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ARTICLE

Bayesian implementation of Skew-Normal distributions for experimental error in the description of pepper growth

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Abstract
The purpose of this work is to implement and compare three types of Skew-Normal distributions together with the Normal submodel for the experimental error through a Bayesian nonlinear modeling of pepper phenotype growth. The posterior means of the parameters (α, β, γ) were shown to be invariant to the experimental error. The Sahu Skew-Normal error showed evidence of null asymmetry for all growth models. In general, all Skew-Normal distributions presented the highest accuracy $(1/\sigma^2)$ in relation to the Normal error. The problematic points stand out for the computational cost in the millions of MCMC iterations and the limitations of the BUGS language. The Skew-Normal distribution of Azzalini and Fernandéz & Steel modeled the asymmetry of the data and provided the best goodness of fit (DIC) and the best precision $(1/\sigma^2)$ for the Gompertz and Von Bertalanffy model in relation to the Normal error.
Keywords: Bayesian Inference; Longitudinal data; Skew-Normal.

1. Introduction

Peppers of the *Capsicum* genus have stood out in Brazil due to their genetic diversity, widespread national consumption, and prominence in Brazilian olive growing (Nunes Ávila & Barbosa, 2019).

In plant growth, some of the phenotypic characteristics follow an exponential growth until the maturation rate is reached. From this inflection point, the plant growth declines until it reaches an asymptotic value. The pattern of this type of growth is called sigmoid. Sigmoid models are non-linear, and the Normal distribution is generally used to adjust these models (Souza, 1998). Asymmetric experimental errors can also be used in plant height modeling (Mangueira *et al.*, 2016; Guedes *et al.*, 2014).

Regarding the issue of normality, Pino (2014) asserts that although the Normal distribution is the default in several statistical procedures, in practice, it is more common for observations to be approximately normal. Some factors contribute to the extrapolation of the normality assumption, such as the presence of outliers, data asymmetry, or support only in R^+ in the variables. In terms of regression, Robust Regression can be used in the presence of outliers. Gelman *et al.* (2013) explain that the student's t distribution because it has heavy tails, is more efficient than the Normal distribution in Bayesian regression. Regarding the asymmetry issue, Eloy *et al.* (2020) explain that several proposals for new distributions address the asymmetry and kurtosis of the data, such as Skew-Normal and Skew-Student t.

The best-known Skew-Normal distribution is the one obtained by Azzalini, through an Azzalini transformation. The methodology adds a new asymmetry parameter (λ) to any distribution in the symmetric family. There are other versions, such as the Sahu Skew-Normal distribution and the Fernandez & Steel Skew-Normal distribution. As Ghaderinezhad *et al.* (2020) assert, the frequentist estimation of the Skew-Normal distribution faces a series of difficulties, such as singularity points, monotonic log-likelihood function for λ, and complex expressions for the estimation of λ using the method of moments or singular Fisher information matrix (Rossi & Santos, 2014). There are distributions whose transformation to Skew-Symmetric models do not have analytical mathematical expressions for moments, expectations, and variances, such as the Azzalini Skew-Logistic distribution studied by Nadarajah (2009). In this context, Ghaderinezhad *et al.* (2020) recommend the Bayesian methodology to overcome the problems of frequentist estimation of the Skew Normal distribution.

In linear models such as the Gauss-Markov Normal model, the significance tests, ANOVA, and confidence intervals are accurate, although they depend on a series of estimability conditions (Luna & Olinda, 2012). When considering an error distribution other than the Normal model, the significance tests generally depend on the asymptotic normality of the maximum likelihood (MV) estimators. In the case of nonlinear Normal models, the distribution of the MV and Gauss-Newton estimators also depend on the asymptotic theory (Cordeiro & Demétrio, 2013), and the ANOVA in these cases is not valid because the decomposition of the sum of total squares into residuals and regression is not valid (Gujarati & Porter, 2012). The gain in the Bayesian methodology of non-linear models consists of the validity of the significance tests and credibility intervals without worrying about the sample size (Martins Filho *et al.* 2008) or the existence of a global maximum of the likelihood function.

In this work, three versions of the Skew-Normal distribution will be implemented: the Skew-Normal distribution of Azzalini (1985), which we will denote as SN1; the Skew-Normal distribution of Sahu *et al.* (2003), which we will denote as SN2, and the Skew-Normal distribution of Fernandéz & Steel (1998) which we will denote as SN3.

The objective of implementing the Skew-Normal distributions in this work is to compare them with the Normal submodel, which we will denote as N, for the experimental error of the Bayesian description of the phenotypic growth of *Capsicum*.

2. Materials and Methods

The database to be worked is composed of 8 accessions of *Capsicum annuum L.*, being these, 1 - Volcano Pepper; 2 - Cayenne Pepper; 3 - Peter Pepper; 4 - Spicy Pepper; 5 - Jamaica Yellow Pepper; 6 - Blocy bell pepper; 7 - Ikeda bell pepper; 8 - Ruby Giant bell pepper. The experiment was conducted in the Plant Science Department of the Federal University of Viçosa (UFV), located in the city of Viçosa, Minas Gerais, Brazil. (20º 45 South and 42º 51 West, average altitude of 650 m). As expressed in Figure 1, the phenotypic characteristics obtained from the experiment are the fruit length - FL (explanatory variable) as a function of the days after flowering - DAF (independent variable).

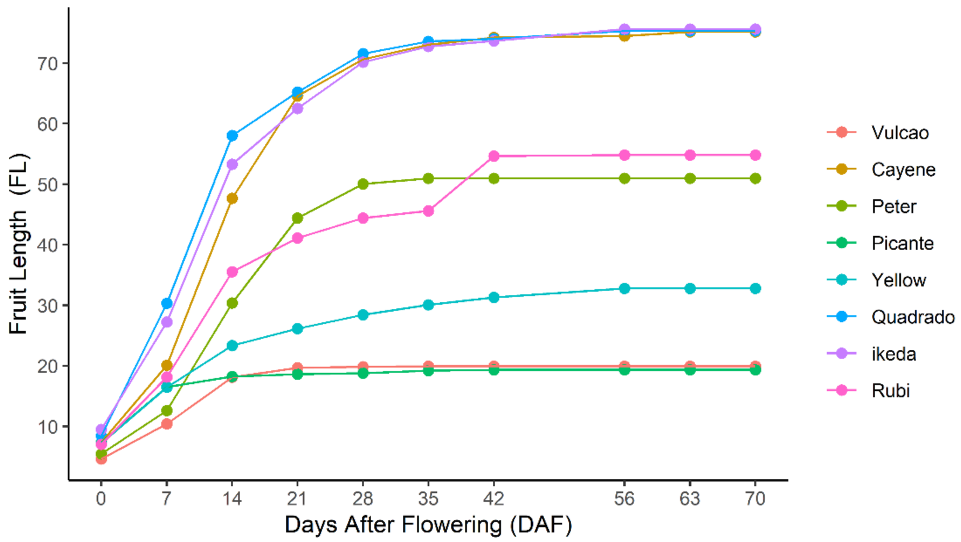

Figure 1. Scatter plot of accessions 1 to 8, plotting Fruit Length (FL) as a function of Days After Flowering (DAF).

Like every niche in agricultural science, plant growth has a series of growth models widely used in modeling longitudinal data. According to Rosa *et al.* (2022), the goal is to find the one that best explains and fits the data from all the varieties of models.

Koya and Goshu (2013) provide a complete review of the main growth models and their mathematical properties.

Sigmoid models such as Velhust's and nonlinear models generally have parameter interpretability depending on the nature of the situation. The parameter α represents the asymptotic weight, that is, the maximum value that a given crop characteristic can reach, the parameter β generally has no biological value, and the parameter γ represents the growth rate.

As explained by Fernandes *et al.* (2015), the most used Logistic, Gompertz, and Von Bertalanffy growth models in the literature owe their frequency of use to their popularity. The author also explains that these models are the furthest from linearity through the Battes curvature and do not have a biological interpretation of β.

In terms of interpretability of the β parameter, adequate reparameterizations of the models allow the inflection point to be equivalent to β and not a function of β. In the most common Logistic model, the inflection point of the curve is represented by $(\log \beta/\gamma, \alpha/2)$, while in the reparameterized Logistic model studied by Fernandes *et al.* (2015):

$$\eta(\theta) = \frac{\alpha}{1+e^{\gamma(\beta-x)}} \quad (1)$$

The biological interpretation of the parameter β becomes the value at which the plant reaches maximum growth speed as shown in Figure 2.

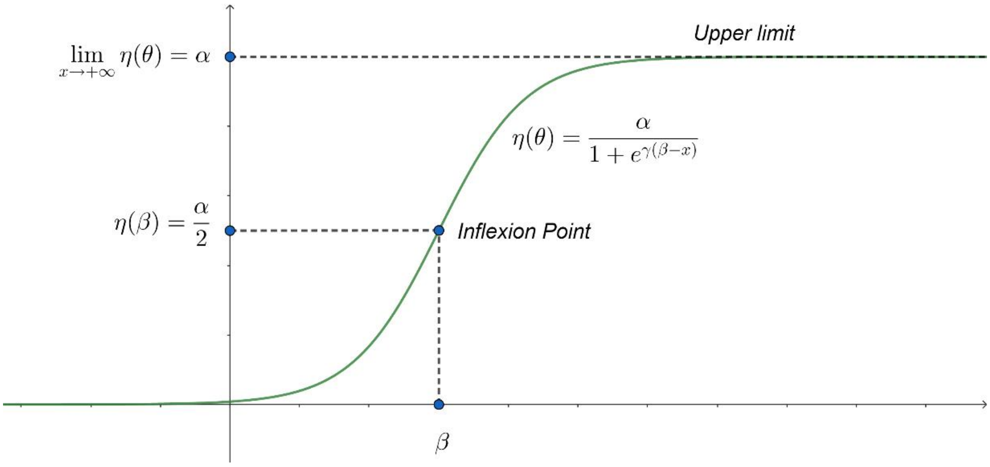

Figure 2. The sigmoid curve of equation (1) with its main elements as an inflection point and asymptotic limit.

Equations 2 and 3 represent other reparameterizations of the Gompertz (Fernandes *et al.*, 2015) and Von Bertalanffy (Fernandes *et al.*, 2020) models with the same biological interpretation for β.

$$\eta(\theta) = \alpha \exp\{-\exp\{\gamma(\beta - x)\} \quad (2)$$

$$\eta(\theta) = \alpha\left(1 - \frac{\exp\{\gamma(\beta - x)\}}{3}\right)^3 \quad (3)$$

2.1 Nonlinear regression with asymmetric errors

In the classical univariate nonlinear regression model, we have a nonlinear response function $\eta(x_i, \theta)$ in the parameter vector θ, a vector of independent variables x, an explanatory variable y, and the experimental error $e_i \sim N(0, \sigma^2)$ which is normally distributed. The nonlinear regression model can also be defined as in equation 4.

$$y_i = \eta(x_i, \theta) + \sigma e_i \quad (4)$$

This is equivalent to saying that $Y_i \sim N(\eta(x_i, \theta), \sigma^2)$, where the error e_i is a random variable, then $\eta(x_i, \theta) + \sigma e_i$ would be as if it were the location-scale transformation of this variable for Y_i, where $e_i \sim N(0,1)$. In normal nonlinear models we have that $E(Y_i) = \eta(x_i, \theta)$ since the distribution of Y_i is symmetric and the location parameter μ is equal to $\eta(x_i, \theta)$.

When it comes to relaxing the assumption of normality of the Gaussian experimental error for the asymmetric error (Gaussian or not), it must be considered that in asymmetric distributions the expectation is not equal to the location parameter $E(Y_i) \neq \mu$, the more asymmetric the distribution, the further the location parameter moves from the expectation. Taking as an example a regression with SN3 errors (see section 2.5), such that $e_i \sim SN3(0, \sigma^2, \lambda)$, in this way we would have the distribution of $Y_i \sim SN3(\eta(x_i, \theta), \sigma^2, \lambda)$, however it is verified that the distribution of each Y_i is not centered in $\eta(x_i, \theta)$ since $E(Y_i) = \eta(x_i, \theta) + \sigma\sqrt{\frac{2}{\pi}}\frac{\lambda^2-1}{\lambda}$, the higher λ, the greater the distance between $E(Y_i)$ and $\eta(x_i, \theta)$, in the absence of asymmetry ($\lambda = 1$) the distortion is canceled.

To correct this distortion let's do $E(Y_i) = \eta(x_i, \theta)$, then $\mu + \sigma\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}} = \eta(x_i, \theta)$, the new value of μ will be:

$$\mu = \eta(x_i, \theta) - \sigma \frac{\lambda^2 - 1}{\lambda} \sqrt{\frac{2}{\pi}} \leftrightarrow e_i \sim SN3\left(-\sigma \frac{\lambda^2 - 1}{\lambda} \sqrt{\frac{2}{\pi}}, \sigma^2, \lambda\right)$$

As can be seen in Figure 3, now using the SN1 case (see section 2.3), the greater the asymmetry, the further the location parameter moves from the center of mass of the distribution, so μ is located in the tails, and when the SN1 distribution undergoes correction then $E(Y) = \mu$, and μ is located in the center of mass of the distribution.

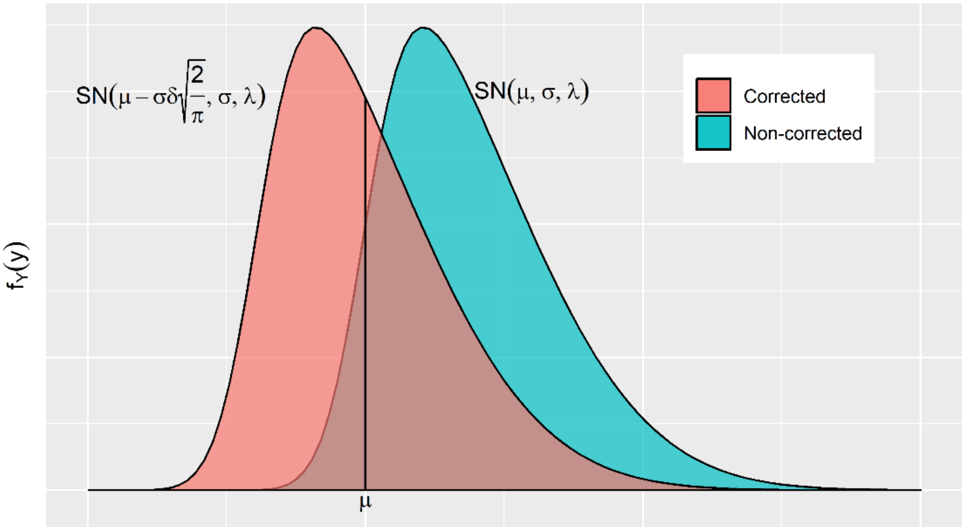

Figure 3. Plot of SN1 densities showing the relative displacement of the location parameter when using the two cases $SN1(\mu, \sigma^2, \lambda)$ – without correction and $SN1\left(\mu - \sigma\delta\sqrt{2/\pi}, \sigma^2, \lambda\right)$ – with correction.

Most skew distributions do not have mathematically tractable expressions for expectation. Due to these difficulties, only three Skew-Normal distributions were selected.

The other distributions underwent the same procedure, Cancho *et al.* (2008) also uses such corrections in their Bayesian implementation of SN2 using $e_i \sim SN2\left(-\lambda\sqrt{\frac{2}{\pi}}, \sigma^2, \lambda\right)$.

2.2 Poisson zero's trick

In Bayesian inference, the likelihood function represents the information coming from the data to be analyzed. The specification of an arbitrary likelihood function can be done indirectly by means of the Poisson zero trick, or the Bernoulli trick; both approaches have the same effect, but Ntzoufras (2008) recommends using the Poisson zero's trick. The Openbugs interface has the *dloglik()* function, which allows the use of likelihood functions that are not included in the package.

The *dloglik()* function implements the Poisson zero trick. The likelihood function of a pdf (probability density function) $f(x_i, \theta)$ can be rewritten:

$$\mathcal{L}(\theta|y) = \prod_{i=1}^{n} f(y_i, \theta)$$

$$\mathcal{L}(\theta|y) = \prod_{i=1}^{n} e^{\log f(y_i, \theta)}$$

$$\mathcal{L}(\theta|y) = \prod_{i=1}^{n} \frac{e^{-\left(-\log f\left(y_i,\theta\right)\right)}\left(-\log f\left(y_i,\theta\right)\right)^0}{0!}$$

$$\mathcal{L}(\theta|y) = \prod_{i=1}^{n} P(Y|y=0)\,; Y \sim \text{Pois}\left(\mu = -\log f\left(y_i,\theta\right)\right)$$

Considering $l_i = \log f\left(y_i, \theta\right)$, the quantity $e^{-(-l_i)}(-l_i)^0/0!$ is equivalent to the probability of $P(Y|y=0)$ such that $Y \sim Pois(\mu = -l_i)$, to ensure that $\mu > 0$, the likelihood function is multiplied by e^{-nK}, in this way, K must have a value such that $K > l_i$.

$$\mathcal{L}(\theta|y) = \prod_{i=1}^{n} \frac{e^{-(K-l_i)}(K-l_i)^0}{0!}$$

$$\mathcal{L}(\theta|y) = \prod_{i=1}^{n} P(Y|y=0)\,; Y \sim Pois(\mu = K - l_i)$$

the constants that l_i may have been removed because they are absorbed by K.

2.3 Azzalini's Skew-Normal Distribution (1985)

The skewed Normal distribution was introduced by Azzalini in 1985. The new probability distribution is obtained by the transformation $f(x) = 2g(x)G(\lambda x)$ where $g(.)$ and $G(.)$ are, respectively, the pdf function and the cdf (cumulative density function) of a symmetric random variable in R of X. With the introduction of a new skewness parameter λ, and with the location-scale transformation $Y = \mu + \sigma X$ where μ and σ are, respectively, the location and scale parameters, the Skew-Normal (SN) distribution is defined as in equation 5.

$$f_Y(y) = \frac{2}{\sigma}\phi\left(\frac{y-\mu}{\sigma}\right)\Phi\left(\lambda\frac{y-\mu}{\sigma}\right) \tag{5}$$

where $\phi(.)$ and $\Phi(.)$ are, respectively, the pdf and cdf of the Normal distribution.

In the case of the Normal distribution, the mean and standard deviation coincide with the location and scale parameters, in other asymmetric distributions, they are functions of these parameters. The asymmetry parameter (λ) denotes the orientation of the curve, values $\lambda > 0$ denote asymmetry to the right, $\lambda < 0$ asymmetry to the left, $\lambda = 0$ returns to the normal distribution which is symmetric as seen in Figure 4.

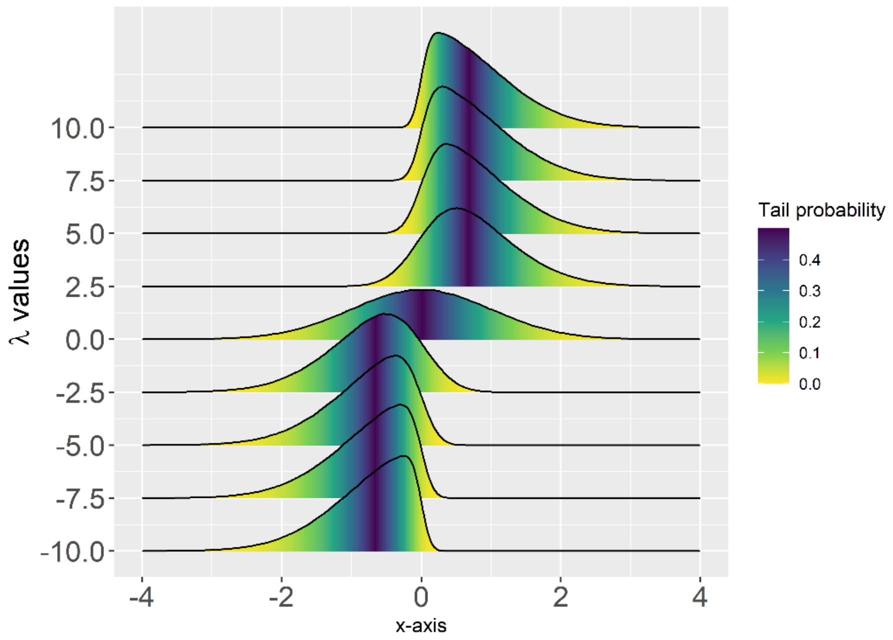

Figure 4. The Behavior of the Azzalini Skew-Normal Distribution by Varying the Skewness Parameter (λ values).

One way to generate random numbers from a Skew-Normal distribution by means of pseudo-realizations of a Normal is through the stochastic representation of Henze (1986). Given $X_0 \sim N(0,1)$ and $X_1 \sim N(\mu, \sigma^2)$ two independent Normal distributions, considering a parameter λ, then the variable Z:

$$Z = \frac{\lambda}{\sqrt{1+\lambda^2}}|X_0| + \frac{1}{\sqrt{1+\lambda^2}}X_1 \quad (6)$$

converges in distribution to $SN1(\mu, \sigma^2, \lambda)$, which denotes in this work the Skew-Normal distribution of Azzalini, based on the stochastic representation, the graphs of the SN1 distribution are constructed - which can also be constructed by the *sn (version 2.2.1)* package - which can be visualized in Figure 4.

The Expectation and Variance of a random variable $Y \sim SN1(\mu, \sigma, \lambda)$ are given by equations (7) and (8) respectively.

$$E(Y) = \mu + \sigma\delta\sqrt{\frac{2}{\pi}} \quad (7)$$

$$V(Y) = \sigma^2\left(1 - \frac{2\delta^2}{\pi}\right) \quad (8)$$

where $\delta = \frac{\lambda}{\sqrt{1+\lambda^2}}$.

In obtaining the likelihood function, a series of steps are followed:

First step: μ is defined according to the procedures in section 2.1 $\mu = \eta(x_i, \theta) - \sigma\delta\sqrt{\frac{2}{\pi}}$

$$f_Y(y) = \frac{2}{\sigma}\phi\left(\frac{y_i - \eta(x_i,\theta) + \sigma\delta\sqrt{\frac{2}{\pi}}}{\sigma}\right)\Phi\left(\lambda\frac{y_i - \eta(x_i,\theta) + \sigma\delta\sqrt{\frac{2}{\pi}}}{\sigma}\right)$$

Second step: Obtain l_i according to the procedures in section 2.2

$$l_i = \log 2 - \log \sigma^2 - 0.5 \log 2\pi - 0.5\left(\frac{y_i - \eta(x_i,\theta)}{\sigma} + \delta\sqrt{\frac{2}{\pi}}\right)^2 + \log \Phi\left(\lambda\left(\frac{y_i - \eta(x_i,\theta)}{\sigma} + \delta\sqrt{\frac{2}{\pi}}\right)\right)$$

Third step: Remove the constants and replace σ^2 with the precision parameter τ such that $\tau = 1/\sigma^2$

$$l_i = \log\tau - 0.5\left(\left(y_i - \eta(x_i,\theta)\right)\sqrt{\tau} + \delta\sqrt{\frac{2}{\pi}}\right)^2 + \log\Phi\left(\lambda\left(\left(y_i - \eta(x_i,\theta)\right)\sqrt{\tau} + \delta\sqrt{\frac{2}{\pi}}\right)\right) \quad (9)$$

2.4 Skew-Normal Distribution of Sahu *et al.* (2003)

In the work of Sahu *et al.* (2003), the authors derive new distributions by adding an Asymmetry parameter to the distributions that belong to the Elliptic class. The new multivariate Skew-Elliptical class is obtained through the conditioned argument method, based on the different density generators $g^{(k)}$, obtaining the Skew-Normal and Skew-t distributions of Sahu. The authors propose these distributions in modeling the asymmetry of the experimental error, instead of using data transformation methodologies, and assert that their implementation is easier than those of Fernandez & Steel (1998). Some advantages of the Skew-Normal distribution of Sahu include the easy implementation of MCMC and invariance to residual autocorrelation (De la Cruz & Branco, 2009). Another advantage, in the context of Bayesian regression, is the obtaining of known posterior distributions.

The Skew-Normal distribution of Sahu *et al.* (2003) is given by:

$$f_Y(y) = 2\phi(\mu, \sigma^2 + \lambda^2)\Phi\left(\frac{\lambda}{\sigma} \times \frac{y-\mu}{\sqrt{\sigma^2+\lambda^2}}\right) \quad (10)$$

If Y is a random variable that follows the Skew-Normal distribution of Sahu *et al.* (2003), then $Y \sim SN2(\mu, \sigma^2, \lambda)$. In terms of skewness, as with SN1, the skewness parameter (λ) denotes the orientation of the curve, values $\lambda > 0$ denote right skewness, $\lambda < 0$ left skewness, $\lambda = 0$ null skewness and convergence to the Normal model. The behavior of SN2 can be visualized in Figure 5.

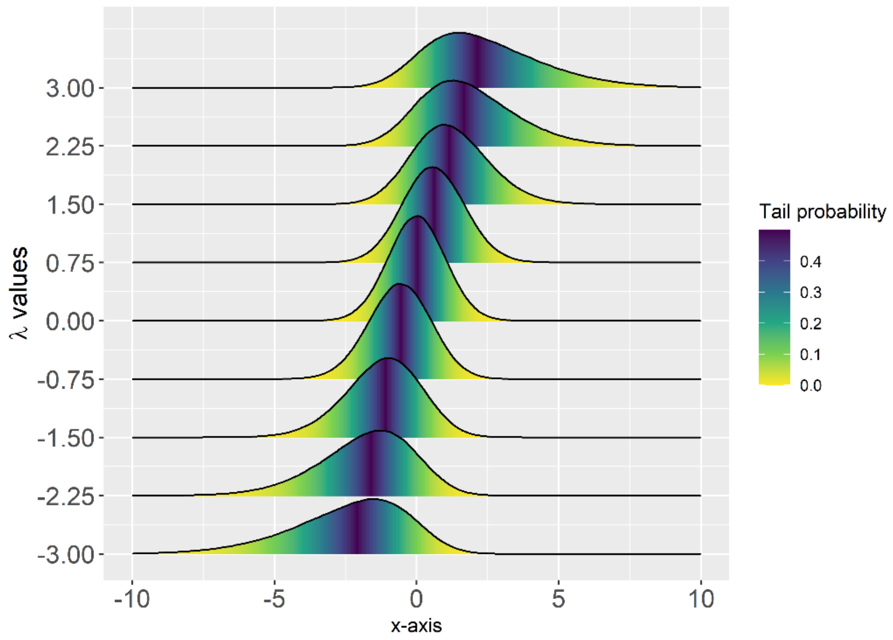

Figure 5. Behavior of the Sahu Skew-Normal Distribution by Varying the Skewness Parameter (λ values).

A stochastic representation of the Sahu Skew-Normal distribution is, similar to the Azzalini distribution:

$$Z \overset{d}{\rightarrow} \lambda|X_0| + X_1 \tag{11}$$

where $X_0 \sim N(0,1)$ and $X_1 \sim N(\mu, \sigma^2)$ are independent, thus $Z \sim SN2(\mu, \sigma^2, \lambda)$. Based on this stochastic representation, it is possible to compute figures of the distribution in question to evaluate its behavior, as shown in Figure 5.

The Expectation and Variance of a random variable $Y \sim SN2(\mu, \sigma^2, \lambda)$ are given, respectively, by equations (12) and (13).

$$E(Y) = \mu + \sqrt{\frac{2}{\pi}}\lambda \tag{12}$$

$$V(Y) = \sigma + \left(1 - \frac{2}{\pi}\right)\lambda^2 \tag{13}$$

For implementation of the likelihood function:

First step: Define μ

$$\mu = \eta(x_i, \theta) - \lambda\sqrt{\frac{2}{\pi}}$$

$$f_Y(y) = 2\phi\left(\eta(x_i, \theta) - \lambda\sqrt{\frac{2}{\pi}}, \sigma^2 + \lambda^2\right)\Phi\left(\frac{\lambda}{\sigma} \times \frac{y - \eta(x_i, \theta) + \lambda\sqrt{\frac{2}{\pi}}}{\sqrt{\sigma^2 + \lambda^2}}\right)$$

Second step: Get l_i

$$\mathrm{l}_i = \log 2 - 0.5\log(\sigma^2+\lambda^2) - 0.5\log 2\pi - 0.5\left(\frac{y-\eta(x_i,\theta)+\lambda\sqrt{\frac{2}{\pi}}}{\sqrt{\sigma^2+\lambda^2}}\right)^2 + \log\Phi\left(\frac{\lambda}{\sigma}\times\frac{y-\eta(x_i,\theta)+\lambda\sqrt{\frac{2}{\pi}}}{\sqrt{\sigma^2+\lambda^2}}\right)$$

Third step: Remove the constants and make $\tau = 1/\sigma^2$

$$\mathrm{l}_i = -0.5\log(\tau^{-1}+\lambda^2) - 0.5\left(\frac{y-\eta(x_i,\theta)+\lambda\sqrt{\frac{2}{\pi}}}{\sqrt{\tau^{-1}+\lambda^2}}\right)^2 + \log\Phi\left(\sqrt{\tau}\lambda\frac{y-\eta(x_i,\theta)+\lambda\sqrt{\frac{2}{\pi}}}{\sqrt{\tau^{-1}+\lambda^2}}\right) \quad (14)$$

2.5 Fernández & Steel (1998) Skew-Normal Distribution

One way to obtain asymmetric probability distributions is through the Fernandéz & Steel methodology. In the work of Fernandes & Steel (1998) the authors proposed, as an application of the methodology, an asymmetric version of the student's t distribution for the residual in a Bayesian implementation of a linear regression. The methodology consists of introducing an asymmetry parameter to any symmetric and unimodal continuous distribution, the transformation is given by:

$$f_X(x) = \frac{2}{\lambda+\lambda^{-1}}\left\{g\left(\frac{x}{\lambda}\right)I_{[0,+\infty)} + g(x\lambda)I_{(-\infty,0)}\right\} \quad (15)$$

where λ is the skewness parameter and $g(.)$ is the density of a symmetric distribution such that $g(x) = -g(-x)$.

In the work of Castillo *et al.* (2011) the authors applied equation (15) to the Normal distribution and then applied a location-scale transformation obtaining the density:

$$f_Y(y) = \frac{2\lambda}{\sigma(1+\lambda^2)}\left\{\phi\left(\lambda\frac{y-\mu}{\sigma}\right)I_{(y<\mu)} + \phi\left(\frac{y-\mu}{\lambda\sigma}\right)I_{(y\geq\mu)}\right\} \quad (16)$$

such as $Y \sim SN3(\mu,\sigma^2,\lambda)$ which represents the density of the Fernández & Steel Skew-Normal distribution. In terms of the asymmetry of this distribution, the asymmetry parameter (λ) denotes the orientation of the curve, values $\lambda > 1$ denote asymmetry to the right, $0 < \lambda < 1$ asymmetry to the left, $\lambda = 1$ null asymmetry (convergence to the Normal distribution), this behavior can be verified in Figure 6 which was generated using the *Skewt (v. 1.0)* package.

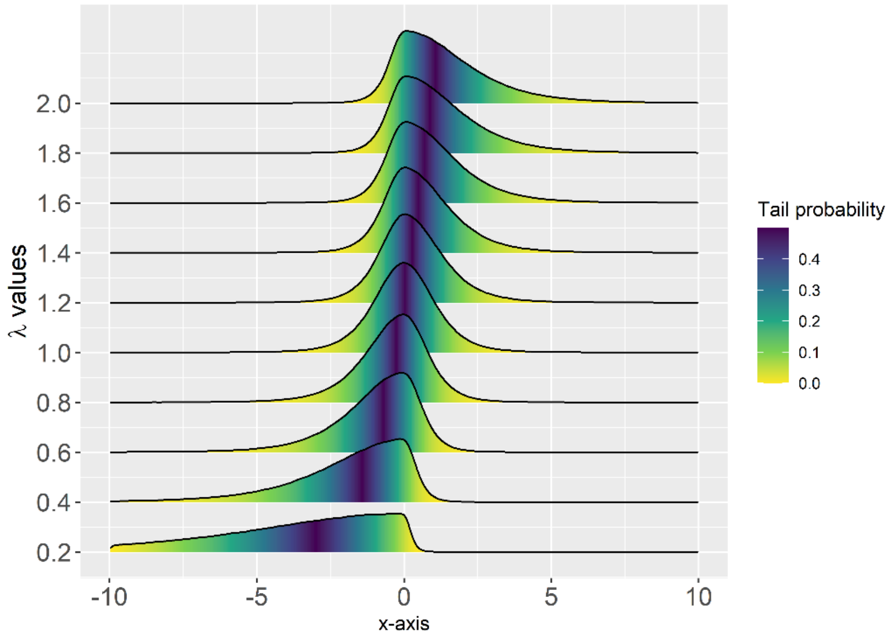

Figure 6. Behavior of the Fernandez & Steel Skew-Normal Distribution by Varying the Skewness Parameter (λ values).

One of the inferential advantages of SN3 consists in the non-singularity of Fisher's expected information matrix for $\lambda = 1$ (SN1 is singular when $\lambda = 0$), which facilitates asymptotic inference (Castillo *et al*, 2011). Another advantage of SN3 consists in not using the cumulant distribution $F(x)$, which does not have analytical expressions for Normal and Student's t (Eloy *et al*, 2019). Castillo *et al.* (2011) demonstrate some properties of SN3 considering the r-th sample moment of Y, in which we obtain the Expectation and Variance of SN3 expressed by equations (17) and (18).

$$E(Y) = \mu + \sigma\sqrt{\frac{2}{\pi}}\frac{\lambda^2 - 1}{\lambda} \tag{17}$$

$$V(Y) = \sigma^2 \frac{(\pi - 2)\lambda^6 + 2\lambda^2(\lambda^2 + 1) + \pi - 2}{\pi\lambda^2(1 + \lambda^2)} \tag{18}$$

In the implementation of the likelihood function:

First step: Define μ

$$\mu = \eta(x_i, \theta) - \sigma\frac{\lambda^2 - 1}{\lambda}\sqrt{\frac{2}{\pi}}$$

$$f_Y(y) = \frac{2\lambda}{\sigma(1+\lambda^2)}\left\{\phi\left(\frac{y-\eta(x_i,\theta)+\sigma\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}}{\lambda\sigma}\right)I_{(y\geq\mu*)} + \phi\left(\lambda\frac{y-\eta(x_i,\theta)+\sigma\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}}{\sigma}\right)I_{(y<\mu*)}\right\}$$

where, $\mu *= \eta(x_i,\theta) - \sigma\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}$

Second step: Rewrite $f_Y(y)$ as a function of the Heavside function $H(x)$ which in OpenBugs is represented by the Step function.

$$f_Y(y) = \frac{2\lambda}{\sigma(1+\lambda^2)}\phi\left(\lambda^{1-2H\left(\frac{y_i-\eta(x_i,\theta)}{\sigma}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)}\frac{y_i-\eta(x_i,\theta)}{\sigma}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)$$

where,

$$H\left(\frac{y_i-\eta(x_i,\theta)}{\sigma}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right) := \begin{cases} 1, & y_i \geq \eta(x_i,\theta)-\sigma\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}} \\ 0, & y_i < \eta(x_i,\theta)-\sigma\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}} \end{cases}$$

Third step: Get l_i

$$\mathrm{l}_i = \log 2 + \log\lambda - \log\sigma - \log(1+\lambda^2) - 0.5\log 2\pi - \log\lambda^{2H\left(\frac{y_i-\eta(x_i,\theta)}{\sigma}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)-1} - \log\sigma - 0.5\left(\lambda^{1-2H\left(\frac{y_i-\eta(x_i,\theta)}{\sigma}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)}\frac{y_i-\eta(x_i,\theta)}{\sigma}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)^2$$

Fourth step: Remove the constants and make $\tau = 1/\sigma^2$

$$\mathrm{l}_i = \log\lambda + \log\tau - \log(1+\lambda^2) - \log\lambda^{2H\left(\left(y_i-\eta(x_i,\theta)\right)\sqrt{\tau}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)-1} - 0.5\left(\lambda^{1-2H\left(\left(y_i-\eta(x_i,\theta)\right)\sqrt{\tau}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)}\left(y_i-\eta(x_i,\theta)\right)\sqrt{\tau}+\frac{\lambda^2-1}{\lambda}\sqrt{\frac{2}{\pi}}\right)^2 \quad (19)$$

2.6 Implementation of empirical priors

A priori is usually determined before accessing the data because it represents the researcher's prior knowledge or accumulated scientific knowledge about a given parameter. The artifice of determining a priori from the data set to be analyzed is called the empirical Bayesian approach, however, it is still an approximation to the classical Bayesian approach (Carlin & Louis, 2008).

One way to determine frequentist estimates for all 8 (see Figure 1) accessions with 3 different growth models is through nonlinear mixed models, in which it is possible to obtain estimates of the fixed and random effects in a single algorithm. Obtaining individual Gauss-Newton estimates for each combination is too laborious, and initial estimates for each case must be obtained. Since this is not the objective of this work, more details can be found in the work of Teixeira *et al.* (2023).

The violin plot and boxplot of residuals in Figure 7 corroborate Pino's (2014) thesis that, despite the primacy of the Normal distribution in several statistical procedures, one cannot assume normality as the standard in practice. It is possible to notice outliers (distributions with heavy tails), asymmetry (asymmetric distributions), or both (asymmetric distributions with heavy tails); however, the focus of this work is on asymmetric normal distributions.

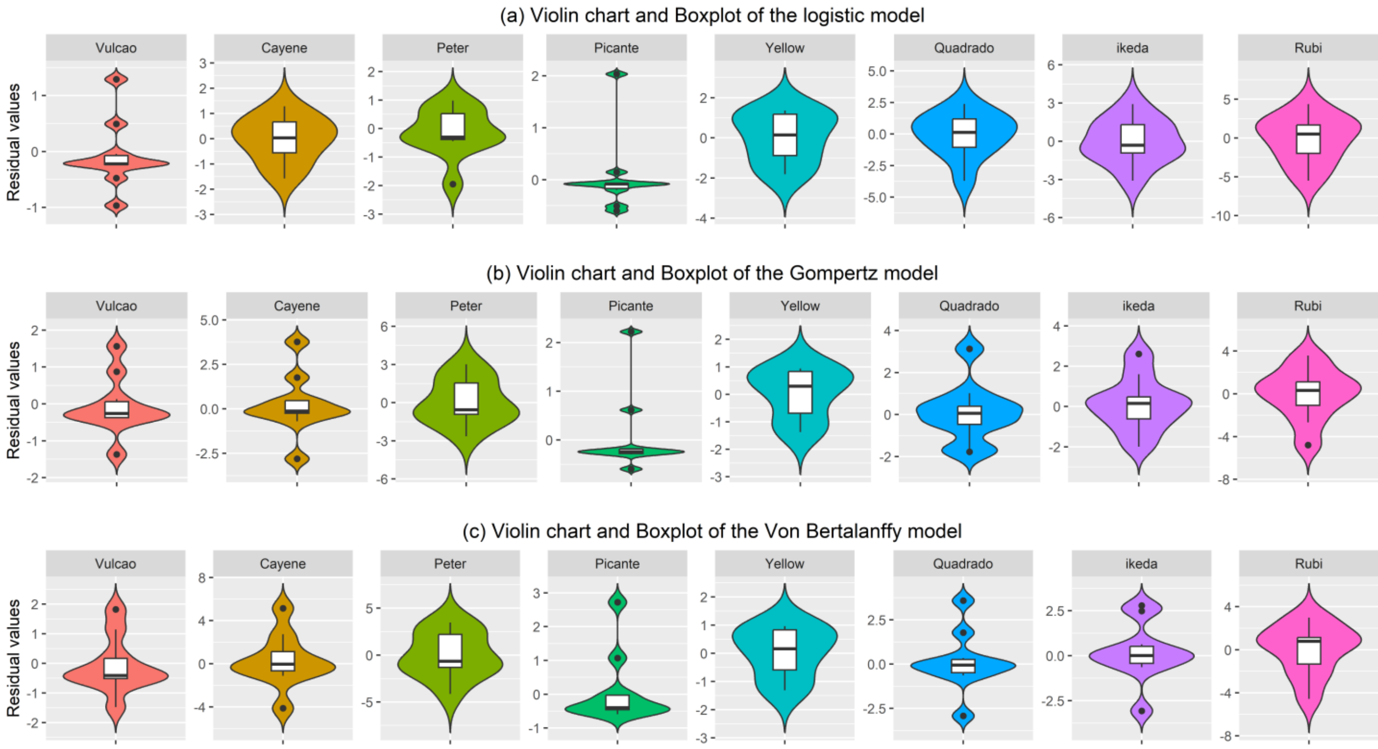

Figure 7. Violin plot together with the Boxplot of the residuals, after adjusting the Logistic, Gompertz and Von Bertalanffy models under the Gaussian error (N) to all accessions represented by Figure 1.

The second step consists of plotting the densities of the histograms of each parameter $(\alpha, \beta, \gamma, \sigma^2)$ of the Logistic, Gompertz and Von Bertallanfy models adjusted to all accessions (see Figure 8). The information of the mean and variance measures (hyperparameters) is incorporated into the Normal distribution, which will be used as prior for (α, β, γ), and for σ^2 the information is incorporated into the gamma distribution.

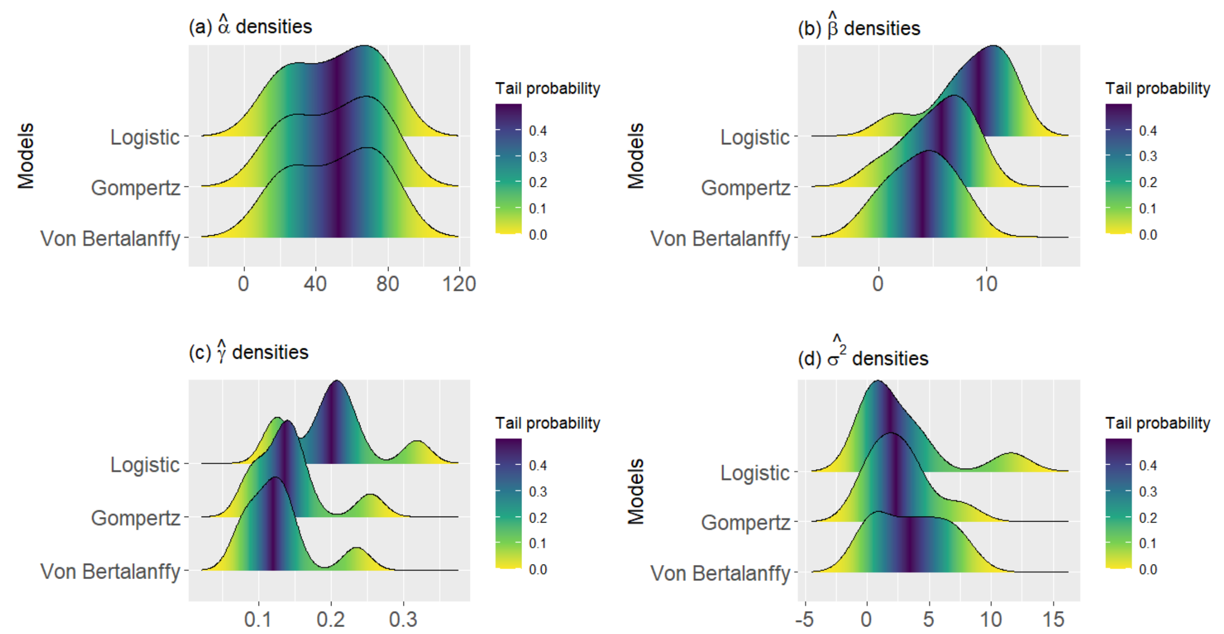

Figure 8. Histogram densities of the estimates of the parameters $(\alpha, \beta, \gamma, \sigma^2)$ of the Logistic, Gompertz and Von Bertallanfy models under the Gaussian error (N) via nonlinear mixed models fitted to all accessions represented in Figure1.

2.7 Bayesian Framework

Considering Bayes' Theorem in which the joint posterior distribution is proportional to the joint distribution of the sample (Likelihood Function) times the joint distribution of the prior distributions with their respective hyperparameters. Considering the Logistic, Gompertz and Von Bertallanfy model.

The posterior distribution considering the different errors is given by: (Perez & Rodriguez, 2018).

$$p(\alpha,\beta,\gamma,\sigma^2,\lambda) \propto \left\{\prod_{i=1}^{n} P(Y|y=0,\lambda=K-l_i)\right\} \times N(\mu_\alpha,\sigma_\alpha^2) \times N\left(\mu_\beta,\sigma_\beta^2\right)$$
$$\times N\left(\mu_\gamma,\sigma_\gamma^2\right) \times IG\left(a_{\sigma^2},b_{\sigma^2}\right) \times N\left(\mu_\lambda,\sigma_\lambda^2\right)$$

Where the hyperparameters are obtained by the results represented in Figure 8, and the l_i's are given by (9), (14) and (19). Except for the SN3 Distribution, which instead of using $\lambda \sim N(\mu_\lambda, \sigma_\lambda^2)$, a Truncated Normal prior $\lambda \sim N(\mu_\lambda, \sigma_\lambda^2)T(0,+\infty)$ is used because of the restrictions of the parameter space.

Based on the results represented in Figure 8 and using $\tau = 1/\sigma^2$ we have the empirical priors:

For the Logistic model:	For the Gompertz model:	For the Von Bertalanffy model:
$\alpha \sim N(49.86, 1.76 \times 10^{-3})$	$\alpha \sim N(50.43, 1.71 \times 10^{-3})$	$\alpha \sim N(50.67, 1.69 \times 10^{-3})$
$\beta \sim N(8.63, 7.74 \times 10^{-2})$	$\beta \sim N(5.42, 0.10)$	$\beta \sim N(3.90, 0.11)$
$\gamma \sim N(0.20, 259.90)$	$\gamma \sim N(0.14, 379.78)$	$\gamma \sim N(0.12, 411.56)$
$\tau \sim IG(2.54, 4.41)$	$\tau \sim IG(3.18, 5.75)$	$\tau \sim IG(3.45, 8.63)$
$\lambda \sim N(0, 10^{-3})$	$\lambda \sim N(0, 10^{-3})$	$\lambda \sim N(0, 10^{-3})$

The Metropolis-Hastings algorithms implemented by the OpenBugs program were used to obtain the MCMC chains for each parameter.

The standardized procedure for implementing all models in the BrgusFit function of the Brugs package was the number of iterations (nIter) 2×10^6, the number of burns (nBurnin) 1% of nIter, and the number of jumps (nThin) of the order of 100. A pilot analysis was performed beforehand to verify the behavior of the results.

3 Results and Discussion

After the procedures adopted in section 2.7, Table 1 shows the results of the a posteriori mean of the MCMC chains of the parameters of interest $(\alpha, \beta, \gamma, \sigma^2, \lambda)$ adjusted to Access 7 (Ikeda bell pepper).

Table 1. Posterior mean of the parameters $(\alpha, \beta, \gamma, \sigma^2, \lambda)$ of the Logistic, Gompertz and Von Bertallanfy models Considering the experimental errors N, SN1, SN2 and SN3, with their respective DIC's

Modelos	Erro	α	β	γ	σ^2	λ	DIC
Logístico	Normal	74,67	9,98	0,18	3,41	0	45,43
Gompertz		75,68	6,56	0,12	2,32	0	40,26
Von Bert.		76,19	4,73	0,1	3,41	0	44,59
Logístico	Azzalini's Skew-Normal	74,77	10,04	0,18	2,52	-2,06	42,16
Gompertz		75,74	6,71	0,12	1,84	7,99	9,8
Von Bert.		75,84	4,44	0,11	2,8	-11,94	20,5
Logístico	Sahu's Skew-Normal	74,65	9,97	0,18	2,32	-0,01	42,79
Gompertz		75,62	6,56	0,12	2	-0,06	39,59
Von Bert.		76,02	4,71	0,11	2,82	-0,34	43,55
Logístico	Fernandez & Steel Skew-Normal	74,94	10,13	0,18	1,74	1,18	48,01
Gompertz		76,13	6,77	0,12	1,21	1,36	35,83
Von Bert.		75,86	4,63	0,11	1,76	0,96	38,78

For the parameter α that represents the asymptotic weight, there is some variation in its values, as can be seen graphically in Figure 9, however there is no clear trend if the experimental errors of N, SN1, SN2 and SN3 influence the values of α. The same can be seen in the works of Mangueira *et al.* (2016) and Faccin & Rossi (2024).

When dealing with the β parameter, the Logistic, Gompertz and Von-Bertalanffy models have different estimates for the inflection point. The Logistic model estimated that Accession 7 has its maximum growth speed around 10 days after flowering (9.98, 10.04, 9.97, and 10.03), while the Gompertz model estimated between 6 and 7 days (6.56, 6.71, 6.56, and 6.67), and the Von Bertalanffy model estimates between 4 and 5 days (4.73, 4.44, 4.71, and 4.63). In this parameter, the different experimental errors of N, SN1, SN2 and SN3 were not able to interfere in the results, as can be seen graphically in Figure 9.

When dealing with the γ parameter, the Gompertz, Logistic and Von Bertalanffy models also presented clear differences in the growth rate of Accession 7. The Logistic model estimated the growth rate at be rorund 0.18, the Gompertz model estimated it around 0.12, and the Von Bertalanffy model estimated it around 0.10. In this parameter, the different likelihood functions of N, SN1, SN2, and SN3 were also not able to influence its behavior, as can be seen graphically with the help of Figure 9. In the work of Mangueira *et al.* (2016) the different experimental errors Normal, Skew-Normal and Skew-t also did not change the values of γ in the frequentist estimation of the Logistic model.

Regarding the parameter σ^2 which is the multiplicative inverse of the precision parameter, the Logistic, Gompertz and Von Bertalanffy models presented substantial differences. With the help of Figure 9 we can see that the Von-Bertalanffy model presented the highest σ^2, followed by the Logistic model, and with the Gompertz model presenting the lowest values of σ^2, or the highest precision. It can also be seen that the different likelihood functions of N, SN1, SN2, and SN3 were b to change the results of σ^2, all the asymmetric versions presented reductions in relation to the Normal, and clearly from Figure 9, the experimental error SN3 obtained primacy with the lowest values. When analyzing the work of Faccin & Rossi (2024), the Bayesian nonlinear regression of the Gompertz model with Skew-Normal and Skew-t errors showed a reduction in σ in relation to the Normal and t submodels.

Regarding the DIC values to verify the quality of the adjustment of each combination according to Table 1:

1) There were significant reductions (difference greater than 5) in the DICs of the Gompertz (9.8) and Von Bertalanffy (20.5) models with the SN1 error in relation to the N error (40.26 and 40.29), the difference was not so great for the Logistic model;

2) There were small reductions in the DIC of the Gompertz (42.79), Logistic (39.59), and Von Bertalanffy (43.55) models with SN2 error with the N error (45.43, 40.26, and 44.59), however nothing greater than 5 as recommended by FIRAT (2017). The asymmetry parameter of these models also presented values close to 0 (-0.01, -0.06, and -0.34);

3) There were significant reductions in DIC for the Gompertz (35.83) and Von Bertalanffy (38.78) models with SN3 error in relation to the N error (40.26 and 44.59); however, for the Logistic model, the quality of fit with the N error (45.43) was superior to the SN3 error (48.01). When consulting the work of Faccin & Rossi (2024), it was also found that the Bayesian fit with Normal and t errors with heteroscedastic errors showed lower DICs than with the Skew-Normal and Skew-t errors.

When analyzing the issue of the asymmetry parameter λ:

1) The SN1 error showed evidence of asymmetry in the three growth models, with the Logistic (-2.06) and Von-Bertalanffy (-11.94) models showing asymmetry to the left, while the Gompertz (7.99) model showed asymmetry to the right. Graphically, Figure 9 shows the discrepancy between the asymmetry parameters of SN1, SN2, and SN3;

2) The SN2 error showed evidence of the absence of asymmetry in the Logistic (-0.01), Gompertz (-0.06) and Von-Bertalanffy (-0.34) growth models;

3) The SN3 error showed evidence of asymmetry to the right (see Figure 9) in all growth models. It was then found that the different experimental errors SN1, SN2, and SN3 affect the orientation of the asymmetry. While the Logistic model has asymmetry to the left with error SN1, the same model has asymmetry to the right with error SN3.

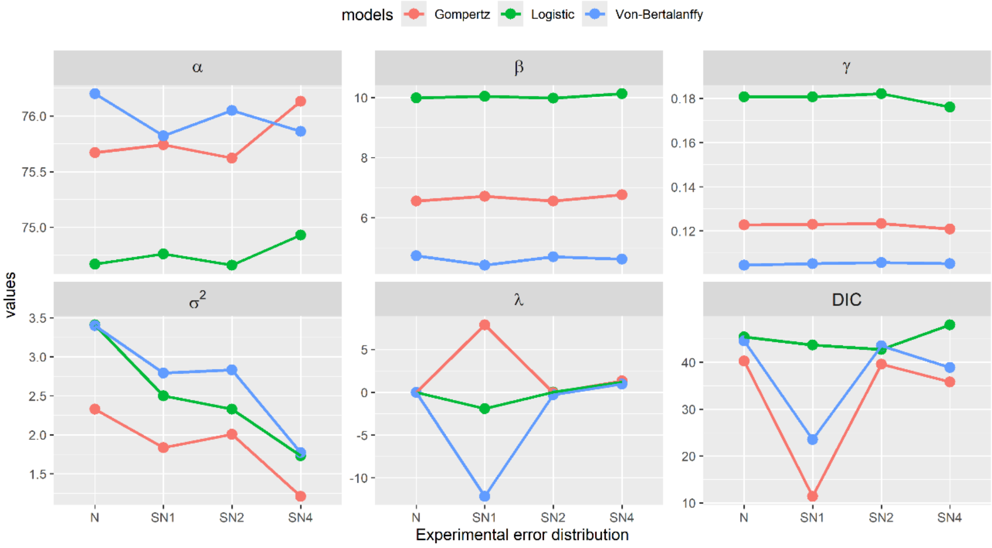

Figure 9. Posterior mean of the parameters $(\alpha, \beta, \gamma, \sigma^2, \lambda)$ of the Logistic, Gompertz and Von Bertallanfy models considering the error distributions N, SN1, SN2 and SN3.

The graph in Figure 10 of the densities of the posterior distributions is helpful to provide informative priors for future studies and to serve as a reference for other works. In item (d) the densities of σ^2 that presented less flattened curves are from the SN3 error. In item (e) which deals with the densities of λ, it can be seen that the lowest precision occurred in the SN2 error with bimodality tendencies; no studies were found that explain this behavior; the less flattened curves are due to the SN3 error, and the SN1 errors, despite appearing to have a bell tendency around 0, the heavy tails affected the estimate of the mean.

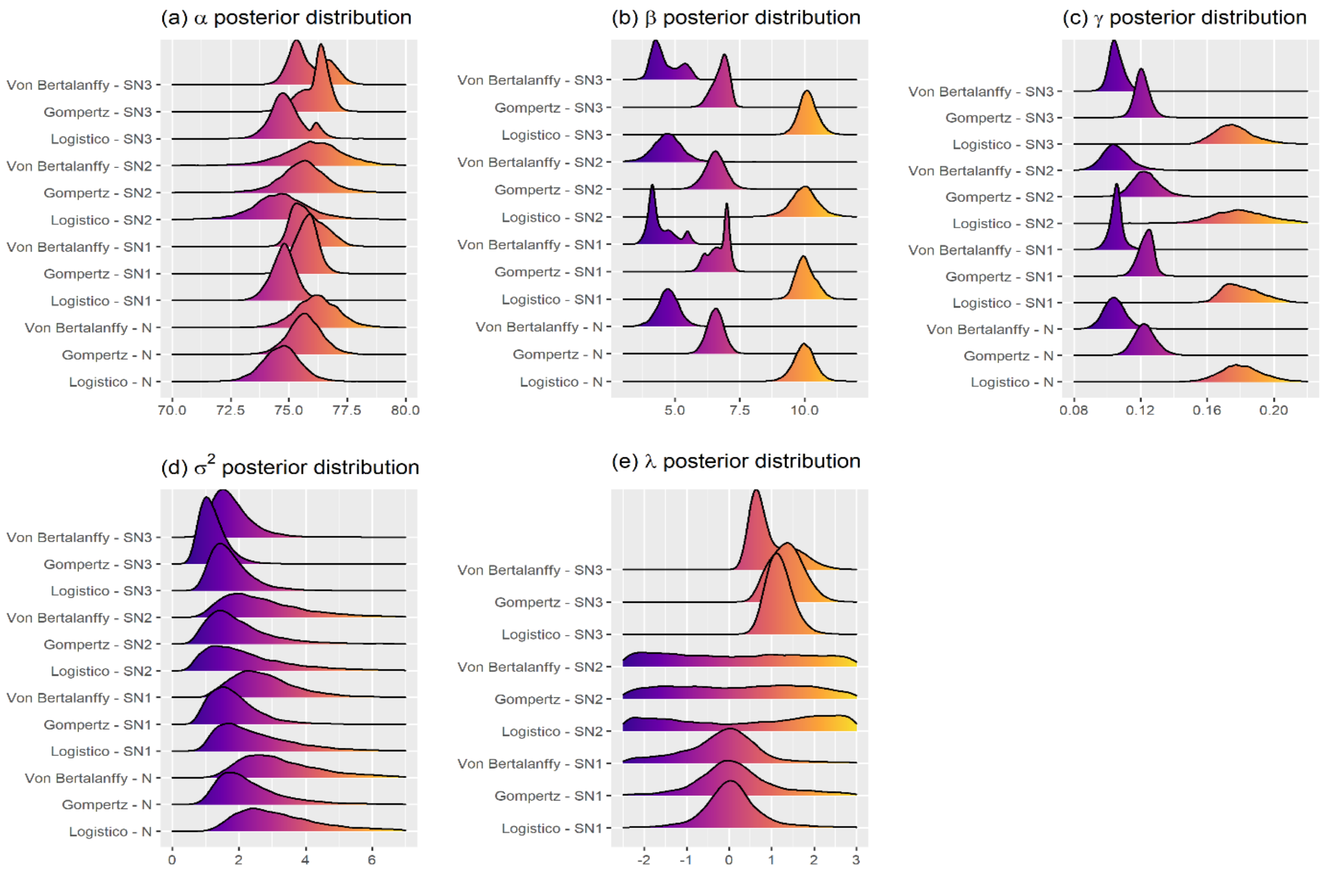

Figure 10. Densities of the posterior distributions of the parameters $(\alpha, \beta, \gamma, \sigma^2, \lambda)$ of the Logistic, Gompertz and Von Bertallanfy models considering the error distributions N, SN1, SN2 and SN3.

When conducting a pilot analysis to verify the models' behavior, all growth models converged when the experimental error N was used, and all passed the Heidelberg-Welch and Geweke criteria using the *coda (v. 0.19-4.1)* package.

When it comes to the Skew-normal error, the parameters $(\alpha, \beta, \gamma, \sigma^2)$ required 100,000 nIter (number of iterations) to achieve convergence of the MCMC chains, values close to those also used by Guedes *et al.* (2014). λ is the only parameter that proved to be problematic, requiring millions of nIter – values also obtained by Rossi & Santos (2014) – to pass the half-width test that makes up the Heidelberg-Welch test. Pereira *et al.* (2020) explain that the author uses the Modified weighted importance resampling methodology as an alternative to Metropolis-Hastings MCMC to overcome the problem of high nIter. The strategy adopted in this work to reduce nIter consists of using estimates close to frequentists, a strategy also used by Rossi & Santos (2014). Figure 11 shows the reduction in nThin values when using or not using estimates from nonlinear Mixed Models as initial values.

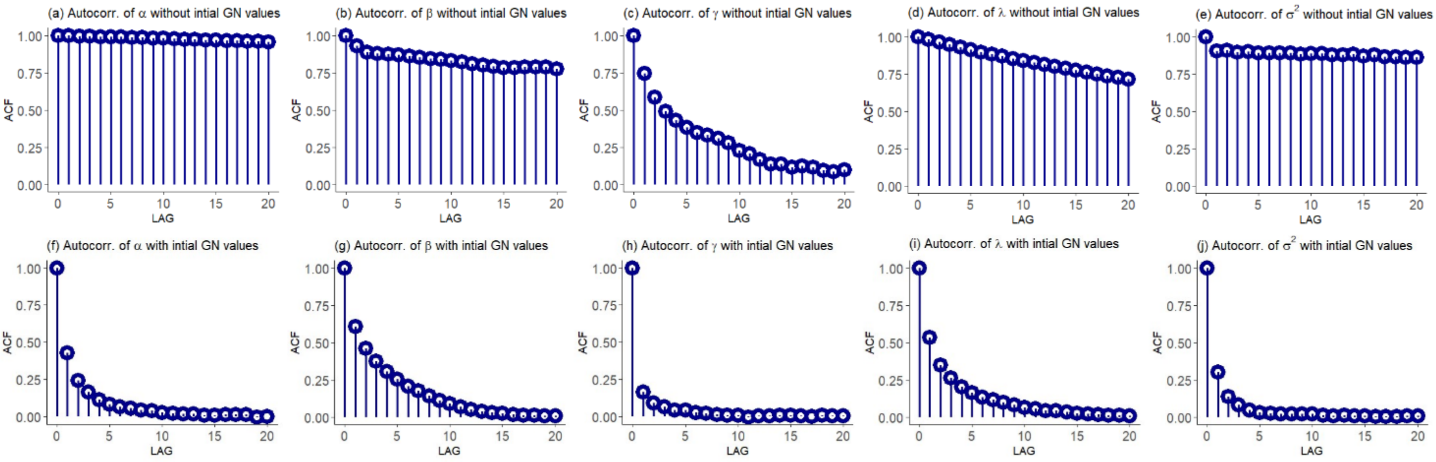

Figure 11. Autocorrelation of the MCMC chains of the parameters $\theta = (\alpha, \beta, \gamma, \sigma^2, \lambda)$ of the Logistic model with SN1 error when considering the initial values $\theta^o = (1,1,1,1,1)$ in comparison when considering the estimates obtained from Access 7 through the adjustment of nonlinear Mixed Models for θ^o.

The negative points to be highlighted in these implementations are due to the complexity of writing these distributions in the Bugs language, which is quite limited. This requires subterfuges such as the use of hierarchical models (Fassin & Rossi, 2024) or approximations of arbitrary likelihood functions. Another observation is the high computational cost for SN1, SN2, and SN3 in the range of millions of MCMC iterations, something that did not occur in the N submodel.

In general, the implementation of the Skew-Normal distributions of Azzalini (1985) and Skew-Normal of Fernandez & Steel (1998) in the experimental error of the Gompertz and Von Bertalanffy growth models proved relevant. They presented a significant gain in the adjustment quality and precision of the models with the Normal submodel. In all scenarios, the Gompertz model proved to be more suitable.

4 Conclusion

Among the distributions implemented, the best-fit quality comes from the Skew-Normal error of Fernandez & Steel and Azzalini with the Gompertz and Von Bertalanffy models.

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Conflicts of Interest

The authors declare no conflict of interest.

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