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Masjkur, Mohammad; Folmer, Henk

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Bayesian estimation of linear and nonlinear mixed models of fertilizer dosing with independent normally distributed random components

M Masjkur^{1,3} and H Folmer^{2,3}

¹Department of Statistics, Faculty of Mathematics and Natural Sciences,
Bogor Agricultural University, Indonesia

²Faculty of Spatial Sciences, University of Groningen, The Netherlands

³Department of Agricultural Economics, College of Economics and Management,
Northwest A&F University, Yangling, Shaanxi, China

Email : m_masjkur@yahoo.com

Abstract. Many linear and nonlinear mixed response models are proposed to predict the optimum dose of fertilizer. However, a major restriction of this class of models is the normality assumption of the random parameter component. The purpose of this paper is to analyze the performance of linear and nonlinear mixed models of fertilizer dosing with independent normally distributed random parameter components. We compare the Linear Plateau, Spillman-Mitscherlich, and Quadratic random parameter models with different random effects distribution assumption, i.e. the normal, Student-*t*, slash, and contaminated normal distributions and the random errors following their symmetric normal independent distributions. The method is applied to datasets of multi-location trials of potassium fertilization of soybeans. The results show that the Student-*t* Spillman-Mitscherlich Response Model is the best model for soybean yield prediction.

1. Introduction

Many linear and nonlinear response models are commonly used to predict the optimum dose of fertilizer. One modeling approach is to fit a general quadratic form to the data by means of least squares under the assumption of a fixed effects model with independent normally distributed random error term with constant variances ([1]-[2]). However, this approach is unrealistic because it neglects the variability that probably exists between sites and/or years.

An alternative model is the mixed effects approach ([3]-[6]). This approach allows the parameters to have a random effect component that represent between sites or years variability. The random parameter models have been found to outperform the fixed parameter models to model dose-response relationships ([5], [7]-[8]). Furthermore, the quadratic functional form commonly used is not always the best model. [7] and [9] showed that the stochastic linear plateau model and the Mitscherlich exponential type functions outperform the quadratic form. In a similar vein, [8] showed that the stochastic linear plateau function is more adequate than the stochastic quadratic plateau function for corn response to Nitrogen fertilizer.

The random parameter components and the errors are usually taken as normally distributed random variables ([5]-[8]). However, the normality and symmetry assumptions may be too restrictive because



in practice departures from normality is common. Particularly, [10] and [11] concluded that the field crop yield distributions are in general non-normal or non-lognormal. The degree of skewness and kurtosis vary by crop and by the amount of nutrients uptake.

Rosa et al. [12] advocated the use of the Normal independent distribution for robust modeling of linear mixed models. Furthermore, [13] considered the Normal independent distribution for modeling of nonlinear mixed models. The Normal independent distribution is a class of symmetric, heavy-tailed distributions that includes the normal distribution, Student- t , slash, and contaminated distributions. The class of Normal independent distributions accommodate observations with heavy tails as well as the normal distribution.

Traditionally, fertilizer-dose response models are estimated by means of maximum likelihood estimation (ML) ([5]-[8]). However, for nonlinear models and small sample sizes ML is frequently biased ([14]). In addition, convergence can be a problem even with careful scaling and good starting values. Bayesian estimation is an alternative to ML. The advantages of Bayesian estimation are that the results are valid in small samples and that convergence in the case of nonlinear models is not an issue ([14]-[15]).

The purpose of this paper is Bayesian estimation of random parameter dose (fertilization)-response (yield) models for yield data that is Normally independently distributed.

2. Mixed effects model and normal independent distributions

2.1. The normal mixed effects model

In general, a Normal mixed effects model reads:

$$Y_i = \eta(\boldsymbol{\phi}_i, \mathbf{X}_i) + \boldsymbol{\epsilon}_i, \quad \boldsymbol{\phi}_i = \mathbf{A}_i \boldsymbol{\beta} + \mathbf{B}_i \mathbf{b}_i, \quad (1)$$

with

$$(\mathbf{b}_i, \boldsymbol{\epsilon}_i) \stackrel{ind}{\sim} N_{n_i+q}(\mathbf{0}, \text{Diag}(\boldsymbol{\Sigma}, \sigma_e^2 \mathbf{I}_{n_i})),$$

where the subscript i is the subject index, $i = 1, \dots, n$; $\mathbf{Y}_i = (y_{i1}, \dots, y_{in_i})^T$ is a $n_i \times 1$ vector of n_i observed continuous responses for subject i , $\eta_i(\boldsymbol{\phi}_i, \mathbf{X}_i) = \{\eta(\boldsymbol{\phi}_i, X_{i1}), \dots, \eta(\boldsymbol{\phi}_i, X_{in_i})\}^T$ with $\eta(\cdot)$ the nonlinear or linear function of random parameters $\boldsymbol{\phi}_i$, and covariate vector \mathbf{X}_i , \mathbf{A}_i and \mathbf{B}_i are known design matrices of dimensions $n_i \times p$ and $n_i \times q$, respectively, $\boldsymbol{\beta}$ is the $p \times 1$ vector of fixed effects, \mathbf{b}_i is the $q \times 1$ vector of random effects, and $\boldsymbol{\epsilon}_i$ is the $n_i \times 1$ vector of random errors, and \mathbf{I}_{n_i} denotes the identity matrix. The matrices $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\boldsymbol{\alpha})$ with unknown parameter $\boldsymbol{\alpha}$ is the $q \times q$ unstructured dispersion matrix of \mathbf{b}_i , σ_e^2 the unknown variance of the error term. When $\eta(\cdot)$ is a nonlinear parameter function, we have the Normal NonLinear Mixed Model (N-NLMM); if $\eta(\cdot)$ is a linear parameter function, we have the N-Linear Mixed Model (N-LMM).

It follows that

$$\mathbf{b}_i \stackrel{ind}{\sim} N_q(\mathbf{0}, \boldsymbol{\Sigma}) \text{ and } \boldsymbol{\epsilon}_i \stackrel{ind}{\sim} N_{n_i}(\mathbf{0}, \sigma_e^2 \mathbf{I}_{n_i})$$

and they are uncorrelated, since $\text{Cov}(\mathbf{b}_i, \boldsymbol{\epsilon}_i) = \mathbf{0}$ ([13],[16]).

2.2. Normal independent (NI) distributions

A Normal independent distribution is defined as the p -dimensional random vector $\mathbf{y} = \boldsymbol{\mu} + U^{1/2} \mathbf{Z}$, where $\boldsymbol{\mu}$ is a location vector, \mathbf{Z} is a multivariate normal random vector with location vector $\mathbf{0}$, scale matrix $\boldsymbol{\Sigma}$ and U is a positive random variable with cumulative distribution function (cdf) $H(u|v)$ and probability density function (pdf) $h(u|v)$, v is a scalar or vector of parameters indexing the distribution of the scale factor U ([12]-[13],[16]). Given U , \mathbf{Y} follows a multivariate normal

distribution with location vector $\mathbf{0}$, and scale matrix $u^{-1}\mathbf{\Sigma}$. Thus, the NI distributions are scale mixtures of the normal distributions denoted by $\mathbf{Y} \sim N_p(\boldsymbol{\mu}, \mathbf{\Sigma}, H)$. The marginal pdf of \mathbf{Y} is

$$f(\mathbf{y}) = \int_0^\infty \phi_p(\mathbf{y}; \boldsymbol{\mu}, u^{-1}\mathbf{\Sigma}) dH(u|\mathbf{v}),$$

The class of normal independent distribution is a group of symmetric heavy-tailed distribution of robust alternative to the routinely used of normal distribution for mixed effects model.

2.3. The NI-mixed effects model

Using the general framework (1), the following general NI-Mixed Model (NI-MM) is defined as:

$$\mathbf{b}_i \stackrel{iid}{\sim} N_q(\mathbf{0}, \text{Diag}(\mathbf{\Sigma}), H) \text{ and } \boldsymbol{\epsilon}_i \stackrel{ind}{\sim} N_{n_i}(\mathbf{0}, \sigma_e^2 \mathbf{I}_{n_i}, H), \quad i = 1, \dots, n. \quad (2)$$

where the random effects are assumed to have a multivariate NI distributions and also the random errors.

3. Bayesian inference

3.1. Prior distributions and joint posterior density

Below, we apply a Bayesian framework based on the Markov Chain Monte Carlo (MCMC) algorithm to infer posterior parameter estimates. Following (1) and (2), the NI mixed model can be formulated in hierarchical for $i = 1, \dots, n$, as:

$$\mathbf{Y}_i | \mathbf{b}_i, U_i = u_i \stackrel{ind}{\sim} N_{n_i}(\eta(\mathbf{A}_i \boldsymbol{\beta} + \mathbf{B}_i \mathbf{b}_i, \mathbf{X}_i), u_i^{-1} \sigma_e^2 \mathbf{I}_{n_i}).$$

$$\mathbf{b}_i | U_i = u_i \stackrel{ind}{\sim} N_q(\mathbf{0}, u_i^{-1} \mathbf{\Sigma}).$$

$$U_i \stackrel{iid}{\sim} H(u_i | \mathbf{v}).$$

([13],[16]).

Let $\mathbf{Y} = (\mathbf{y}_1^T, \dots, \mathbf{y}_n^T)^T$, $\mathbf{b} = (\mathbf{b}_1^T, \dots, \mathbf{b}_n^T)^T$, $\mathbf{u} = (u_1, \dots, u_n)^T$. Then, the complete likelihood function associated with $(\mathbf{y}^T, \mathbf{b}^T, \mathbf{u}^T)^T$, is given by

$$L(\boldsymbol{\theta} | \mathbf{Y}, \mathbf{b}, \mathbf{u}) \propto \prod_{i=1}^n [\phi_{n_i}(\mathbf{y}_i; \eta(\mathbf{A}_i \boldsymbol{\beta} + \mathbf{B}_i \mathbf{b}_i, \mathbf{X}_i), u_i^{-1} \sigma_e^2 \mathbf{I}_{n_i}) \phi_q(\mathbf{b}_i; \mathbf{0}, u_i^{-1} \mathbf{\Sigma}) h(u_i | \mathbf{v})].$$

To complete Bayesian specification, we need to consider prior distributions for all the unknown parameters $\boldsymbol{\theta} = (\boldsymbol{\beta}^T, \sigma_e^2, \boldsymbol{\alpha}^T, \mathbf{v}^T)^T$. We consider $\boldsymbol{\beta} \sim N_p(\boldsymbol{\beta}_0, \mathbf{S}_\beta)$, $\sigma_e^2 \sim IG(\tau/2, T/2)$, $\mathbf{\Sigma} \sim IW_q(\mathbf{M}, l)$ ([13],[16]). For \mathbf{v} we take $\mathbf{v} \sim \text{Exp}(\tau/2) \mathbb{I}_{(2, \infty)}$ for the Student- t (t) model, Gamma (a, b) for the slash (SL) model. Furthermore, $U(0, 1)$ for v_1 and Beta (ρ_0, ρ_1) for v_2 for the contaminated normal (CN) model.

Assuming independency of the parameter vector, the joint prior distribution of all unknown parameters is

$$\pi(\boldsymbol{\theta}) = \pi(\boldsymbol{\beta}) \pi(\sigma_e^2) \pi(\boldsymbol{\alpha}) \pi(\mathbf{v})$$

Combining the likelihood function and the prior distribution, the joint posterior density of all unknown parameters is

$$\pi(\boldsymbol{\theta}, \mathbf{b}, \mathbf{u}|\mathbf{y}) \propto \prod_{i=1}^n [\phi_{n_i}(\mathbf{y}_i; \boldsymbol{\eta}(\mathbf{A}_i \boldsymbol{\beta} + \mathbf{B}_i \mathbf{b}_i, \mathbf{X}_i), u_i^{-1} \sigma_e^2 \mathbf{I}_{n_i}) \phi_q(\mathbf{b}_i; \mathbf{0}, u_i^{-1} \boldsymbol{\Sigma}) h(u_i|\boldsymbol{\nu})] \pi(\boldsymbol{\theta})$$

3.2. Model comparison criteria

The expected Akaike information criterion (EAIC) and the expected Bayesian information criterion (EBIC) are a deviance-based measure appropriate for Bayesian model selection ([17]-[18]).

Let $\boldsymbol{\theta}$ and $\mathbf{Y} = (y_1, \dots, y_n)^T$ be the entire model parameters and data, respectively. Define $D(\boldsymbol{\theta}) = -2 \ln f(\mathbf{y}|\boldsymbol{\theta}) = -2 \sum_{i=1}^n \ln f(\mathbf{y}_i|\boldsymbol{\theta})$, where $f(\mathbf{y}_i|\boldsymbol{\theta})$ is marginal distribution of y_i , then $E[D(\boldsymbol{\theta})]$ is a measure of fit and can be approximated by using the MCMC output in a Monte Carlo simulation. This index is given by $\bar{D} = \frac{1}{K} \sum_{k=1}^K D(\boldsymbol{\theta}^{(k)})$. Where $\boldsymbol{\theta}^{(k)}$ is the k^{th} iteration of MCMC chain of the model and K is the number of iterations.

The expected Akaike information criterion (EAIC) and the expected Bayesian information criterion (EBIC) define as follows

$$\widehat{EAIC} = \bar{D} + 2p, \text{ and } \widehat{EBIC} = \bar{D} + p \log(N)$$

where \bar{D} is the posterior mean of the deviance, p is the number of parameters in the model, N is the total number of observations. These criteria penalizing models with more complexity. Smaller value of EAIC and EBIC indicate a better fit ([19]).

4. Case study

4.1. Data

The dataset is obtained from 19 multi-location trials of potassium fertilization of soybeans. The experiments were carried out between 2002 and 2014. The soil types are Ultisols, Inceptisols, Vertisols, and Oxisols with soil potassium contents varying from very low to very high. Common soybean varieties were used. Each experiments consisted of five levels of potassium fertilization. The doses applied were 0, 40, 80, 160 and 320 kg ha⁻¹ of KCl. The plots were 6 by 5 m, or 4 by 5 m arranged in a randomized complete block design with three to nine replications. The response variable was soybean yield (t ha⁻¹). The yields reported are averages over replications ([20]-[22]).

4.2. Response functions

We consider three response functions: the Linear Plateau (LP), the Spillman-Mitscherlich (SM) and the Quadratic functions (Q).

The stochastic LP is defined as follows:

$$Y_i = \min(\alpha_1 + (\alpha_2 + b_{2i})X_i; \mu_p + b_{3i}) + b_{1i} + \varepsilon_i \quad (3)$$

where for location i , Y_i is the soybean yield; X_i the potassium fertilizer dose; α_1 the intercept parameter; α_2 the linear response coefficient; μ_p the plateau yield; b_{1i} , b_{2i} , and b_{3i} are the random effects; and ε_i is the random error term. In term of (1), $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)^T$ $\mathbf{b}_i = (b_{1i}, b_{2i}, b_{3i})^T$; $\mathbf{b}_i \stackrel{iid}{\sim} N_q(\mathbf{0}, \boldsymbol{\Sigma}, H)$ and $\varepsilon_i \stackrel{ind}{\sim} N_{n_i}(\mathbf{0}, \sigma_e^2 \mathbf{I}_{n_i}, H)$.

The stochastic SM reads:

$$Y_i = \beta_1 - (\beta_2 + b_{2i}) \exp((- \beta_3 + b_{3i}) X_i) + b_{1i} + \varepsilon_i \quad (4)$$

where β_1 is the maximum yield attainable by potassium fertilization; β_2 is the yield increase; β_3 is the ratio of consecutive increments of the yield; all other parameters, variables and distributions as in (3).

The stochastic Q is defined as:

$$Y_i = \gamma_1 + (\gamma_2 + b_{2i})X_i + (\gamma_3 + b_{3i})X_i^2 + b_{1i} + \varepsilon_i \quad (5)$$

where γ_1 is the intercept parameter whose position (value) can be shifted up or down by the random effect b_{1i} ; γ_2 is the linear response coefficient with random effect parameter b_{2i} ; γ_3 is the quadratic response coefficient whose position can be shifted up or down by the random effect b_{3i} ; $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \gamma_3)^T$; all other variables and distributions as in (3) ([7]-[9]).

4.3. Statistical analysis

The datasets was used to identify the model with the best fit among the random parameter models of fertilizer dosing. Several statistical models with differing distribution in the random effects and random errors are compared. These models are :

Model 1: Normal distribution for the random effects and for the random errors (N-N)

Model 2: Student- t distribution for the random effects and for the random errors (t - t)

Model 3: Slash distribution for the random effects and for the random errors (SL-SL)

Model 4: Contaminated normal distribution for the random effects and for the random errors (CN-CN).

The following independent priors were considered to perform the Gibbs sampler, $\boldsymbol{\beta}_k \sim N(0, 10^3)$, $\sigma^2 \sim IG(0.1, 0.1)$, $\boldsymbol{\Sigma} \sim IG(0.1, 0.1)$, and $v \sim Exp(0.1)I(2,)$ for the t - t model, $v \sim Gamma(0.1, 0.01)$ for the slash model, $v_1 \sim Beta(1, 1)$ and $v_2 \sim Beta(2, 2)$ for the contaminated normal model, respectively.

For each of the models, we ran three parallel independent chains of the Gibbs sampler with size 50 000 iterations for each parameter with thinning of 5 and an initial burn in of 25 000. We monitored chain convergence using trace plots, autocorrelation plots and the Brooks-Gelman-Rubin scale reduction factor (\hat{R}) ([23]). To avoid non-convergence, we normalized the original doses (subtracted the mean and divided by the standard deviation) which gave: -1.06, -0.70, -0.35, 0.35, and 1.76, respectively ([24]). We fitted the models using the R2jags package available in R ([25]).

5. Results and discussion

5.1. Soybean yield data

Figure 1 shows the histogram and normal Q-Q plot of soybean yield data for 19 locations, while the boxplot is presented in figure 2. The figures indicates non-normality (heavy-tailed) pattern. The Q-Q plot does not show a straight line, while the boxplot shows asymmetry and an outlier. Thus, it seems appropriate to fit a heavy-tailed model to the data.

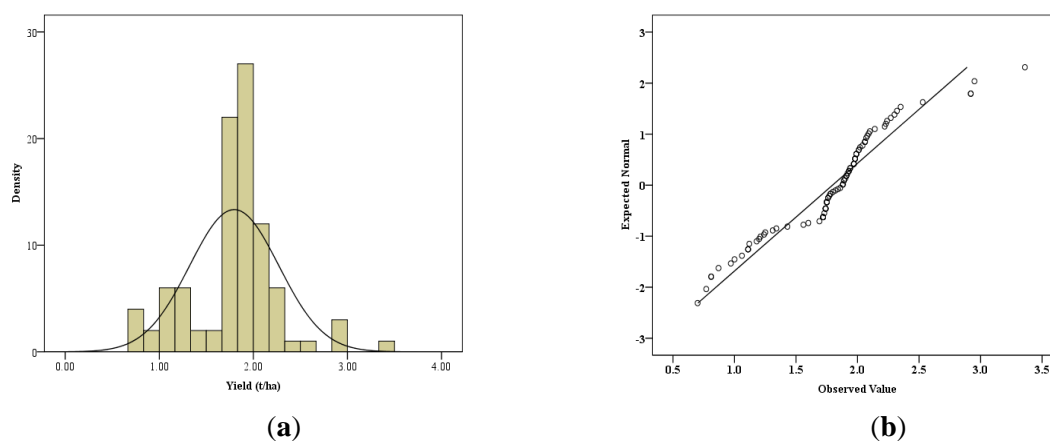


Figure 1. Soybean yield data: (a) Histogram; (b) Normal Q-Q plot.

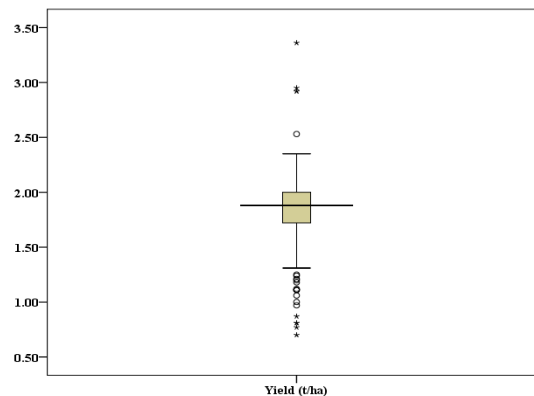


Figure 2. Boxplot of soybean yield data.

5.2. Linear plateau response models

Based on the EAIC and the EBIC in table 1, we find that among the NI models the Student- t (t - t) Model gives the best fit, followed by the contaminated normal (CN-CN), slash (SL-SL), and normal (N-N) Model. We furthermore find that the heavy-tailed distributions outperform the normal distributions. Thus, the t - t Model is the best Linear Plateau Response Model.

Table 1. The Linear plateau models

Parameter	N-N		t - t		SL-SL		CN-CN	
	Mean	SD	Mean	SD	Mean	SD	Mean	SD
α_1	1.473	0.114	1.555	0.109	1.482	0.110	1.521	0.125
α_2	39.968	20.482	29.274	19.480	30.780	19.899	29.061	19.030
μ_p	1.878	0.129	1.853	0.111	1.854	0.122	1.867	0.119
σ_ε^2	0.139	0.014	0.014	0.004	0.012	0.004	0.012	0.006
d_1	0.467	0.095	0.374	0.098	0.355	0.085	0.340	0.113
d_2	13.135	11.964	2.534	4.694	3.684	6.048	2.452	3.937
d_3	0.306	0.081	0.241	0.074	0.227	0.068	0.227	0.077
ν (ν_1)			5.043	3.039	2.697	1.620	0.515	0.253
ν_2							0.450	0.226
EAIC	-93.56		-104.91		-95.86		-97.21	
EBIC	-93.71		-105.09		-96.04		-97.41	

Table 1 furthermore shows that for the t - t Model, all the fixed effects, i.e., the intercept parameter (α_1), the linear response coefficient (α_2), the plateau yield u_p and the random effects (d_1, d_2, d_3) are significant.

5.3. Spillman-Mitscherlich response models

Based on the EAIC and EBIC in table 2 we find the following rankings of the NI models: t - t < N-N < SL-SL < CN-CN. Therefore, the t - t Model is the best Spillman-Mitscherlich Response Model.

Table 2. The Spillman-Mitscherlich models

Parameter	N-N		<i>t-t</i>		SL-SL		CN-CN	
	Mean	SD	Mean	SD	Mean	SD	Mean	SD
β_1	1.950	0.111	1.919	0.092	1.945	0.103	1.955	0.106
β_2	0.032	0.013	0.054	0.021	0.069	0.024	0.067	0.023
β_3	2.495	0.415	1.848	0.312	1.765	0.300	1.808	0.305
σ^2_ε	0.104	0.010	0.009	0.003	0.009	0.003	0.010	0.003
d_1	0.465	0.087	0.371	0.087	0.355	0.080	0.401	0.086
d_2	0.008	0.006	0.053	0.012	0.051	0.012	0.052	0.012
d_3	0.623	0.199	0.441	0.240	0.463	0.198	0.490	0.222
$v(v_1)$			4.754	2.731	3.139	1.735	0.321	0.235
v_2							0.544	0.203
EAIC	-147.72		-153.88		-138.45		-135.19	
EBIC	-147.88		-154.06		-138.63		-135.39	

For the *t-t* Model, the fixed effects, i.e., the maximum yield coefficient (β_1), the increase in yield (β_2), the ratio of successive increment (β_3) and the random effects (d_1, d_2, d_3) are significant.

5.4. The Quadratic response models

Comparison of the EAIC and EBIC in table 3 leads to the following rankings: *t-t* < SL-SL < CN-CN < N-N. The results furthermore show that the heavy-tailed distributions outperform the normal distribution, and that overall the *t-t* Model is the best Quadratic Response Model.

Table 3. The Quadratic models

Parameter	N-N		<i>t-t</i>		SL-SL		CN-CN	
	Mean	SD	Mean	SD	Mean	SD	Mean	SD
γ_1	1.796	0.107	1.825	0.079	1.783	0.096	1.788	0.096
γ_2	0.510	0.072	0.330	0.056	0.398	0.072	0.391	0.076
γ_3	-0.386	0.072	-0.246	0.052	-0.297	0.067	-0.292	0.069
σ^2_ε	0.033	0.006	0.014	0.005	0.011	0.005	0.014	0.006
d_1	0.445	0.085	0.327	0.085	0.297	0.074	0.315	0.092
d_2	0.046	0.030	0.082	0.023	0.075	0.020	0.077	0.021
d_3	0.030	0.022	0.072	0.019	0.066	0.017	0.068	0.018
$v(v_1)$			2.516	1.329	1.617	0.868	0.366	0.160
v_2							0.265	0.141
EAIC	-45.32		-104.44		-83.22		-80.59	
EBIC	-45.47		-104.62		-83.40		-80.79	

For the *t-t* Model, all the fixed effects, i.e., the intercept parameter (γ_1), the linear response coefficient (γ_2), the quadratic response coefficient (γ_3), and the variance component (d_1, d_2, d_3) are significant.

5.5. Comparing the Linear plateau, Spillman-Mitscherlich and Quadratic models

Comparing the Linear Plateau (LP), Spillman-Mitscherlich (SM) and Quadratic (Q) models under four distributional assumptions, we find that the *t-t* Spillman-Mitscherlich model has the smallest EAIC and EBIC values among the competing models indicating that this is the best fit model for the soybean yield data (table 4).

Table 4. Comparison of LP, SM and Q models

Distribution	LP		SM		Q	
	EAIC	EBIC	EAIC	EBIC	EAIC	EBIC
N	-93.56	-93.71	-147.72	-147.88	-45.32	-45.47
<i>t</i>	-104.91	-105.09	-153.88	-154.06	-104.44	-104.62
SL	-95.86	-96.04	-138.45	-138.63	-83.22	-83.40
CN	-97.21	-97.41	-135.19	-135.39	-80.59	-80.79

6. Conclusion

We investigated the performance of linear and nonlinear mixed response models with normal independent (NI) distributions of random effects. We applied the Bayesian estimation framework to datasets of multi-location trials of potassium fertilization of soybeans. We compared the Linear Plateau, Spillman-Mitscherlich, and Quadratic random parameter models with different distributions of the random parameter component, i.e. the normal, Student-*t*, slash, and contaminated normal distributions and the random errors following their symmetric normal independent distributions.

The overall results showed that for all three models of fertilizer dosing, the Student-*t* distributions outperform the normal distributions. The best model for soybean yield prediction is the Student-*t* Spillman-Mitscherlich Response Model.

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