  $\tau_n^2$  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  $\theta_i$  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  $\theta_i$ . 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  $\theta_i$  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  $\theta_i$  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  $\tau_b^2$ . 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  $\mu_{BMAX}.$

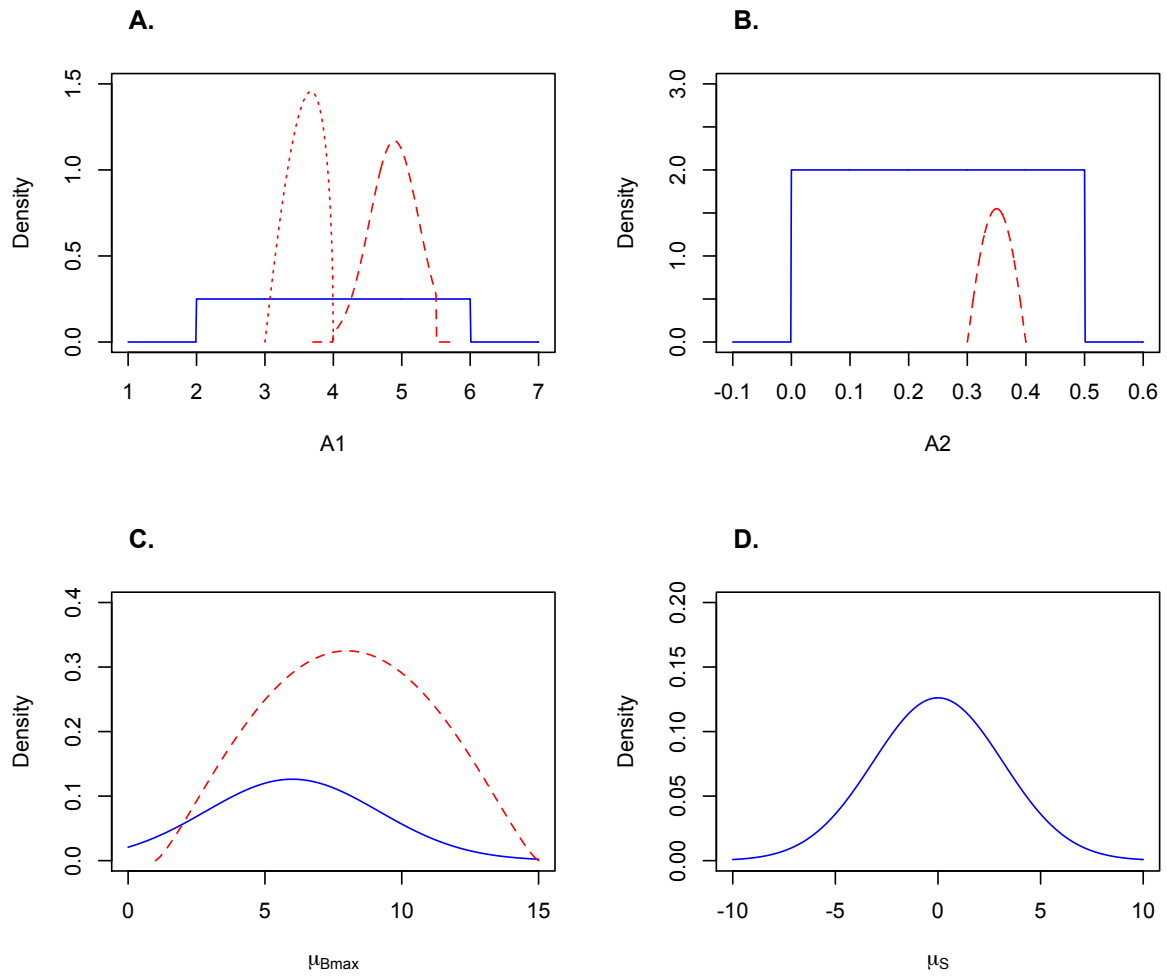
248 The elicitation was conducted following the procedure described in details by Chen et al.  
249 (2019). As maize is a C4 crop, the expert chose to define two distributions for  $A_1$ , one for  
250 maize and one for the two C3 crop species considered (wheat and rice). For wheat and rice,  
251 the 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  $A_1$ ,  $A_2$ ,  $\mu_{BMAX}$ , and  $\mu_S$ .  
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),  $\mu_{BMAX}$  (C), and  $\mu_S$  (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  $\mu_{BMAX}$  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  $\mu_{BMAX}$ , 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  $A_1$ ,  $A_2$ ,  $\mu_{B_{MAX}}$ ,  $\mu_S$ ,  $B_{MAX_i}$  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

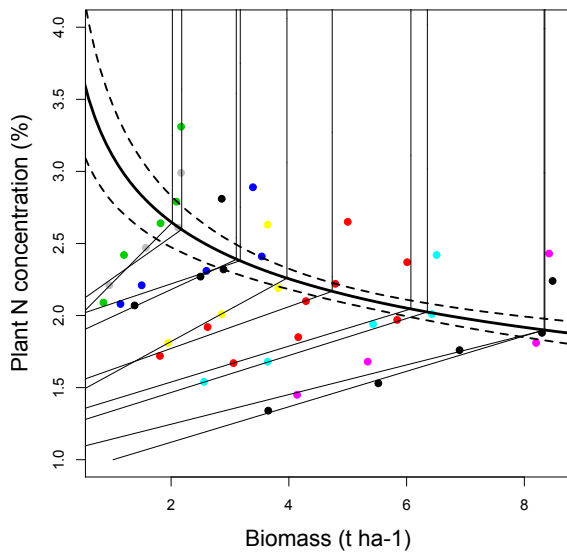
294 The fitted critical N curve and its 95% critical interval obtained for the maize cultivar DH605  
295 with prior 1 are shown in Figure 3a. The width of the critical interval describes the level of  
296 uncertainty in the fitted curve and directly reflects the distributions of the values of the  
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<sup>-1</sup> and  
300 becomes lower than 0.25% when the biomass is higher than 4 t ha<sup>-1</sup>. 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

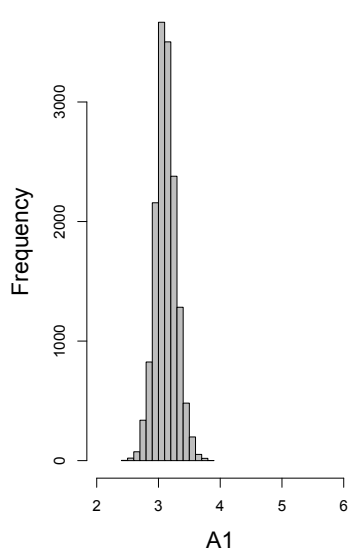
311 **Figure 3.** Fitted critical N curve obtained for the maize cultivar DH605 and its 95% credibility interval. In graphic  
312 3a, continuous and dashed thick lines represent the posterior median and the 95% credibility interval,  
313 respectively. The thin lines represent the linear-plus-plateau 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.

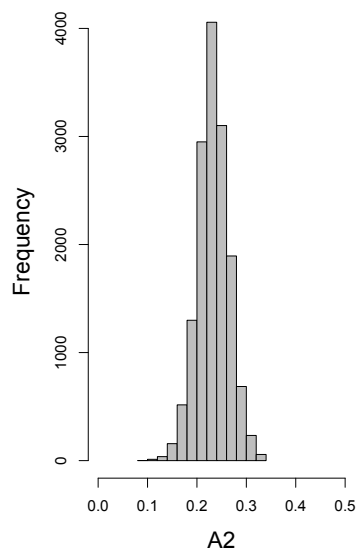


320

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<sup>-1</sup>  
327 <sup>1</sup>, 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).

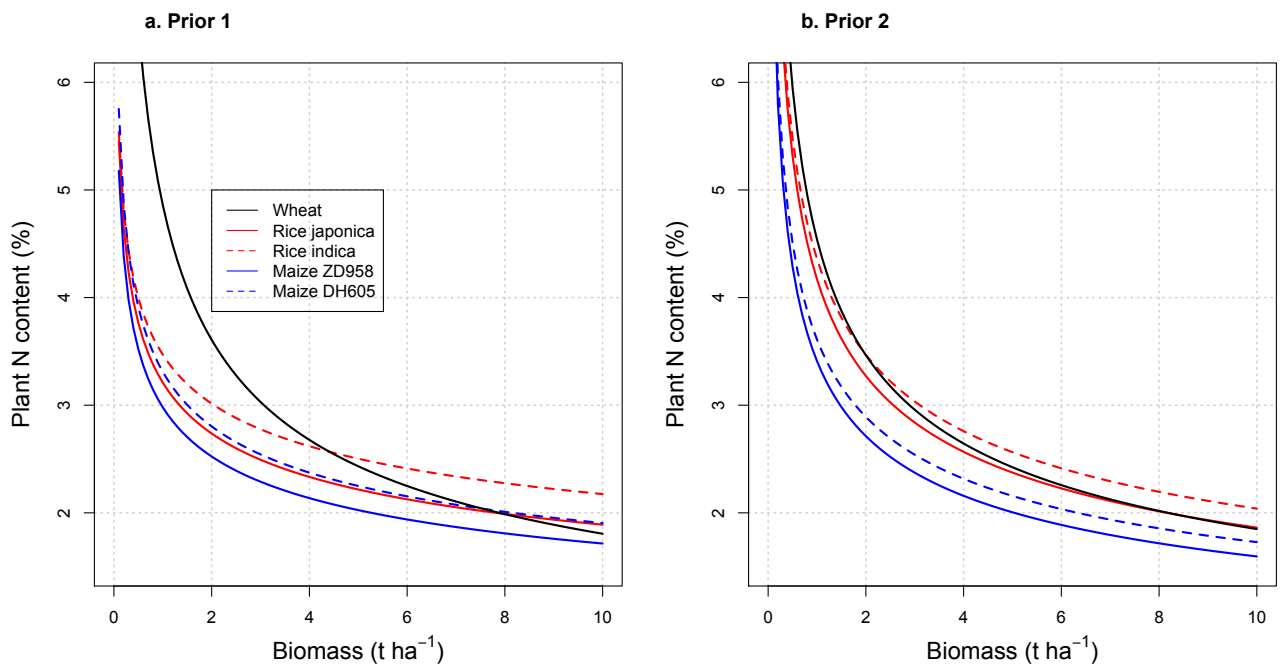
331 The curve obtained for wheat with prior 2 (Figure 4B) is very similar to the curve obtained  
332 with prior 1. For wheat, the fitted critical N curve is thus insensitive to the choice of prior. On  
333 the contrary, the curves obtained for rice indica and japonica are much higher with prior 2  
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

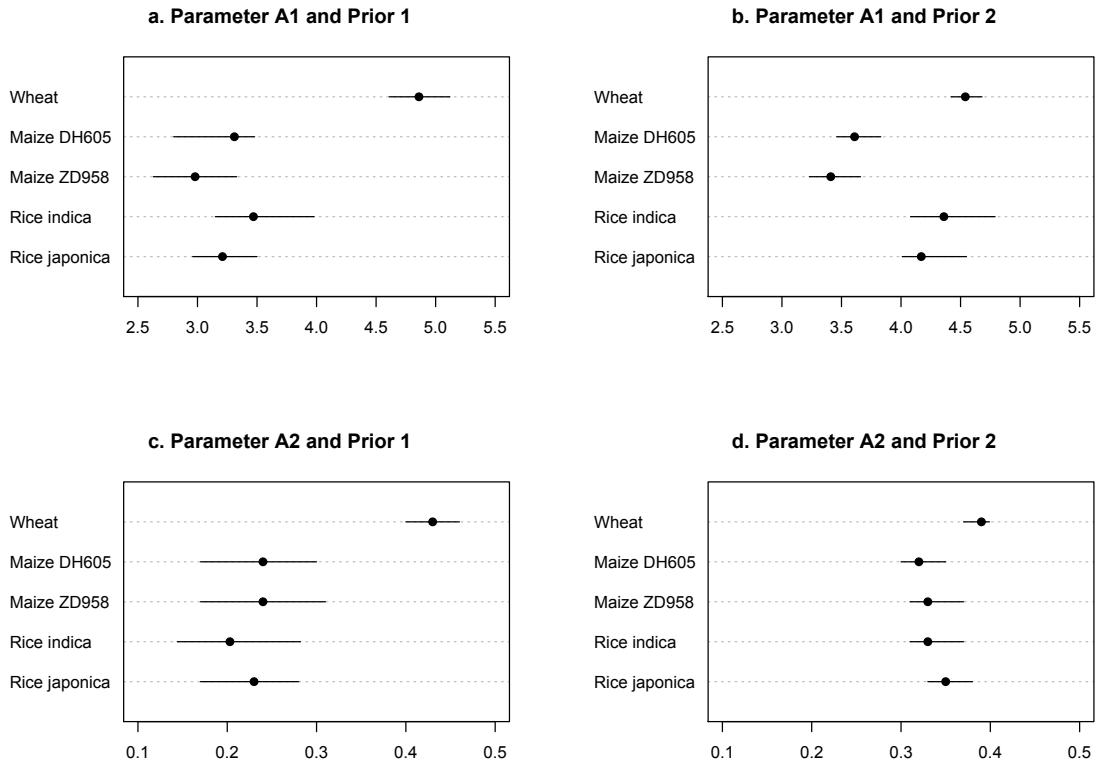
346

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.

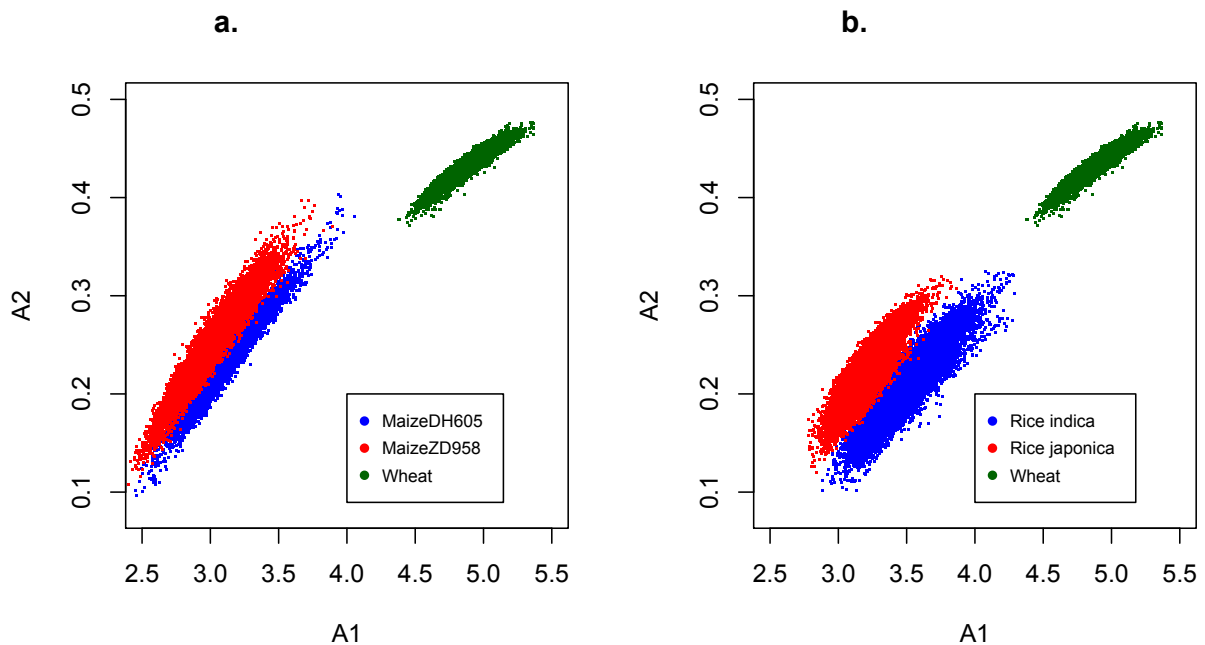
379

380

381

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

## 480 [Acknowledgments](#)

481 This work is part of the project Licite (Institut Carnot Plant2Pro) and of the project CLAND  
482 (16-CONV-0003).

483

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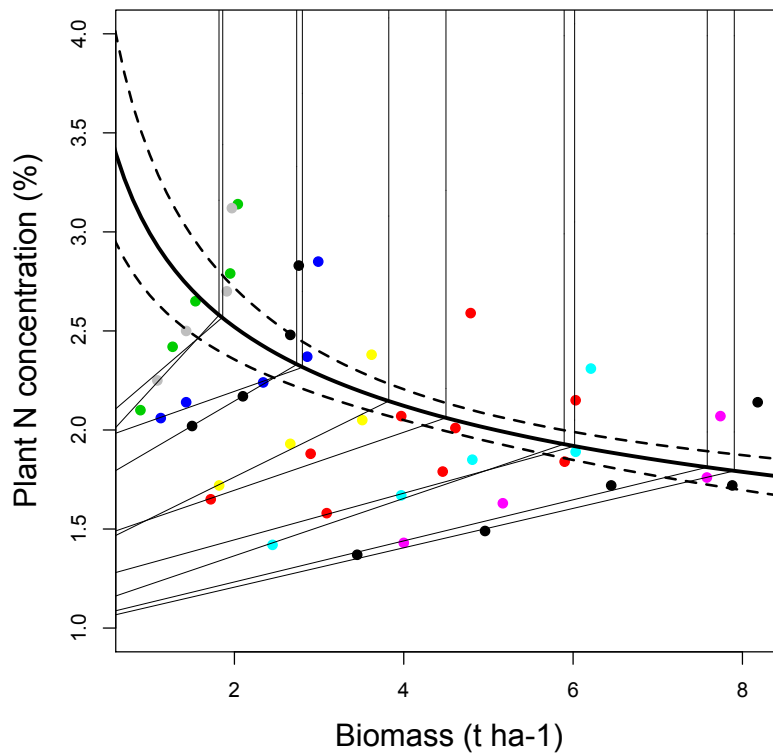
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527 Appendix A: Individual fitted critical N curves

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

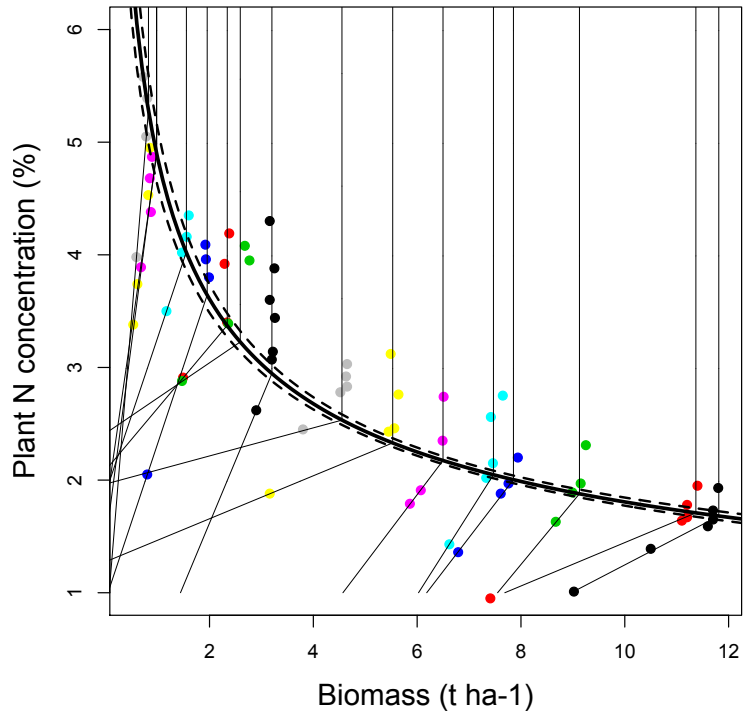
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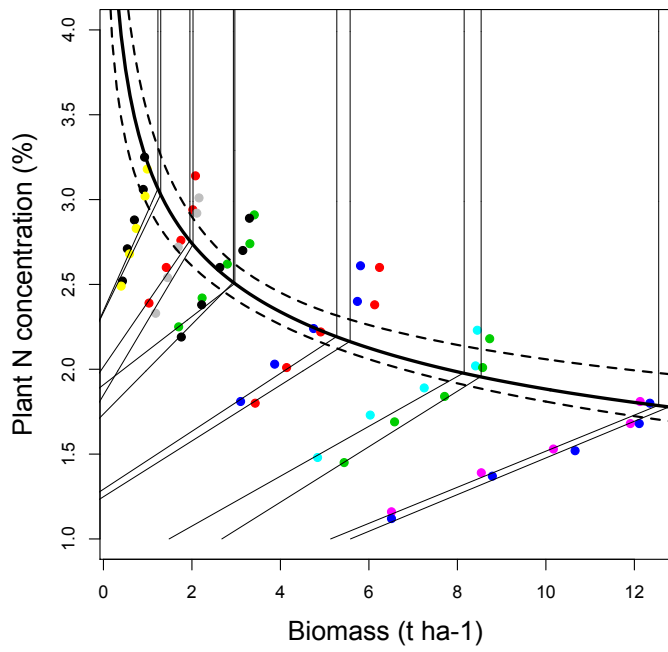
539 A2. Wheat



540

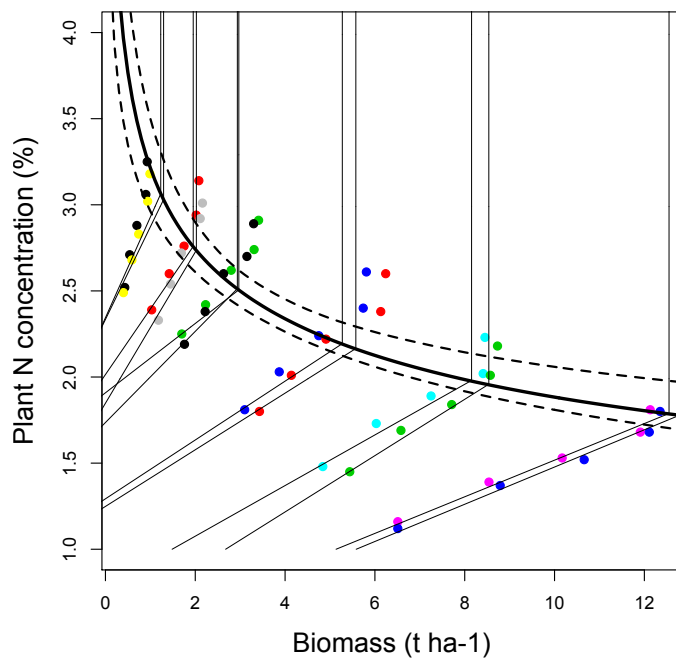
541

542 A3. Rice Japonica



543

544 A4. Rice Indica



545

546

547



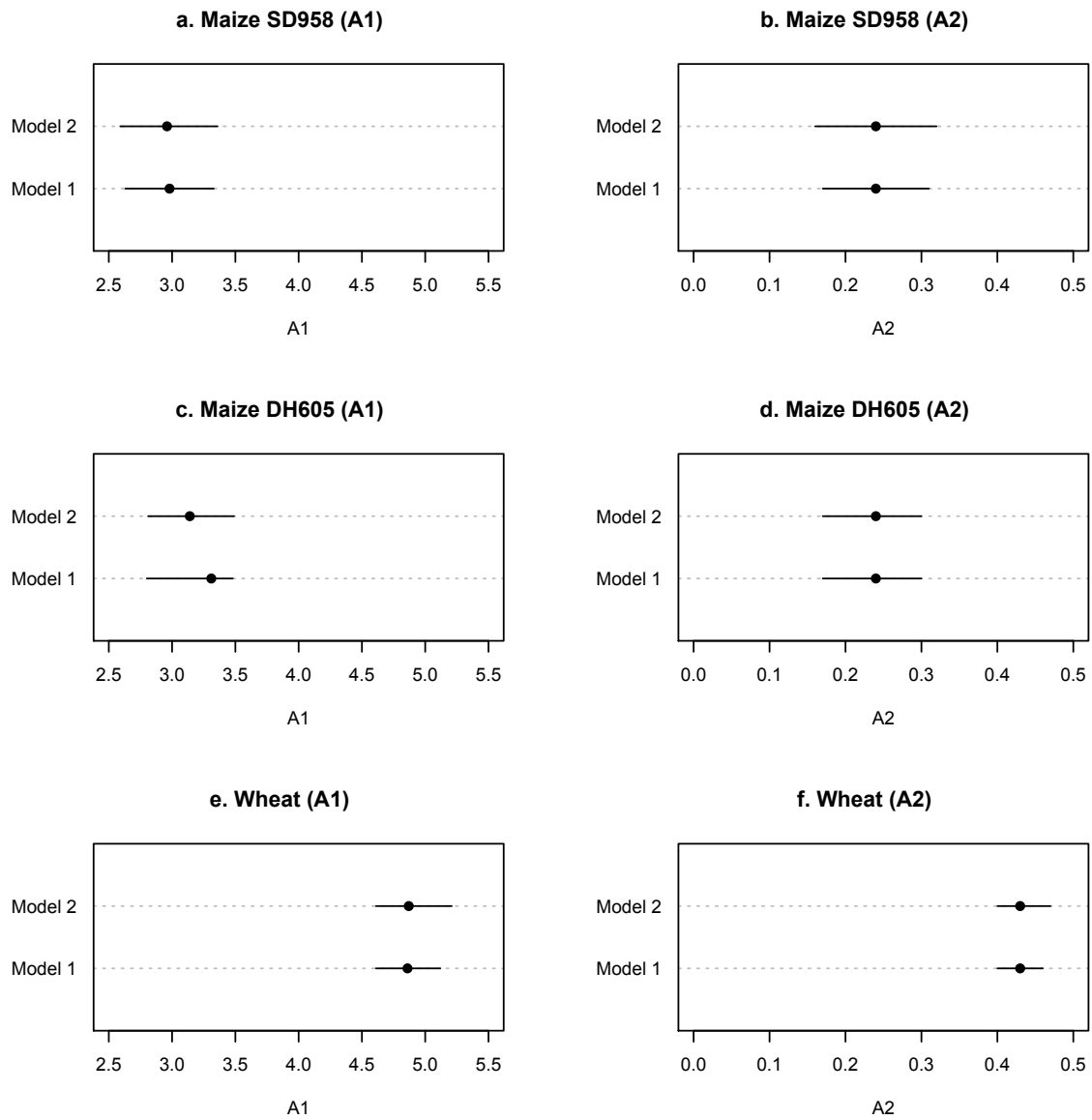
## 548 Appendix B: Characteristics of the maize experiments

549

Experiment No.	Sowing/Harvesting date	Soil characteristics	Cultivar	N(kg N ha <sup>-1</sup> )	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 <sup>-1</sup>	(ZD958)	75 (N1)	Bell stage
		Total N: 0.74 g kg <sup>-1</sup>		150 (N2)	Tasseling stage
		Olsen-P: 35.67 mg kg <sup>-1</sup>		225 (N3)	Anthesis stage
		NH <sub>4</sub> OAc-K <sup>+</sup> : 84 mg kg <sup>-1</sup>		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 <sup>-1</sup>	(DH605)	75 (N1)	Bell stage
		Total N: 0.61 g kg <sup>-1</sup>		150 (N2)	Tasseling stage
		Olsen-P: 33.94 mg kg <sup>-1</sup>		225 (N3)	Anthesis stage
		NH <sub>4</sub> OAc-K <sup>+</sup> : 76 mg kg <sup>-1</sup>		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 <sup>-1</sup>	(ZD958)	90 (N1)	Bell stage
		Total N: 0.83 g kg <sup>-1</sup>		180 (N2)	Tasseling stage
		Olsen-P: 44 mg kg <sup>-1</sup>		270 (N3)	Anthesis stage
		NH <sub>4</sub> OAc-K <sup>+</sup> : 90 mg kg <sup>-1</sup>			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 <sup>-1</sup>	(DH605)	90 (N1)	Bell stage
		Total N: 0.57 g kg <sup>-1</sup>		180 (N2)	Tasseling stage
		Olsen-P: 23.51 mg kg <sup>-1</sup>		270 (N3)	Anthesis stage
		NH <sub>4</sub> OAc-K <sup>+</sup> : 58.45 mg kg <sup>-1</sup>			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
```