

Description of blackberry fruit growth by nonlinear regression models

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Abstract- Blackberry is a small fruit with several properties beneficial to human health and its cultivation is an alternative for small producers due to its fast and high financial return. Studying the growth of fruits over time is extremely important to understand their development, helping in the most appropriate crop management, avoiding post-harvest losses, which is one of the aggravating factors of blackberry cultivation, being a short shelf life fruit. Thus, growth curves are highlighted in this type of study and modeling through statistical models helps understanding how such growth occurs. Data from this study were obtained from an experiment conducted at the Federal University of Lavras in 2015. The aim of this study was to adjust nonlinear, double Logistic and double Gompertz models to describe the diameter growth of four blackberry cultivars ('Brazos', 'Choctaw', 'Guarani' and 'Tupy'). Estimations of parameters were obtained using the least squares method and the Gauss-Newton algorithm, with the "nls" and "gls" functions of the R statistical software. The comparison of adjustments was made by the Akaike information criterion (AIC_c), residual standard deviation (RSD) and adjusted determination coefficient (R^2_{aj}). The models satisfactorily described data, choosing the Logistic double model for 'Brazos' and 'Guarani' cultivars and the double Gompertz model for 'Tupy' and 'Choctaw' cultivars.
Index terms: Regression analysis; Model Selection; Fit quality; Sigmoid; Small fruits; Fruit development.

Descrição do crescimento de frutos de amora-preta por modelos de regressão não linear

Resumo- A amora-preta é um pequeno fruto com várias propriedades benéficas à saúde humana, e seu cultivo é uma alternativa para os pequenos produtores. Estudar o crescimento de frutos, ao longo do tempo, é extremamente importante para entender seu desenvolvimento, auxiliando no manejo mais adequado da cultura, evitando, por exemplo, perda após a colheita, que é um dos fatores agravantes da amora-preta, por ser um fruto de curto período de prateleira. Sendo assim, as curvas de crescimento ganham destaque, nesse tipo de estudo, e a modelagem, por meio de modelos estatísticos, ajuda a entender como tal crescimento acontece. Conduziu-se este trabalho com o objetivo de ajustar modelos não lineares, duplo Logístico e duplo Gompertz, para descrever o crescimento do diâmetro de quatro cultivares da amora-preta (Brazos, Choctaw, Guarani e Tupy). As estimativas dos parâmetros foram obtidas por meio do método de mínimos quadrados, utilizando o algoritmo de Gauss-Newton, por meio do software R. A comparação dos ajustes foi feita pelo critério de informação Akaike (AIC_c), desvio padrão residual (DPR) e coeficiente de determinação ajustado (R^2_{aj}). Os modelos descreveram de forma satisfatória os dados, sendo escolhido o modelo duplo Logístico para as cultivares Brazos e Guarani e o duplo Gompertz para as cultivares Tupy e Choctaw.

Termos de indexação: Análise de regressão; seleção de modelos; qualidade de ajuste; sigmoide; pequenas frutas; desenvolvimento de frutos.

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Introduction

Small fruits, such as blackberry, strawberry, raspberry, currant, blueberry, among others, are growing in importance, quality and production volume. The cultivation of these fruits is characterized by the low implantation and production cost and good economic return. The ideal consumption of these fruits is fresh, maintaining their physicochemical, nutritional and biological properties. However, most of the production is destined to the consumption of the processed fruit, in the form of jellies, juices, ice cream, among others. The processing of these fruits is justified by the fact that they are highly perishable, that is, they have short shelf life (TULLIO, 2013).

According to Antunes et al. (2014), the fresh fruit consists of 85% water, 10% carbohydrates, minerals, vitamins A and B and calcium, with some benefits to human health, such as bleeding control, blood pressure, sedative effect, action oxidant, among others.

Blackberry belongs to the genus *Rubus*; it is a small fruit, with good adaptation to the mild climate. Its cultivation for commercialization began in Europe, in the 16th century, later taken to the USA and arriving in Brazil in the 1970s (RASEIRA; FRANZON, 2012). This is a culture of quick financial return for producers; however, it is still little explored in Brazil, with plantations located in the states of Rio Grande do Sul, Espírito Santo, Rio de Janeiro and Southern Minas Gerais (FACHINELLO et al., 2011; ANTUNES et al., 2014).

Fruit harvesting is subjectively performed by color and size (CAVALINI et al., 2006). The preservation time of fresh blackberry fruits is short and knowing the best harvesting time is very important, increasing the consumption time of fresh fruits (GONÇALVES et al., 2012; SOUZA et al., 2018). With rapid loss of post-harvest quality, there is a very large consumption limitation in its natural form; therefore, it is very important to use additional post-harvest techniques to prolong this time. Therefore, choosing the right time to objectively harvest these fruits is very important, and having knowledge about the growth pattern of fruits can be useful in this process, reducing the rapid loss of post-harvest quality, which is the main problem found for the consumption of fresh blackberry fruits (GONÇALVES et al., 2012).

Some authors have studied fruit development, observing the sigmoid growth pattern and using nonlinear regression models, as, in these cases, they are more suitable than linear ones, synthesizing data information in few parameters and with biological interpretations (MARO et al., 2012; PRADO et al., 2013a; PRADO et al., 2013b; FERNANDES et al., 2014). Nonlinear models have been used in a fruit growth study with satisfactory results, providing good estimates of parameters and practical interpretation, with green dwarf coconut

(PRADO et al., 2013b), cashew (MUIANGA et al., 2016), cacao (MUNIZ et al., 2017), Asian pear (RIBEIRO et al., 2018a), pequi (RIBEIRO et al., 2018b) and strawberry fruits (DIEL, 2019).

Most fruit growth studies have used simple sigmoid models. However, in the case of stone fruits, growth occurs in two development stages, and in the first, growth is slow, in the initial stage, passing to fast and stabilizing at the end, with a second stage of the same form. This behavior makes the biometric measurements of fruits to present the shape of a double “S” over time, with characteristics of a curve with two sigmoids (COOMBE, 1976; FERNANDES et al., 2017). Double sigmoid models have been satisfactorily used in growth studies (ALVAREZ and BOCHE, 1999; GOMES et al., 2008; CUNHA JUNIOR et al., 2007; BEBBINGTON et al., 2009; FAMIANE et al., 2012; BRUCKNER et al., 2012; MARTINEZ et al., 2017; FERNANDES et al., 2017; SILVA et al., 2019).

The estimation of parameters in nonlinear models, in general, is performed by minimizing the sum of squares of errors, leading to a system of normal nonlinear equations, requiring the use of iterative methods to obtain estimates. Among iterative methods, the most used is Gauss-Newton (ZEVIANI et al., 2012; SOUSA et al., 2014; CARNEIRO et al., 2014; FERNANDES et al., 2015; FURTADO et al., 2019; SILVA et al., 2019).

Some authors do not take into account, when adjusting nonlinear models, the interpretation of the parameter associated with the inflection point, arguing that it is a scale parameter (SILVEIRA et al., 2011; CASSIANO and SAFADI, 2015). However, Fernandes et al (2015) suggest a parameterization for Logistic and Gompertz models that have a direct interpretation for this parameter. In addition, SARI et al. (2019) pointed out that the inflection point is the point at which the growth rate reaches its maximum, which can be estimated, therefore, by equating the first derivative in relation to the model time to zero.

The aim of this study was to characterize the growth of blackberry fruits of four cultivars (‘Choctaw’, ‘Tupy’, ‘Brazos’ and ‘Guarani’), in relation to their diameter using double Logistic and double Gompertz nonlinear regression models.

Material and methods

Data were taken from Tadeu (2014), which experiment was carried out at the Federal University of Lavras from January 2012 to January 2014. The climate is altitude tropical, with dry winters and rainy summers (ALVARES et al., 2013). The variable under study was the diameter in millimeters (mm) of blackberry of ‘Brazos’, ‘Choctaw’, ‘Guarani’ and ‘Tupy’ cultivars. Seedlings were

planted in 2009 with a T-wire cordon, 60 cm apart and 80 cm in height, with 3.0 m x 0.5 m spacing.

From this study, the diameters of 12 fruits of each cultivar were measured. To obtain these measurements, digital caliper (King Tools 150 mm model, Cia, São Paulo, SP) was used. The choice of fruits, for the study, was made by the development stage, that is, fruits that lost petals and anthers (called anthesis) at the same time.

The Logistic double (1) and double Gompertz (2) growth models were used, described by the following expressions, with parameters taken from Fernandes et al. (2017):

$$Y_i = A_1 / \{1 + \exp(B_1 - K_1 t_i)\} + (A_2 - A_1) / \{1 + \exp(B_2 - K_2 t_i)\} + u_i, (1)$$

$$Y_i = A_1 \exp(-\exp(B_1 - k_1 t_i)) + (A_2 - A_1) \exp(-\exp(B_2 - k_2 t_i)) + u_i, (2)$$

in which, $u_i = \phi_1 u_{i-1} + \dots + \phi_p u_{i-p} + \varepsilon_i$ with $i = 1, 2, \dots, n$ and $n = 13$ the number of times in which blackberry fruits were measured; u_i is the fit residue in the i -th time; ϕ_1 is the autoregressive parameter of order 1; u_{i-1} is the residue of the time fit immediately before the i -th measurement; ϕ_p is the autoregressive parameter of order p ; u_{i-p} is the fit residue in p times before the i -th measurement; ε_i is the model's random error, which by assumption has normal distribution. When residues are independent, parameters ϕ_1 will be null and, consequently, $u_i = \varepsilon_i$ (FURTADO, 2019).

In equations (1) and (2), Y_i defines the average values of diameters (mm) of blackberry fruits in times t_i in days; A_1 indicates the maximum expected value of the first phase, A_2 is the asymptotic value of the second growth phase, that is, the diameter value when the fruit is fully developed; B_1 and B_2 represent the abscissa of the inflection point of the respective curves; K_1 and K_2 represent the fruit maturity indices in the respective curves; t_i refers to the time of the i -th measurement, expressed in days after anthesis (FERNANDES et al., 2015, FERNANDES et al., 2017). To adjust the models, the R software (R DEVELOPMENT CORE TEAM, 2018) was used to estimate parameters using least squares and the nlme, car, lmtest and qpcr packages. The initial values for the iterative method to start the iteration was a graphical analysis with the manipulate function of the R software (ALLAIRE, 2014; DIEL et al., 2019).

Studying other points on the growth curve can be extremely important, as it can help the researcher to know the precocity, acceleration and growth rate of the phenomenon under study and to know these points, the derivatives of models are used in relation to the time variable (SARI et al., 2019). In this work, the first derivative of the double Logistic and double Gompertz models was made in order to know how the growth rate behaves in the two phases and in a complementary way to the Student t test to verify if the two phases are statistically equal.

The Breusch-Pagan (BREUSCH; PAGAN,

1979) and Shapiro-Wilk (SHAPIRO; WILK, 1965) tests were used to verify the homogeneity of variances and normality of residues, respectively. To assess the existence of residual autocorrelation, the Durbin-Watson test (DURBIN; WATSON, 1951) was used. In addition to hypothesis tests, graphical analysis was used to verify these assumptions. Models were compared using the following criteria: i) Residual standard deviation (RSD), calculated by the expression, $DPR = \sqrt{QME}$ where QME is the residual mean square; ii) Adjusted determination coefficient (R^2_{aj}), obtained by $R^2_{aj} = 1 - \left[\frac{(1-R^2)(n-1)}{n-p} \right]$, where R^2 is the determination coefficient, n the number of times in which measurements were taken and p the number of model parameters. iii) Corrected Akaike information criterion (AKAIKE, 1974), given by $AIC_c = AIC + \frac{2p(p+1)}{n-p-1}$, with, $AIC = n \ln \left(\frac{SQR}{n} \right) + 2p$ where SQR is the sum of the squares of residues, p is the number of model parameters, n is the sample size and \ln is the natural logarithmic operator. For all analyses, the significance level adopted was 5%.

Results and discussion

Table 1 shows the results obtained for the Shapiro-Wilk (SW), Breusch-Pagan (BP) and Durbin-Watson (DW) tests and Figures 1, 2, 3 and 4 show the graphical analysis of the residual vector of the double Logistic and double Gompertz models to diameter data of the four blackberry cultivars. The normality assumption was met in all analyses, except for the double Gompertz model of 'Brazos' cultivar; thus, the modeling of this cultivar was not presented and discussed in this study. Regarding variance homogeneity, for all models and all cultivars, this assumption was not violated.

Table 1. P-value for Shapiro-Wilk (SW), Breusch-Pagan (BP) and Durbin-Watson (DW) tests in the residue analysis after adjusting the double Logistic and double Gompertz models to diameter data of 'Tupy', 'Brazos', 'Guarani' and 'Choctaw' cultivars.

| Cultivar | Model | Test | | |
|-----------|-----------------|---------------|---------------|---------------|
| | | SW P-value | BP P-value | DW P-value |
| 'Tupy' | double Logistic | 0.9900 | 0.1002 | 0.0221 |
| | double ompertz | 0.9512 | 0.1301 | 0.0178 |
| 'Brazos' | double Logistic | 0.0970 | 0.6996 | 0.7492 |
| | double Gompertz | 0.0066 | 0.7004 | 0.9980 |
| 'Guarani' | double Logistic | 0.9674 | 0.0536 | 0.8480 |
| | double Gompertz | 0.6917 | 0.9800 | 0.0591 |
| 'Choctaw' | double Logistic | 0.5120 | 0.4120 | 0.0001 |
| | double Gompertz | 0.3974 | 0.4976 | 0.0025 |

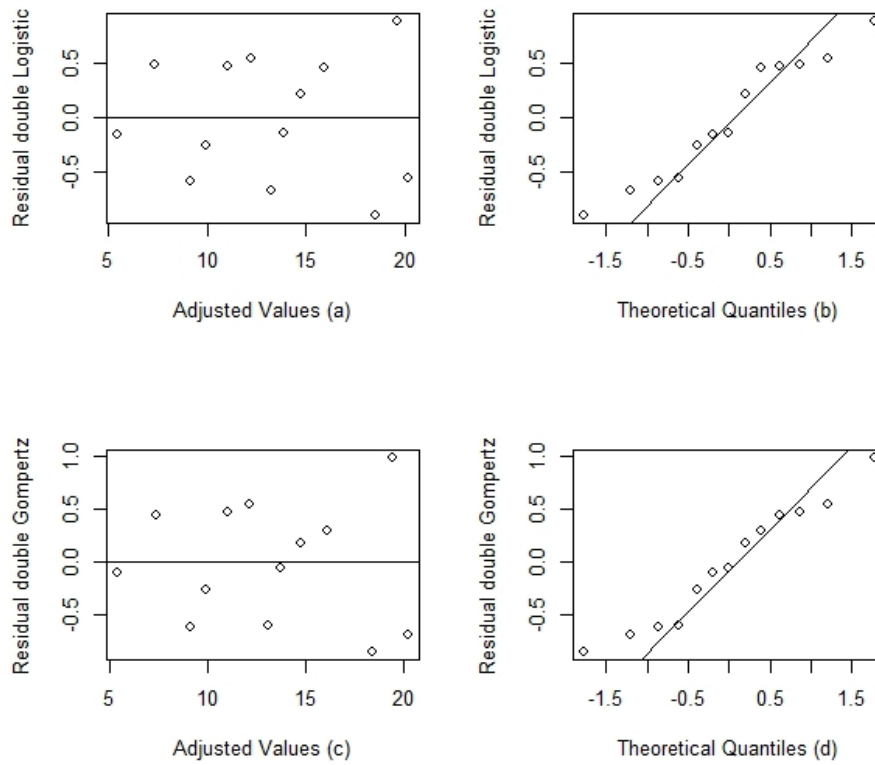


Figure 1. Residual analysis for the diameter (mm) of ‘Tupy’ cultivar, where (a) and (c) represent the adjusted values in relation to residues, and (b) and (d) represent the residual values in relation to the theoretical quantiles for the double Logistic and double Gompertz models, respectively.

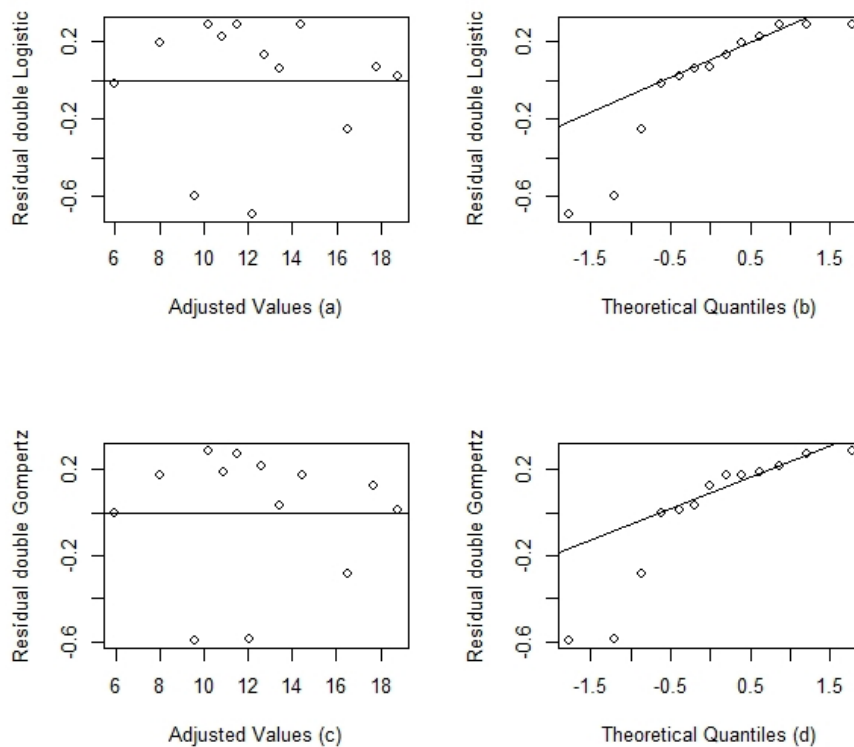


Figure 2. Residual analysis for the diameter (mm) of ‘Brazos’ cultivar, where (a) and (c) represent the adjusted values in relation to residues, and (b) and (d) represent the residual values in relation to the theoretical quantiles for the double Logistic and double Gompertz models, respectively.

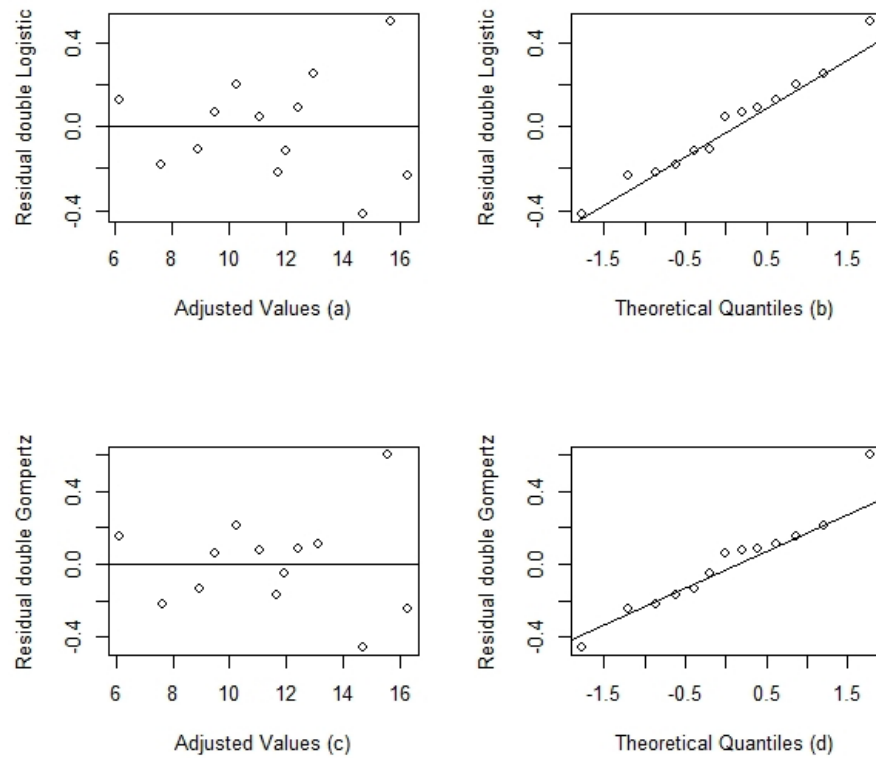


Figure 3. Residual analysis for the diameter (mm) of ‘Guarani’ cultivar, where (a) and (c) represent the adjusted values in relation to residues, and (b) and (d) represent the residual values in relation to the theoretical quantiles for the double Logistic and double Gompertz models, respectively.

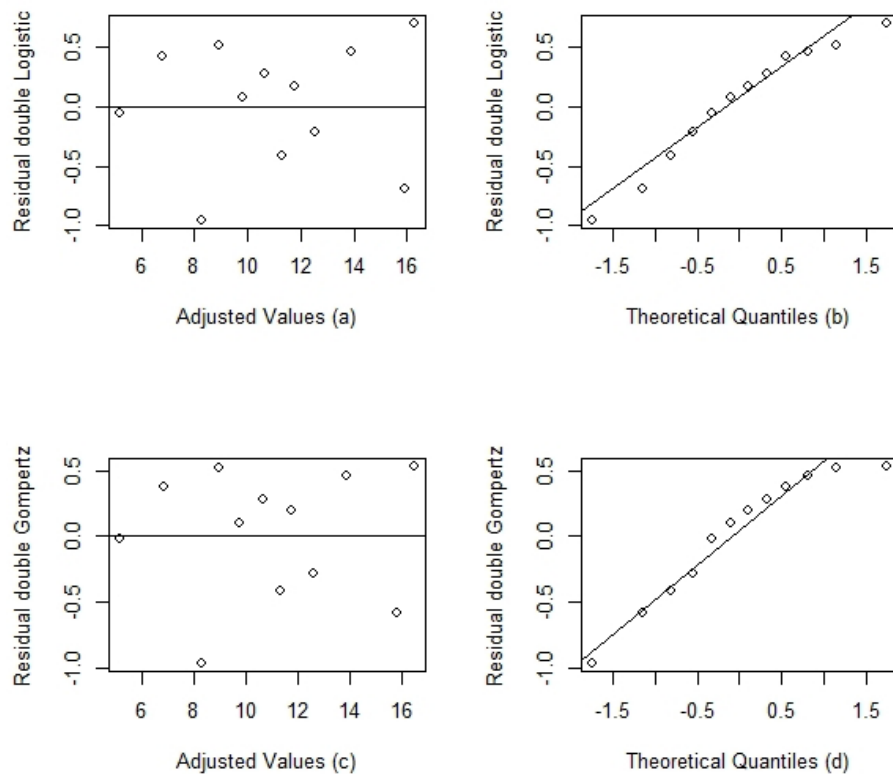


Figure 4. Residual analysis for the diameter (mm) of ‘Guarani’ cultivar, where (a) and (c) represent the adjusted values in relation to residues, and in (b) and (d) represent the residual values in relation to the theoretical quantiles for the double Logistic and double Gompertz models, respectively.

Analyzing the results presented in Table 1, for the independence of the residual vector, this assumption was violated for the double Logistic model and the double Gompertz model for ‘Tupy’ and ‘Choctaw’ cultivars. Therefore, these models were again adjusted and the first-order autoregressive term was added to model this dependency. This result was similar to that found by Lúcio et al. (2015), Muniz et al. (2017) and Ribeiro et al. (2018b) in tomato, cocoa and pear growth studies, respectively. Other studies with measures taken from the same individuals over time had results similar to those found for ‘Brazos’ and ‘Guarani’ cultivars, not violating the independence assumption, such as the works of Muianga et al. (2016) and Fernandes et al. (2014), for cashew and coffee, respectively.

Table 2. Fit quality evaluators, adjusted determination coefficient (R^2_{aj}), corrected Akaike information criterion (AIC_c) and residual standard deviation (RSD) for adjusting the double Logistic and double Gompertz models to diameter data (mm) of blackberry fruits of ‘Tupy’, ‘Brazos’, ‘Guarani’ and ‘Choctaw’ cultivars.

| Cultivar | Model | Parameters | | |
|-----------|-----------------------|---------------|----------------|---------------|
| | | R^2_{aj} | AIC_c | RSD |
| ‘Tupy’ | double Logistic | 0.9746 | 32.8388 | 0.7317 |
| | double Gompertz (AR1) | 0.9751 | 32.1388 | 0.7304 |
| ‘Brazos’ | double Logistic | 0.9871 | 20.5857 | 0.4248 |
| ‘Guarani’ | double Logistic | 0.9888 | 18.7370 | 0.3194 |
| ‘Choctaw’ | double Logistic | 0.9587 | 23.6090 | 0.6954 |
| | double Gompertz (AR1) | 0.9635 | 23.3321 | 0.6382 |

Table 3. Estimates of parameters and their Confidence Intervals (LI; LS) for adjusting the double Logistic and double Gompertz models to diameter data (mm) of blackberry fruits of ‘Tupy’, ‘Brazos’, ‘Guarani’ and ‘Choctaw’ cultivars.

| Cultivar | Model | Parameters | | | | | | |
|-----------|----------------------|---------------|-------------|-------------|---------------|---------------|-------------|-------|
| | | A_1 | B_1 | K_1 | A_2 | B_2 | K_2 | phi |
| ‘Tupy’ | Double | 15.71 | 3.66 | 0.08 | 21.15 | 29.99 | 0.27 | 0,56 |
| | Gompertz (AR1) IC | [11.29;20.13] | [0.88;6.44] | [0.03;0.13] | [19.35;22.94] | [28.09;31.89] | [0.17;0.47] | ----- |
| ‘Brazos’ | Double Logistic | 11.71 | 2.76 | 0.18 | 19.31 | 32.08 | 0.28 | ----- |
| | IC | [9.75;13.68] | [0.86;4.67] | [0.07;0.28] | [17.56;21.07] | [29.78;34.37] | [0.09;0.46] | ----- |
| ‘Guarani’ | Double Logistic | 12.74 | 3.58 | 0.11 | 16.52 | 32.94 | 0.43 | ----- |
| | IC | [10.75;14.73] | [1.04;6.12] | [0.06;0.16] | [15.71;17.33] | [30.86;35.02] | [0.05;0.80] | ----- |
| ‘Choctaw’ | Double | 12.97 | 2.10 | 0.09 | 17.23 | 29.40 | 0.36 | 0,70 |
| | Gompertz (AR1) IC | [10.73;15.22] | [0.62;3.58] | [0.04;0.14] | [15.69;18.77] | [27.85;30.95] | [0.16;0.56] | ----- |

Regarding the asymptotic value parameter (A_2), a conclusion made concerns the overestimation of this value, as can be seen in Figure 5, and this estimate (A_2) was close to the maximum growth found in data, with expected value of 21.15 mm. Another parameter of the double Gompertz model is the growth rate, and for the first and second growth phases, values were, respectively, 0.0841mm /

day and 0.2714mm / day and the Student’s t-test result was significant for these values, that is, K_1 and K_2 differ statistically. According to this result, it could be concluded that the second growth phase is more accelerated than the first, as observed by Silva et al (2013) for peach data.

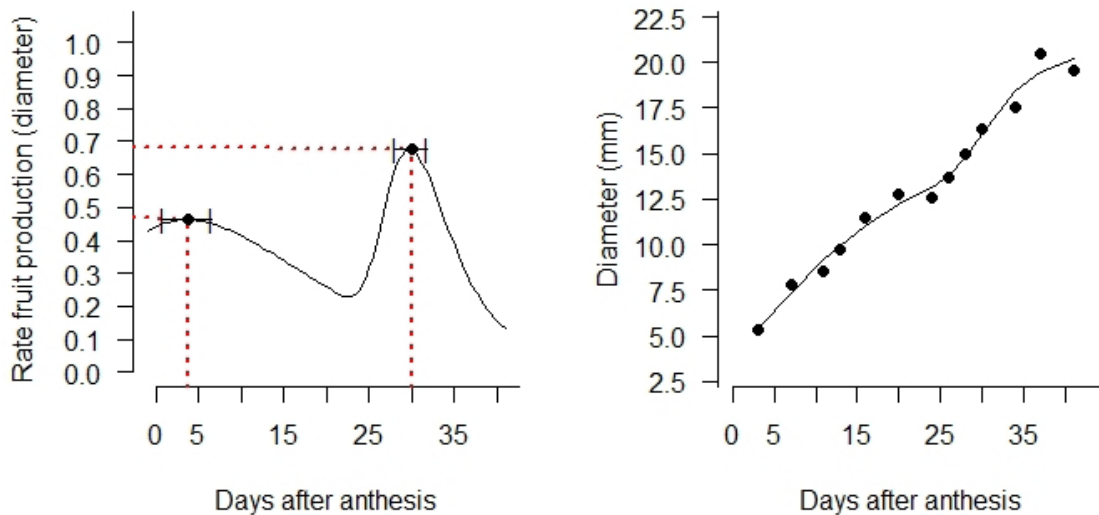


Figure 5. Growth rate graph (left) and adjustment graph of the double Gompertz model (right) to fruit diameter data for 'Tupy' cultivar.

For 'Brazos' cultivar, normality was violated and the abscissa parameter of the inflection point for the first growth phase (B_1) of the double Gompertz model was not significant, since the confidence interval contained zero; in addition, as can be seen in Table 2 and Table 3, respectively, only the double Logistic model was used. The model chosen for this cultivar obtained determination coefficient greater than 98%, indicating good fit. Checking the information of parameters of this model, the horizontal asymptote was 19.31 mm, being a good estimate of the

diameter in the final stage of fruit maturation, as shown in Figure 6. Values are related to the growth rate of both phases, which are presented in Table 3, with values of 0.1829 mm / day and 0.2814 mm / day for K_1 and K_2 , respectively, these two phases being statistically equal by the Student's t test (p -value < 0.05). This result is inconsistent with those found by Silva et al. (2013) and Fernandes et al (2017), because in both works, phases were different.

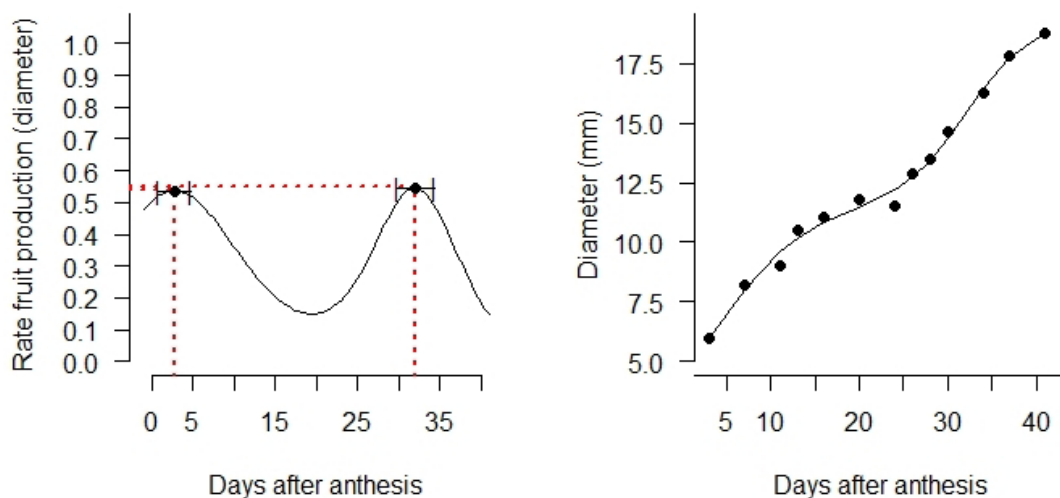


Figure 6. - Growth rate graph (left) and adjustment graph of the Logistic double model (right) to fruit diameter data for 'Brazos' cultivar.

Analyzing results in Table 3, for ‘Guarani’ cultivar, the confidence interval of the B_1 parameter of the double Gompertz model contained zero, this parameter being unreliable to draw conclusions about its result. Therefore, as verified for the double Gompertz model for ‘Brazos’ cultivar, the results of this model were not discussed below. As a result, it was not necessary to make a comparison with the double Logistic model by AICc and RSD evaluators, the double Logistic model being the only model tested and adequate to describe the diameter growth of the ‘Guarani’ cultivar. Even though there is no way to compare the models proposed in this work, Table 2 shows

that the determination coefficient of the double Logistic model, the only one suitable for these data, was greater than 98.5%, suggesting that this model has excellent fit quality in the description of the diameter growth of this cultivar. Analyzing the results of the ‘Guarani’ cultivar, the asymptotic value (A_2) had good estimate, with value close to the maximum growth found in data, with estimate of 16.52 mm, as can be seen in Figure 7. The values of estimates for both growth phases were 0.11 for the first phase and 0.43 for the second, with the Student t test being significant (p -value > 0.05), that is, phases are statistically different.

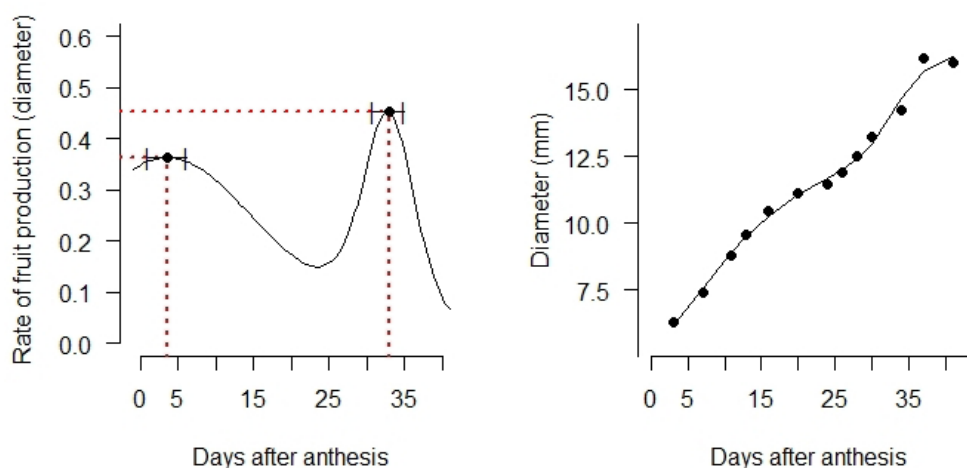


Figure 7. Growth rate graph (left) and adjustment graph of the Logistic double model (right) to fruit diameter data for ‘Guarani’ cultivar.

For ‘Choctaw’ cultivar, estimates and the 95% confidence interval are in Table 3, showing that all confidence intervals for parameters did not contain zero. Both models had good adjustments, with R^2_{aj} showing values greater than 95%. As observed for ‘Tupy’ cultivar, any of the models could be chosen to characterize this growth, but the double Gompertz model presented lower AICc and RSD values and higher R^2_{aj} value, as can be seen in Table

2, which was chosen to comment about these results. The horizontal asymptote value (A_2) did not overestimate this value, with estimate 17.2366 mm, this verification being made in Figure 8. Growth rate estimates were 0.0904 mm / day and 0.3609 mm / day for the first and second growth phases, respectively, and Student’s t test was significant (p -value > 0.05), as in the works by Silva et al. (2013) and Fernandes et al. (2017), the second growth phase is faster than the first one.

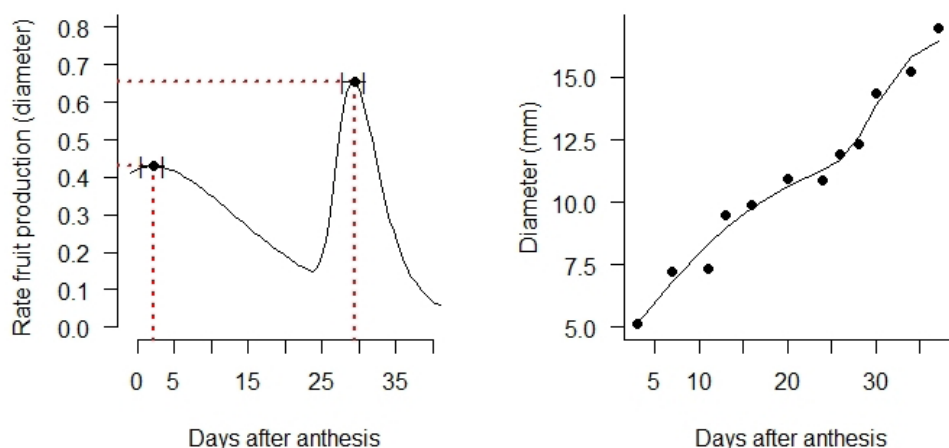


Figure 8. Growth rate graph (left) and adjustment graph of the double Gompertz model (right) to fruit diameter data for ‘Choctaw’ cultivar.

The inflection point of the first growth phase occurred before the fifth day after anthesis, as can be seen in Figures 1, 2, 3 and 4 (left) and the second point occurred, approximately, on the thirtieth day after anthesis and other information was in relation to the growth pattern, as Figures 1, 2, 3 and 4 (left) corroborate pattern found in Figures 1, 2, 3 and 4 (right), that is, the growth of cultivars under study follows a characteristic of double sigmoid. Martins et al. (2019) evaluated the phenology of the 'Tupy' cultivar and concluded that it has the same double sigmoid growth pattern. For other fruits, such as coffee, Fernandes et al. (2017) and peach, Silva et al. (2013) and Silva et al. (2019) also observed the same curve shape in their studies.

The model chosen to represent the nonlinear relationship between time and days after anthesis of the 'Tupy' cultivar presented final diameter growth estimate of 21.1522 mm; Martins et al. (2019) and Campagnolo and Pio (2012) observed value within the confidence interval of estimates found, and in this work, these values were, respectively, 21.40 mm and 21.00 mm. However, Ferreira et al. (2018) found value of 24.00 mm, which can be explained by the fact that these authors used castor bean cake as fertilizer.

Conclusions

The fruit diameter growth pattern of blackberry cultivars under study was the double sigmoidal, adequately described by nonlinear double Logistic and double Gompertz models. For 'Tupy' and 'Choctaw' cultivars, the most appropriate model was the Logistic double and for 'Brazos' and 'Guarani' cultivars, the double Gompertz was the most appropriate. 'Tupy' and 'Choctaw' cultivars presented the second growth phase more quickly than the first, while for 'Brazos' and 'Guarani' cultivars, these phases were statistically equal. At harvest time, fruits of the different cultivars presented diameters between 17.2 mm and 21.1 mm.

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