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Parameterization effects in nonlinear models to describe growth curves

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ABSTRACT. Various parameterizations of nonlinear models are common in the literature.In addition to complicating the understanding of these models, these parameterizations affect the nonlinearity measures and subsequently the inferences about the parameters. Bates and Watts (1980) quantified model nonlinearity using the geometric concept of curvature. Here we aimed to evaluate the three most common parameterizations of the Logistic and Gompertz nonlinear models with a focus on their nonlinearity and how this might affect inferences, and to establish relations between the parameters under the various expressions of the models. All parameterizations were adjusted to the growth data from pequi fruit. The intrinsic and parametric curvature described by Bates and Watts were calculated for each parameter. The choice of parameterization affects the nonlinearity measures, thus influencing the reliability and inferences about the estimated parameters. The most used methodologies presented the highest distance from linearity, showing the importance of analyzing these measures in any growth curve study. We propose that the parameterization in which the estimate of B is the abscissa of the inflection point should be used because of the lower deviations from linearity and direct biological interpretation for all parameters.

Keywords: biological interpretation, Gompertz model, logistic model, measures of curvature, nonlinearity.

Efeito da parametrização em modelos não lineares na descrição de curvas de crescimento

RESUMO. Diferentes parametrizações de modelos não lineares são comuns na literatura, mas além de complicar seu entendimento, podem afetar as medidas de não linearidade e as inferências sobre os parâmetros. Bates and Watts (1980) quantificaram a não linearidade presente no modelo utilizando o conceito geométrico de curvatura. O objetivo deste trabalho foi avaliar as três parametrizações mais comuns dos modelos não lineares Logístico e Gompertz, quanto à sua não linearidade, as implicações nas inferências e estabelecer relações entre os parâmetros nas diferentes formas de expressar os modelos. Todas as parametrizações foram ajustadas a dados de crescimento do fruto de pequi do cerrado. Para cada parametrização foram calculadas as medidas de curvatura intrínseca e paramétrica descritas por Bates e Watts. A escolha da parametrização afeta as medidas de não linearidade, consequentemente, influencia na confiabilidade e nas inferências sobre os parâmetros estimados. As formas mais utilizadas na literatura apresentaram os maiores afastamentos da linearidade, evidenciando a importância de se analisar estas medidas em qualquer estudo sobre curva de crescimento. Devem ser utilizadas as parametrizações na qual a estimativa de B representa a abscissa do ponto de inflexão por apresentarem menores desvios de linearidade e interpretação biológica direta para todos os parâmetros.

Palavras-chave: interpretação biológica, modelo Gompertz, modelo logístico, medidas de curvatura, não linearidade.

Introduction

To study a growth curve is to track over time some features linked to the development, for example, weight, height, length, diameter, among others. This type of curve generally has a sigmoid al appearance (S-shaped) well adjusted by nonlinear regression. Besides, the parameters of this class of models have direct practical interpretation. Thus, nonlinear models are widely used in growth studies of different species (CARNEIRO et al., 2014; FERNANDES et al., 2014).

Among the various nonlinear models in the literature, the most used are Logistic and Gompertz. Many authors have used different parameterizations of these models to describe animal, vegetable and fruit growth curves (GBANGBOCHE et al., 2008; TERRA et al., 2010; UEDA et al., 2010; GAZOLA et al., 2011; SILVA et al., 2011; MAZUCHELI et al., 2011; TEIXEIRA et al., 2012; OLIVEIRA et al., 2013; PRADO et al., 2013; AMANCIO et al., 2014; ANDRADE et al., 2014; PEREIRA et al., 2014; SOUSA et al., 2014).

The use of reparameterization is common in nonlinear regression models so that the parameters are rearranged to have convenient interpretations to the study area in question. However, some reparameterization confuses authors and students, making the use of linear regression more complicated than it really is. According to Cordeiro et al. (2009), usually the model is not expressed in a suitable parametric form, which would facilitate rapid convergence of the iterative process used to obtain the parameters estimates, being necessary to seek a more appropriate parameterization.

The statistical properties of nonlinear models, parameter estimation and the validity of asymptotic inferences are functions of the linear approximation of these models, which is affected mainly by the parameter considered. Expressions used to assess the suitability of the linear approximation and its effects on inferences are known as nonlinearity measures. The greater the nonlinearity in the model the farther from linear is the approximation, making the inferences about the parameters less reliable (SEBER; WILD, 2003; CORDEIRO et al., 2009; TJORVE; TJORVE, 2010).

Bates and Watts (1980) quantified the nonlinearity present in the models, based on geometric concept of curvature, and showed that this nonlinearity can be decomposed into two components: intrinsicc^{ι}, which is the nonlinearity characteristic of the model, and parametricc^{θ}, which represents the effect of the nonlinearity parameter in the model. According to Souza et al. (2010), the intrinsic curvature measured does not vary according to a chosen parameter. However, the curvature parameter is sensitive to this change, so that a model reparameterization can significantly change the value of the parametric curve, thus affecting the reliability of the estimates.

Great values of the intrinsic curvature c^{ι} indicate the nonlinearity intensity of the response function and the high value for the parametric curve c^{θ} indicates that the parameterization of the model is responsible for higher distance from the linear form. A model can be preferred when it has lower values for these statistics, its nonlinearity is smaller and hence the linear approximation is better. Among the characteristics of a good linear approximation is the guarantee of unbiased estimators, normally distributed with minimal variance even in small samples (MAZUCHELI; ACHCAR, 2002; SEBER; WILD, 2003; ZEVIANI et al., 2012).

The aim of this work was to evaluate the three most common parameterizations of the Logistic and Gompertz nonlinear models with a focus on their nonlinearity and how this might affect inferences, and to establish relations between the parameters under the various expressions of the models.

Material and methods

The data used to illustrate the fit of nonlinear models were taken from Rodrigues et al. (2009) and correspond to 8 longitudinal values of pequi fruits mass growth (g), collected in Itumirim, southern Minas Gerais State, Brazil. The samples were collected every 15 days, from an thesis to abscission of the fruits.

Table 1 shows the three parameterizations of Logistic and Gompertz models most often found in the literature.

Table 1. Most used parameterization of Logistic and Gompertz models.

Logistic 1	$Y = \frac{A}{1 + e^{[k*(B-X)]}} + \varepsilon$	Gompertz 1	$Y = A * e^{-e^{[k*(B-X)]}} + \varepsilon$
Logistic 2	$Y = \frac{A}{1 + B * e^{-k*X}} + \varepsilon$	Gompertz 2	$Y = A * e^{-e^{(B-k*X)}} + \varepsilon$
Logistic 3	$Y = \frac{A}{1 + \left(\frac{1}{B} - 1\right) * e^{-k*X}} + \varepsilon$	Gompertz 3	$Y = A * e^{-B*e^{-k*X}} + \varepsilon$

In the models presented in Table 1, it follows that: Y is the dependent variable; X is the independent variable, usually related to time; A is the upper asymptote of the model or weight (size) maturity; B is associated with the abscissa of the inflection point; k is the precocity index of the species, i.e., the higher value of k the less time is required for the trait under study to reach its maximum A; ε is the random error of the model, which is assumed to be independent and identically normal distributed so that ε ~ N (0, Iσ^2).

Of the models presented, the most used are Logistic 2 and Gompertz 3. The main difference between the parameterizations, both for Logistic and Gompertz, occurs for the parameter B, commonly called scale parameter. Problems of interpretation generally appear for this parameter, so that some authors claim that this parameter has no biological interpretation. In fact, this 'lack' of interpretation is due to confusion caused by the parameterization adopted, creating the mistaken consensus that this is only a scale parameter without biological interpretation.

If using parameterization Logistic 1 or Gompertz 1 (Table 1), the B value has practical interpretation because it is the abscissa of the inflection point (point at which the growth changes from ascending to descending).That is, when $X = B$ the characteristic under study reaches the maximum of its growth and starts to 'grow less' to stabilize. According to Fernandes et al. (2014), the Logistic model is symmetric with respect to this point and, at the inflection point, 50 % of mature weight (A) is reached. For the Gompertz model at that point, about 37 % of A is reached.

Most parameterizations shown in Table 1 can be found in Seber and Wild (2003). Logistic 3 is specific to the epidemiology of plant diseases and was first proposed by Van Der Plank (1963) when studying the polycyclic diseases progress.

Table 2 shows the relations between the parameters for the three Gompertz model parameterizations studied. Note that in all of them, parameters A and k are the same, whereas the value of B undergoes great changes. For the Logistic model A and k values are also the same in the three parameterizations, varying only the parameter B which relations are shown in Table 3.

Table 2. Relation between the parameters in the three parameterizations studied for the Gompertz model.

	Gompertz 1	Gompertz 2	Gompertz 3
Gompertz 1		$A_2 = A_1$ $B_2 = k_1 * B_1$ $k_2 = k_1$	$A_3 = A_1$ $B_3 = e^{k_1 * B_1}$ $k_3 = k_1$
Gompertz 2	$A_1 = A_2$ $B_1 = \frac{B_2}{k_2}$ $k_1 = k_2$		$A_3 = A_2$ $B_3 = e^{B_2}$ $k_3 = k_2$
Gompertz 3	$A_1 = A_3$ $B_1 = \frac{\ln(B_3)}{k_3}$ $k_1 = k_3$	$A_2 = A_3$ $B_2 = \ln(B_3)$ $k_2 = k_3$	

Table 3. Relations between parameters B in the three parameterizations studied for the Logistic model.

	Logistic 1	Logistic 2	Logistic 3
Logistic 1		$B_2 = e^{k_1 * B_1}$	$B_3 = \frac{1}{e^{k_1 * B_1} + 1}$
Logistic 2	$B_1 = \frac{\ln(B_2)}{k_2}$		$B_3 = \frac{1}{B_2 + 1}$
Logistic 3	$B_1 = \frac{\ln(\frac{1}{B_3} - 1)}{k_3}$	$B_2 = \frac{1}{B_3} - 1$	

As noted by Tjorve and Tjorve (2010) and Ueda et al. (2010), expressions relating the parameters shown in Tables 2 and 3 show that these parameterizations are all forms of the same model, differing only in the interpretation of the parameter B. Knowing these relations, the model parameters can be estimate with the parameterization that most closely matches the linear behavior (CORDEIRO et al., 2009) and then the estimates for the parameterization that have the interpretation of interest can be calculated.

The parameters of both models were estimated for the description of the growth curves of pequi fruit in each of the three parameterizations studied (Table 1). Estimates of these parameters were obtained by iterative method of Gauss-Newton implemented in the *nls ()* function of the R software (R DEVELOPMENT CORE TEAM, 2015). The significance of the parameters ($\neq 0$) was verified by the t-test at 5%. Initially it was considered that all assumptions about errors (ε) are met. From the error vector of this setting the residuals analysis was made based on statistical tests. If any of the conditions is not met, the deviation must be corrected or incorporated into the parameter estimation process. Statistical tests of Shapiro-Wilk, Durbin-Watson and Breusch-Pagan were used to verify the normality, independence and residual homoscedasticity.

The nonlinearity measures described by Bates and Watts (1980) were obtained by *rms.curv ()* function of the R software. To evaluate the fit the following parameters were also calculated: adjusted determination coefficient $\left(R_a^2 = \frac{(n-1)(1-R^2)}{n-p}\right)$ and Akaike information criteria ($AIC = -2ln\,(like) + 2p$), wherein: R^2 is the determination coefficient; n is the sample size; p is the number of parameters and *like* is the maximum of the likelihood function. These evaluators were obtained using *Rsq.ad ( ),* of package *qpcR,* and *AIC ( )* functions of software R, respectively.

Results and discussion

Table 4 presents the parameter estimates and their standard errors for all three forms of Logistic and Gompertz models in adjusting to growth data from pequi fruit. As already mentioned and shown in Tables 2 and 3, the estimates of parameters A and k were identical in parameterization of the same model, but estimates of B vary widely. All parameters were significant by t-test and residual analysis found that all assumptions about the error vector have been met, considering a nominal significance level of 5%.

Table 4. Estimates with their standard error (SE) for the parameters of the three forms of Logistic and Gompertz models in the description of pequi fruits growth.

	A	SE	B	SE	k	SE
Logistic 1	107.7960	(1.5821)	51.4186	(0.8066)	0.1047	(0.0075)
Logistic 2	107.7960	(1.5821)	218.3489	(81.8104)	0.1047	(0.0075)
Logistic 3	107.7960	(1.5821)	0.0045	(0.0017)	0.1047	(0.0075)
Gompertz 1	110.1785	(1.3365)	45.2989	(0.5385)	0.0687	(0.0037)
Gompertz 2	110.1785	(1.3365)	3.1148	(0.1741)	0.0687	(0.0037)
Gompertz 3	110.1785	(1.3365)	22.5308	(3.9231)	0.0687	(0.0037)

Estimates for the mature weight of pequi fruit (A) are consistent with Rodrigues et al. (2009)

where the maximum weight was 109 g. Analyzing estimates of parameter B which has direct biological interpretation in parameterizations Logistic 1 and Gompertz 1, the estimate by Logistic model for the inflection point is around 51 days after anthesis. For the Gompertz model the estimate is around 45 days after an thesis. This fact corroborates with Fernandes et al. (2014), where Gompertz reaches the inflection point slightly before the Logistic model. If necessary to obtain the estimate of the inflection point using other parameterizations, simply proceed with the changes indicated for the parameter B in Tables 2 and 3.

Figure 1 shows the models fitted for the growth of pequi fruits using parameters estimated in Table 4. As can be seen the three parameterizations of both models overlap each other, giving the impression of being only two models, corroborating the statements of Tjorve and Tjorve (2010) and Ueda et al. (2010).

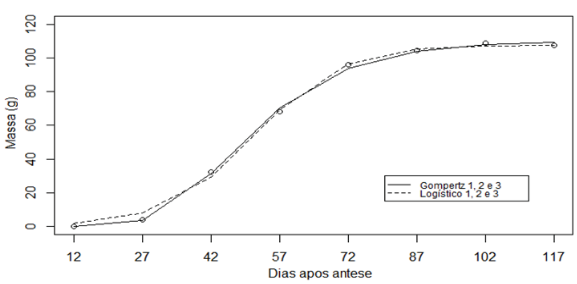

Figura 1. Description of development of pequi fruit using three parameterization of Gompertz and Logistic models.

Table 5 presents measures of intrinsic c^{ι} and parametric c^{θ} nonlinearity for each model type. As mentioned by Souza et al. (2010) the intrinsic curvature values remain constant for the three parameterizations for both models.

Table 5. Goodness of fit evaluators for the three parameterizations of Logistic and Gompertz models in describing the growth of pequi fruits and number of Gauss-Newton algorithm iterations required for convergence.

	R^2_a	AIC	c^{ι}	c^{θ}	Nº iterations
Logistic 1	0.9968	41.8062	0.1608	0.3008	7
Logistic 2	0.9968	41.8062	0.1608	3.4942	14
Logistic 3	0.9968	41.8062	0.1608	3.5099	12
Gompertz 1	0.9986	35.9526	0.1519	0.3007	8
Gompertz 2	0.9986	35.9526	0.1519	0.3176	6
Gompertz 3	0.9986	35.9526	0.1519	1.6701	9

Values greater than 0.5 are considered significant in both measures and indicate departure from linearity (BATES; WATTS, 1980; ZEVIANI et al., 2012). Intrinsic nonlinearity is usually the smallest measure and hence, is not significant. However, even if it is not significant, the parametric nonlinearity can be significant, impairing the quality of inferences about the parameters (MAZUCHELI; ACHCAR, 2002).

In this work, the intrinsic nonlinearity was not significant in all adopted parameterizations, and slightly lower for the Gompertz model. The parametric nonlinearity was not significant in the parameterizations Logistic 1, Gompertz 1 and Gompertz 2. But it far surpasses the critical value in the parameterization 2 and 3 of the Logistic model and parameterization 3 of the Gompertz model, indicating departure from linearity and compromising the reliability of the estimates obtained under these parameterization (CORDEIRO et al., 2009; ZEVIANI et al., 2012).

Interestingly the most used parameterizations, Logistic 2 and Gompertz 3, are the ones with the largest standard error for the estimate of the parameter B (Table 4). In addition, these parameterizations also showed significant values for parametric curve 3.49 and 1.67 respectively, greater than 0.5. It also highlights the need for greater computational effort because these parameterizations need more iteration to achieve convergence (Table 5), as was also noted by Rossi and Santos (2014). Most authors choose these parameterizations without considering this fact, simply because they are the most common, which can compromise the quality of the fitting as they present departure from linearity, thus damaging inferences about the parameters. To choose the appropriate parameterization in the fit of a nonlinear model it is important to consider the difference between getting or not convergence to the solution and obtainment of estimates (MAZUCHELI; ACHCAR, 2002).

Some parameterization compromise inferences about the parameters because their nonlinearity measures are significant. As mentioned by Mazucheli and Achcar (2002), non-linear models with behavior distant of linear can have their asymptotic results invalidated, especially in situations where small samples are available. However, the choice of the best parameter cannot be generalized, because the effect of parameterization on the curvature measures is data dependent, (SEBER; WILD, 2003). Thus it is evident the importance of analyzing the nonlinearity in any study of growth curves that use nonlinear models, in order to always work with the parameterization in which the nonlinearity measures are the smallest possible.

In describing the growth curve of pequi fruit, Logistic 1 and Gompertz 1parameterizations have the lowest values of parametric curve, thus ensuring the best quality of linear approximation in the estimation of the parameters and greater reliability in estimates (SEBER; WILD, 2003; CORDEIRO et al., 2009; ZEVIANI et al., 2012). Furthermore, these parameterizations have the advantage of ensuring direct practical interpretation for all parameters involved.

Both for Logistic and Gompertz models, the values of adjusted determination coefficient and Akaike information criterion were the same for all three parameterizations (Table 5). They evaluate the goodness of fit offered and, although reparametrized, the model is still the same (TJORVE; TJORVE, 2010).What changes is the space of solutions and interpretations of parameter *B*. Therefore, it is important to make clear that the parameterization does not affect the goodness of fit but the reliability and inferences about the estimated parameters.

Conclusion

The choice of parameterization affects the nonlinearity hence influences the reliability and the inferences about the estimated parameters. Thus, the nonlinearity measures should be analyzed in any growth curve study that uses nonlinear models. Logistic and Gompertz models parameterizations in which the estimate of *B* is the abscissa of the inflection point should be used because have direct biological interpretation for all parameters. In addition, for pequi fruit growth, these parameterizations presented the lower values for parametric nonlinearity.

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