Brazilian Journal of Biometrics (2022), **40**, 393–406
doi:10.28951/bjb.v40i4.623

BRAZILIAN JOURNAL OF
BIOMΣTRICS
ISSN:2764-5290

ARTICLE

Bayesian estimation of nonlinear models parameters in the description of growth coffee fruits

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(Received: June 1,2022; Revised: December 14,2022; Accepted: December 14,2022; Published: December 30,2022)

Abstract

Coffee is one of the main products of Brazilian agriculture and the country is currently the largest producer and exporter in the world. The coffee fruit has a double sigmoidal growth pattern, however, as well as in other fruits that also show such a growth pattern, the authors generally do not estimate parameters of regression models to describe such curve. In the study of fruit growth curves, the sample size is generally small, so the estimation of the parameters should preferably be done by the Bayesian methodology, since a priori information is incorporated, reducing the effects of having few observations. The Markov Chain Monte Carlo algorithms are the most used computational tool in Bayesian statistics. However, these generate dependent samples, can be complicated to implement and, mainly, to teach. There are also other alternatives to the MCMC algorithms to obtain approximations of integrals of interest in Bayesian inference, the main ones are based on the importance resampling techniques. The objective of this work is to use Bayesian inference with the weighted importance resampling technique in the estimation of parameters of double sigmoidal nonlinear regression models to the description of coffee fruit growth. The double nonlinear logistic model was used in the description of the accumulation of fresh weight in coffee fruits. All prioris used have Beta distribution and were obtained by the called prior of specialist technique. Bayesian methodology was efficient, since it provided parameters with practical interpretation to coffee fruit growth, consistent with the reality. Thus, Bayesian inference by weighted importance resampling was a good alternative for the parameters estimation of nonlinear double sigmoid regression models. The logistic model showed that the growth of coffee fruits is more intense in the first sigmoid (until 162 DAF) of the growth curve and stabilizes in its final weight after 262 daf.

Keywords: Double Logistic; Prior of specialist; Regression; Weighted importance resampling.

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1. Introduction

The importance of coffee in the world is highlighted, with great impact on the economy of countries. Brazil is the world's largest coffee producer and exporter, accounting for about 35% of all coffee trade, and is the second largest consumer market (Voltolini *et al*., 2020). Studies describing growth curves of fruits with identifications of his critical points can help the producer to identify possible points of intervention during fruit development, thus obtaining a better final quality of the product (Silva *et al*., 2021).

The growth pattern of coffee berries, considering the fresh mass accumulated over time, is double sigmoid (Fernandes *et al*., 2017). The nonlinear regression models are able to describe diverse situations, providing a better fit quality and, mainly, present practical interpretation of the parameters. Therefore are been widely used, especially in the study of growth curves (Allaman and Jelihovschi, 2022; Fernandes *et al*., 2019; Fruhalf et al, 2020; Mischan *et al*., 2015; Oliveira *et al*., 2021; Salles *et al*., 2020; Silva *et al*., 2020).

Growth models are commonly estimated by frequentist approach, however the parameter estimation process is based on asymptotic theory and, when there is small sample data, the obtention of the estimates is very affected, generating atypical growth curves (Pereira *et al*., 2022; Martins Filho *et al*., 2008; Salles *et al*., 2020). However, few longitudinal observations are common in the study of fruit growth, due to the short fruiting period.

Another methodology for obtaining parameter estimates of these models is the Bayesian approach. In this methodology, already existing information about the growth is incorporated into the parameter estimation process, thus reducing the effect of having few data. Monte Carlo via Markov Chains (MCMC) algorithms are the most used computational tool in Bayesian statistics (Peres *et al*., 2022). Thus, recent researches sought to improve its implementation, and propose techniques to facilitate the convergence analysis (Liu *et al*., 2016; Pensar *et al.* 2020; Vanderwerken and Schmidler, 2017; Witmer, 2017).

An alternative to the MCMC is the weighted importance resampling, that unlike MCMC, it generates independent samples, requires a short computational time for implementation, and has a more attractive theory (Pereira *et al*., 2022; Cole *et al*., 2012; Lopes *et al*., 2012).

The objective of this work is to use Bayesian inference with the weighted importance resampling technique in the estimation of parameters of double sigmoidal nonlinear regression models to the description of coffee fruit growth.

2. Matherials and Methods

2.1 Database

Fresh fruit weight (in grams) data of coffee (Coffea arabica cv. Obatã IAC 1669-20) extracted from Cunha and Volpe (2011) were used. Fruit growth was monitored from 96 days after flowering (DAF) to 293 DAF. Fourteen collections at 15-day intervals were performed.

2.2 Double sigmoidal model

The double sigmoidal expression was composed using the nonlinear logistic model, since it is the most indicated for the description of characteristics that present sigmoidal growth, following the parameterization suggested by Fernandes *et al.* (2017). Thus, the model was defined as:

$$Y|\mu, \sigma^2 \sim N(\mu, I\sigma^2),$$

where: Y is the fruit fresh weight; I is identity matrix; μ is mean and σ^2 is variance of a normal distribution. Here, μ is the expression of double logistic model:

$$\mu = \frac{a_1}{1 + e^{-k_1(DAF - b_1)}} + \frac{a_2 - a_1}{1 + e^{-k_2(DAF - b_2)}} \tag{1}$$

where DAF is the fruit age in which the fresh weight was measured; a_1 is the maximum fresh weight expected for the first growth stage; a_2 is the final fruit fresh weight, or fruit weight at maturity; b_1 and b_2 represent the abscissa of the inflection point in the respective steps; k_1 and k_2 represent the growth index in steps 1 and 2. The higher the k value the shorter the time the fruit takes to reach its maximum fresh weight (a_1 or a_2) (Fernandes *et al.*, 2017).

Thus, the parameter vector for the model is given by: $\theta' = [a_1, b_1, k_1, a_2, b_2, k_2]$. The next step for implementing a Bayesian analysis is the specification of prior distributions.

2.3 Constructing the Prior and Posterior distributions

The basic idea in eliciting prior distributions for a parameter, based on practical knowledge, is to establish descriptive statistics as a range of plausible values and some measure of position for it, with the help of specialists. Then, distributions for the parameters can be established; this technique is called prior of specialist (Garthwaite *et al.*, 2005).

In the present work, all prior distributions used have Beta distribution since, according to Moala and Penha (2016), this is one of the most used distributions to model prior of specialist. Thus, the prior for each of the six parameters had the following expression:

$$P(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}, \tag{2}$$

where: $\alpha > 0$ and $\beta > 0$ are (known) hyperparameters of the Beta distribution.

The parameters of the nonlinear models have practical interpretation, thus, based on previous knowledge on the coffee fruit growth and information obtained from specialists to identify hyperparameters, the following prior distributions for vector θ' were well established.

Table 1. Prior distributions with his hyperparameters (α, β) for all parameters of double sigmoidal model

Parameter	Prior distribution
a_1	$Beta(2,2)$
b_1	$[104 * Beta(2,2) + 96]$
k_1	$Beta(2,10)$
a_2	$2 * Beta(2,2)$
b_2	$[200 * Beta(2,2) + 200]$
k_2	$Beta(2,20)$

Assuming independence of the priors, the joint prior distribution is defined for the parameter vector as the product of the individual prior distributions, denoted by $P(\theta)$. The likelihood is defined under the assumption of normality of the model, thus, the expression of the posterior $P(\theta|Y)$ is:

$$\begin{aligned} P(\theta|Y) &\propto \left(2\pi\sigma^2\right)^{\frac{-n}{2}} exp\left\{\frac{-(Y-\mu)'(Y-\mu)}{2\sigma^2}\right\} \times P(\theta) \\ P(\theta|Y) &\propto exp\left\{\frac{-(Y-\mu)'(Y-\mu)}{2\sigma^2}\right\} \times P(\theta) \end{aligned}$$

where: Y is the observed data, μ, σ^2 and θ were previously defined.

The expression presented above is the joint posterior distribution of the models. Information about the posterior behavior of each parameter, average, and credibility interval for example, can be obtained by calculating integrals, such as:

$$E[h(\theta)|Y] = \int_D h(\theta)P(\theta|Y)d(\theta)$$

where $h(\theta)$ is a suitably chosen function.

However, due to the complexity of the expressions of the nonlinear double sigmoidal models, these integrals are impossible to be solved analytically, and a modification of the weighted importance resampling technique presented in Smith and Gelfand (1992) will be used to generate samples of the distributions of interest.

2.4 Weighted Importance Resample

The methodology proposed by Smith and Gelfand (1992) consists of the following idea. Suppose it is necessary to generate samples from an unknown distribution with probability density function $f(\theta)$, but it's difficult to generate samples directly from it. Then consider a distribution $g(\theta)$ that is known and consequently sampled, defined in the same domain (or parametric space) of $f(\cdot)$. Based on the theory of importance sampling (RUBIN, 1987) expression of $f(\cdot)$ is multiplied and divided the by the expression $g(\cdot)$, obtaining:

$$\frac{f(\theta)}{g(\theta)} \times g(\theta)$$

Then, samples of $g(\theta)$ are generated and weighted by calculated weights based on $\frac{f(\theta)}{g(\theta)}$. Then, an approximate sample of f(θ) is found. The algorithm develops as follows:

i) generation of a sample of size M, $(\theta_1, \theta_2, ..., \theta_M)$ of the distribution $g(\theta)$;
ii) calculation of the weights for each sample generated:

$$w_j = \frac{f(\theta_j)}{g(\theta_j)}$$

where $1 \leq j \leq M$;
iii) normalization of these weights:

$$q_j = \frac{w_j}{\sum_{t=1}^{M} w_t}$$

iv) removal a sample of size m making $m \leq M$ of the sample $(\theta_1, \theta_2, ..., \theta_M)$ taking only the θ_j with the highest values of q_j, i.e, a weighted resampling with weights calculated based on the distribution of interest, obtaining a new sample $(\theta_1^*, \theta_2^*, ..., \theta_m^*)$.

Smith and Gelfand (1992) showed that the sample obtained in step *iv*) forms a sample of a distribution $f(\theta^*)$ that converges in distribution to $f(\theta)$ as m grows. The only requirement for the candidate generating distribution $g(\theta)$ is that it is defined in the same parametric space as the distribution of interest $f(\theta)$.

In Bayesian inference problems, $f(\theta)$ is the posterior distribution $(P(\theta|Y))$ and a natural choice, according to Smith and Gelfand (1992), is to consider $g(\theta)$ as the prior distribution. On the other hand, the present work proposes to consider the distribution $g(\theta)$ as an approximation of the likelihood, denoted by Q(θ). The candidate generating distribution Q(θ) is an approximate of the real likelihood, created based on the maximum likelihood estimate and the Cholesky decomposition of the covariance matrix of the parameters. As we have already assuming a normal distribution for the model, as $M \to +\infty$, $Q(\theta)$ converges in distribution for $L(Y|\theta)$.

Thus, a sample of size M of the likelihood is taken and the weights in step ii) are calculated as follows:

$$w_j = \frac{f(\theta_j)}{g(\theta_j)} = \frac{P(\theta_j|Y)}{Q(\theta_j)} = \frac{L(Y|\theta_j)P(\theta_j)}{Q(\theta_j)} \simeq \frac{L(Y|\theta_j)P(\theta_j)}{L(Y|\theta_j)} = P(\theta_j)$$

and in the step *iii*) as:

$$q_j = \frac{w_j}{\sum_{t=1}^{M} w_t} = \frac{P(\theta_j)}{\sum_{t=1}^{M} P(\theta_t)} = P(\theta_j). \tag{3}$$

The denominator of expression 3, tends to 1 as M grows, so the weights are obtained directly in the prior distribution, which facilitates the calculations.

The estimation of $Q(\theta)$, requires getting the maximum likelihood estimate $(\hat{\theta})$ and the covariance matrix $(\hat{\Sigma})$ of the model parameters. They were estimated by the *gnls* function. Thus, the algorithm for obtaining the samples of the posterior distribution was implemented as follows:

i) a sample of size $M = 10000$ of $Q(\theta)$ of the model was generated;

$Q(\theta)_j$ values were generate considering $Q(\theta) \sim N_6(\hat{\theta}, \hat{\Sigma})$.

Then the Cholesky decomposition (L) of $\hat{\Sigma}$, with $\hat{\Sigma} = LL'$ was performed and simulated a vector Z_j that follow a multivariate standard normal distribution $N_6(\emptyset, I_6)$. The desired vector was obtained using the linear transformation $Q(\theta)_j = \hat{\theta} + LZ_j$.This process was repeated ten thousand times, with $j = 1, 2, ..., 10000$.

ii) the weights in the prior distribution $P(\theta)$, were calculated for each value generated;
iii) a resampling was performed, with replacement weighted by the weights obtained in the prior distribution of size m=10000, from sample obtained in the first step.

Thus, the marginal density of each parameter was approximately recreated from samples. The sample mean, standard deviation and highest posterior density interval (HPD - 95%) were calculated for each marginal distribution of the parameters to obtain a specific estimate to be used for substitution in the expression of the model and thus obtain the estimated curve.

2.5 Markov chain Monte Carlo - MCMC

The MCMC algorithm, which is the consolidated form for the obtaining samples of marginal posterior distributions, was also implemented to compare the results and mainly the computational time required to obtain the samples of the marginal distributions of each parameter. The joint posterior and complete conditional distributions were not known, thus, it's necessary to use the Metropolis-Hastings algorithm.

To implement the Metropolis-Hastings algorithm were used the same prior distributions $P(\theta)$, same size of the chains (M=10000) and the likelihood approximation $Q(\theta)$ as candidate generating distribution ensuring the parity of the comparison. The convergence analysis was done by using the Raftery & Lewis and Geweke criteria. After verifying te convergence for each marginal distribution of the parameters were calculated the sample mean, standard deviation and highest posterior density interval (HPD - 95%).

2.6 Computational Resources

All computational procedures involved, the processes of sampling and resampling to obtain the estimates for the parameters and the analyses of the data were made using the statistical software R (R Development Core Team, 2020). The maximum likelihood estimate and the covariance matrices of the parameters were obtained by the gnls function of the nlme package (Pinheiro *et al.*, 2022). The coda package (Plummer *et al.*, 2006) of the R program was used in the summary of the marginal distributions and analysis of convergence of the chains generated by MCMC.

3. Results and Discussion

The algorithm was implemented to obtain samples of the marginal distributions of each parameter by weighted importance resample. Particularity on the MCMC, as observed by Blasco *et al.* (2003), was used the Metropolis-Hastings algorithm in the process of obtaining samples of the marginals distributions, due to the nonlinearity of the model. The sample means, standard deviations are presented in Tables 2 and 3 together with the highest posterior density interval (HPD - 95%) for the parameters of the nonlinear double sigmoidal logistic model obtained by the weighted importance resampling, and MCMC, respectively.

Table 2. Mean, standard deviation, and HPD interval for parameters of the double logistic model obtained by modified weighted importance resampling in the description of coffee fruit growth curve

			HPD	
Parameter	mean	standard deviation	2.5%	97.5%
$\hat{a}_1$	0.6708	0.0421	0.5863	0.7494
$\hat{b}_1$	148.1257	1.5725	145.0599	151.1921
$\hat{k}_1$	0.1659	0.0284	0.1099	0.2194
$\hat{a}_2$	1.0817	0.0258	1.0316	1.1336
$\hat{b}_2$	225.6010	5.1857	215.1511	235.7878
$\hat{k}_2$	0.0631	0.0191	0.0239	0.0998

Table 3 shows the results of the marginal distributions obtained by MCMC. All chains reached convergence by the criteria of Raftery and Lewis and Geweke, however, the results of the convergence analysis are not presented because they are not the objective of this work.

A very low standard deviation of the estimates is shown in Table 2 and Table 3, indicating a high reliability of the parameters estimated by the model. This denotes the efficiency of the Bayesian methodology for the estimation of parameters of nonlinear regression models, as found by Blasco *et al.* (2003), Martins Filho *et al.* (2008), Pereira *et al.* (2022), Salles *et al.* (2020) and Zheng and Zhu (2008).

Table 3. Mean, standard deviation, and HPD interval for parameters of the double logistic model obtained by MCMC in the description of coffee fruit growth curve

			HPD	
Parameter	mean	standard deviation	2.5%	97.5%
$\hat{a}_1$	0.6889	0.0402	0.6047	0.7632
$\hat{b}_1$	148.5727	1.5166	145.6022	151.4618
$\hat{k}_1$	0.1589	0.0276	0.1023	0.2104
$\hat{a}_2$	1.0763	0.0265	1.0268	1.1287
$\hat{b}_2$	227.0296	5.0265	217.2921	236.9215
$\hat{k}_2$	0.0695	0.0195	0.0317	0.1076

The parameter a_2, is the most interesting one because it represents the final weight of the fruit, and coffee is marketed according to its weight. It was very well estimated, with credibility intervals for a_2 (Table 2 and 3) containing the latest fresh weight observations measured in practice by Cunha and Volpe (2011). This reinforces the practical interpretation of the parameters and the quality of the methodology in obtaining the estimates. Besides better precision, the Bayesian approach may allow consistent inferences from few observations, like observed too by Salles *et al.* (2020).

Tables 2 and 3 also show that the estimates for the parameter k_1 were always greater than those of parameter k_2, indicating that the development of coffee fruit is accelerated in the first growth stage (or first sigmoid). This rapid expansion in the first stage of development of the coffee fruit can be explained by the phenological scale proposed by Nunes *et al.* (2010), in which the authors point out the rapid fruit growth in this first stage. This process is different in peach fruits, for example, which have increased growth in the second stage (Fernandes *et al.*, 2022).

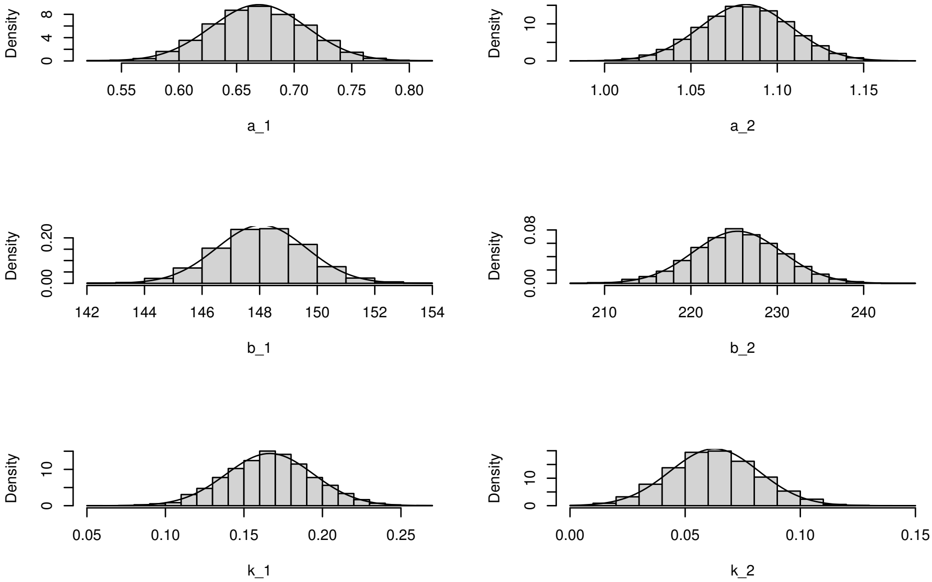
Unlike what happens with coffee fruit, Silva *et al.* (2020) observed that in blackberry fruits the difference in intensity between the growth stages depends on the cultivar under study. So that in some cultivars k_2 were greater than k_1, but in others cultivars they are statistically equals.

As commented by several authors such as Allaman and Jelihovschi (2022), Silva *et al.* (2020) and Teixeira *et al.* (2021), the identification of points of physiological importance in the growth curve can be of fundamental importance for the most appropriate management. One of these points is the asymptotic deceleration point (ADP), at this point, the characteristic under study stabilizes its growth. As presented in Silva *et al.* (2020), for the Logistic model the ADP can be estimated by: $\left(\frac{k*\beta+2.2924}{k}\right)$. Based on the results of this work (Table 2), describing the growth of the coffee fruits, the estimate of ADP was 162 and 262 DAF for the first and second sigmoid respectively. Which means that at 162 daf the coffee fruit stops growing and after a few days it starts to grow again (slowly, because $k2<k1$) and finally stabilizes in its final weight after 262 daf.

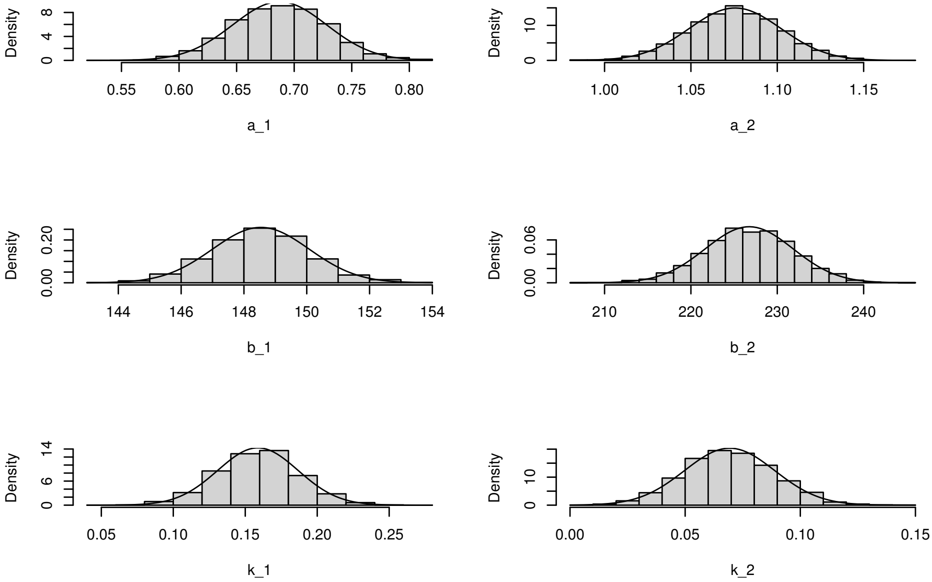
Figure 1 shows the sample histogram of the marginal distributions of each parameter for the double logistic model, obtained by the weighted importance resampling method and by MCMC. The solid line is the density of the normal distribution generated with the mean and variance information obtained in the marginal distribution. These marginal distributions were very similar even obtained by different methodologies.

The mean estimates of each parameter were similar for the two estimation methods (Tables 2 and 3). According to Smith and Gelfand (1992), the resampling method forces the obtaining of a greater number of samples in the most important parts of the problem. Straub and Papaioannou (2015) claim that this technique no need chain convergence analysis and is easy to understand. Thus, researchers can focus on the main parts of Bayesian problems, which are the elicitation of priors and summary of posterior information. However, in accord with Witmer (2017) the use of this technique in practical courses of Bayesian inference for undergraduates is little emphasized.

One difficulty in using MCMC algorithms is the requirement of large number of samples to control the Monte Carlo error and avoid generating nonsense values that can only be detected after a careful analysis of convergence (Liu *et al.*, 2016). After the convergence analysis and elimination of burn-in and thin, the final effective size of the samples generated by MCMC was less than half the final effective size obtained by weighted importance resampling. Since the weighted importance resampling uses all 10,000 values, the final chain when using MCMC had 4,897 values after eliminating the burn-in (206 first values) and thin (lag 2).



(a) Modified weighted importance resampling.



(b) Markov chain Monte Carlo - MCMC.

Figure 1. Sample histogram with Normal density curves of the marginal distributions of each parameter of the double logistic model obtained by the modified weighted importance resampling (a) and MCMC (b).

The double sigmoid model studied was very efficient in describing the growth curve of coffee fruits (Figure 2). The credibility intervals were obtained using the predictive distribution, contain all observed data and were small (Figure 2), thus confirming the double sigmoidal growth pattern of the coffee fruits, which is corroborated by Fernandes *et al.* (2017) and Nunes *et al.* (2010).

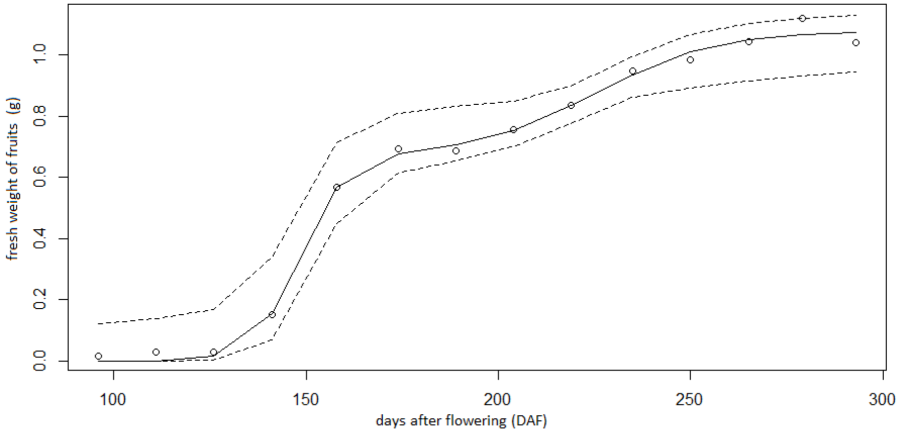


Figure 2. Double logistic model in description of fresh weight fruits growth versus days after flowering (DAF). Dotted lines depict 95% credibility interval.

The fitting quality obtained was very high (Figure 2) with determination coefficient R^2 = 99.54%. The estimated parameters are consistent with the literature, confirming the efficiency of the weighted importance resampling method as an alternative for the estimation of parameters of double sigmoid regression models. Therefore, this approach can be used to estimate parameters of any growth curves (animal, vegetable and fruit). Specifically in fruits such as plum, peach, guava, gabiroba and blackberry, which also present a double sigmoidal growth pattern, according to Famiani *et al.* (2012), Fernandes *et al.* (2022), Nava *et al.* (2014), Santos *et al.* (2015) and Silva *et al.* (2020), respectively.

It's important to note that the efficiency of the Bayesian methodology is associated with the "good quality" of the prior distribution, like commented too by Pereira *et al.* (2022) and Salles *et al.* (2020). Thus, the weighted importance resampling is strongly indicated for the study of growth curves, since the nonlinear models present practical interpretation for the parameters, thus facilitating the obtaining of prior of specialist suggested by Garthwaite *et al.* (2005).

4. Conclusions

Bayesian inference by weighted importance resampling method was a good alternative for the parameters estimation of nonlinear double sigmoid regression models, providing parameters for coffee fruit growth that have practical interpretation and consistent with the literature.

The logistic model showed that the growth of coffee fruits is more intense in the first sigmoid (until 162 DAF) of the growth curve and stabilizes in its final weight after 262 daf.

Acknowledgments

This work was supported by the Coordenação de Aperfeiçoamento de Pessoal do Ensino Superior - CAPES.

Conflicts of Interest

The authors declare no conflict of interest.

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Appendices

Software R codes to implement weighted importance resample

```
##############
library(nlme)
library(coda)
library(car)
rm(list=ls())
###########  81° 261°  ##############################################
daf=c(96,111,126,...,293)
freshWeight=c(0.016,0.031,0.03,...,1.040)
####### SIR #######################
## Weighted Importance Resampling
inicio<- proc.time()
##### LL model ##################
reg=gnls(freshWeight~alfa1/(1+exp(-k1*(daf-beta1)))+
(alfa2-alfa1)/(1+exp(-k2*(daf-beta2))),
start=list(alfa1=0.6, beta1=170, k1=0.2, alfa2=1, beta2=250, k2=0.15))
summary(reg)
round(coef(reg),2)

plot(daf,freshWeight)
lines(daf,fitted(reg))
###################### Sample Importance Resample ######################
## priors
lPriori <- function(theta){
  dbeta(theta[1],2,2,log=TRUE)+
    dbeta(theta[4]/2,2,2,log=TRUE)+
    dbeta(theta[2]/200,4,4,log=TRUE)+
    dbeta((theta[5]-theta[2])/200,2,2,log=TRUE)+
    dbeta(theta[3],2,10,log=TRUE)+
    dbeta(theta[6],2,20,log=TRUE)
}

### obtaining Q() aproximation
theta.v <- reg$coefficients
Sigma.v <- reg$varBeta

L <- t(chol(Sigma.v))

N <- 10000
n <- 10000
w <- 0*1:N
THETA <- matrix(0,N,6)

for(i in 1:N){
  THETA[i,1:6] <- theta.v+L%*%rnorm(6)
  w[i] <- lPriori(THETA[i,1:6])
}
```

```
index <- sample(1:N,n,replace=TRUE,prob=exp(w)) # weighted positions of sampling
tail(index)

Posterior.Sample <- THETA[index,]  # resampling

am <- mcmc(Posterior.Sample)
summary(am)
raftery.diag(am)
HPDinterval(am)

proc.time() - inicio

par(mfrow=c(3,2))
hist(am[,1],prob=T, xlab = "a_1", main = "")
curve(dnorm(x, mean(am[,1]), sd(am[,1])), add= TRUE)
hist(am[,4],prob=T, xlab = "a_2", main = "")
curve(dnorm(x, mean(am[,4]), sd(am[,4])), add= TRUE)
hist(am[,2],prob=T, xlab = "b_1", main = "")
curve(dnorm(x, mean(am[,2]), sd(am[,2])), add= TRUE)
hist(am[,5],prob=T, xlab = "b_2", main = "")
curve(dnorm(x, mean(am[,5]), sd(am[,5])), add= TRUE)
hist(am[,3],prob=T, xlab = "k_1", main = "")
curve(dnorm(x, mean(am[,3]), sd(am[,3])), add= TRUE)
hist(am[,6],prob=T, xlab = "k_2", main = "")
curve(dnorm(x, mean(am[,6]), sd(am[,6])), add= TRUE)
```