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Nonlinear Regression Models and Measures of Nonlinearity: An Overview

Marcelo Teixeira Leite
Department of Sugar and Ethanol Technology, Federal University of Paraíba, Brazil, Zip code 58058-600
Corresponding Author: Marcelo Teixeira Leite

ABSTRACT :In nonlinear estimation, the degree of nonlinearity must be sufficiently small so that the usual estimation techniques developed for linear regression can be used as a reliable approximation for the nonlinear model. Both the effectiveness of least squares algorithms and the validity of inferences made regarding the parameters of a nonlinear model will be affected by the closeness of the linear approximation to the model. Since most asymptotic inferences for nonlinear regression models are based on analogy with linear models, and since these inferences are approximate, some measures of nonlinearity have been proposed as a guide for understanding how good linear approximations are likely to be. This study discusses the most used measures of nonlinearity: the curvature measures of Bates and Watts, the bias measure of Box, and the Hougaard's measure of skewness.
KEYWORDS:*Nonlinearregression models*, curvatures of Bates and Watts, bias measure of Box, Hougaard's measure of skewness.

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I. NONLINEAR REGRESSION MODELS

The concept of nonlinear regression model and its consequences to statistical inference can be explained by using the following regression model:

$\mathbf{y} = \mathrm{f}(\mathbf{x}, \boldsymbol{\theta}) + \boldsymbol{\varepsilon}$(1)

Where **y** is the vector of the response variables, **x** is the vector of the independent variables, **θ** is the vector of regression parameters, **ε** is the vector of the random errors and f (**x**, **θ**) is a function of the independent variables and the parameters, known as regression function. Generally, it is assumed that the errors ε_i are independently and normally distributed with mean zero and constant variance.

When$\partial \mathrm{f}(\mathrm{x_i}, \boldsymbol{\theta})/\partial\theta_j$is independent of **θ** or$\partial^2 \mathrm{f}(\mathrm{x_i}, \boldsymbol{\theta})/\,\partial\boldsymbol{\theta}_j^2 = 0$, the regression model is called *linear* with respect to the parameters. If at least one derivative of **y** with respect to a parameter is a function of that parameter, the regression model is called *nonlinear*(Seber and Wild, 1989). An important consequence of the fact that a regression model is nonlinear is that the least squares estimators of its parameters do not possess the desirable properties of their counterparts in linear regression models, that is, they are not unbiased, minimum variance, normally distributed estimators (Ratkowsky, 1983).

II. NONLINEAR ESTIMATION

Assuming that the regression function in Equation (1) is twice continuously differentiable in **θ**, the residual sum of squares is given by:

$\mathrm{S}(\boldsymbol{\theta}) = \sum_{i=1}^{n}[\mathrm{y_i} - \mathrm{f}(\mathrm{x_i}, \boldsymbol{\theta})^2]$(2)

The least-squares estimators of the parameters$\hat{\theta}$ are the values of **θ** which minimize the sum of squares S(**θ**). For linear models, there is an analytical solution which leads to the minimum value of S(**θ**). For nonlinear models, the search for the minimum value of S(**θ**) is performed by iterative numerical methods, and the algorithms used is based on a linear approximation to the regression function (Draper and Smith, 1998). Thus, in nonlinear estimation, the degree of nonlinearity must be sufficiently small so that the usual estimation techniques developed for linear regression can be used as a reliable approximation for the nonlinear model. Both the effectiveness of least squares algorithms and the validity of inferences made regarding the parameters of a nonlinear model will be affected by the closeness of the linear approximation to the model (Box, 1971). The closer the linear behavior of a nonlinear model is, the more accurate the asymptotic results and consequently the more reliable inferences are. There are some nonlinear regression models whose estimators come close to being unbiased, normally distributed, minimum variance estimators. Such models have been termed *close to linear* models by Ratkowsky (1983).

III. MEASURES OF NONLINEAR BEHAVIOR

Since most asymptotic inferences for nonlinear regression models are based on analogy with linear models, and since these inferences are approximate, some measures of nonlinearity have been proposed as a guide for understanding how good linear approximations are likely to be (El-Shaarawi and Piegorsch, 2002).

One of the first relevant attempts to quantify the nonlinearity of a nonlinear regression was presented by Beale (1960), who proposed four measures. However, these measures should not be used in practice, since they tend to underestimate the true nonlinearity (Seber and Wild, 1989). Box (1971) presented a formula for estimating the bias in the least squares estimators, and Gillis and Ratkowsky (1978) concluded that this formula not only predicted bias to the correct order of magnitude but also gave a good indication of the extent of nonlinear behavior of the model, using simulation studies. Bates and Watts (1980) developed measures of nonlinearity based on the geometric concept of curvature. They demonstrated the relationship between their measures and those of Beale, explained why measures of Beale generally tend to underestimate the true nonlinearity and also showed that the bias measure of Box is closely related to their measure of parameter-effects nonlinearity (PE).

Currently, the most used measures of nonlinearity are the curvature measures of Bates and Watts, the bias measure of Box, and the Hougaard's (1985) measure of skewness. These measures are discussed as follows. For further details, see the original works.

Definitions and formulas[1]

Let **X** be the Jacobian matrix for the model:

$$\mathbf{X} = \frac{\partial \mathbf{f}}{\partial \boldsymbol{\theta}} \quad (3)$$

Let **Q** and **R** be the components of the **QR** decomposition of **X** = **QR**of **X**, where **Q** is an $(n \text{ x } n)$ orthogonal matrix. Finally, let **B** be the inverse of the matrix constructed from the first p rows of the $(n \text{ x } p)$ dimensional matrix **R**. Next define:

$$[\mathbf{H}_j]_{kl} = \frac{\partial^2 \mathbf{f}_j}{\partial \theta_k \, \partial \theta_l} \quad (4)$$

$$[\mathbf{U}_j]_{kl} = \textstyle\sum_{mn} \mathbf{B}'_{km} \, [\mathbf{H}_j]_{mn} \, \mathbf{B}_{nl} \quad (5)$$

$$[\mathbf{A}_j]_{kl} = \sqrt{p.mse} \textstyle\sum_m Q'_{jm} \, [\mathbf{U}_m]_{kl} \quad (6)$$

Where **H**, **U**, and the acceleration array **A** are three-dimensional $(n \text{ x } p \text{ x } p)$ matrices. The first p faces of the acceleration array constitute a $(p \text{ x } p \text{ x } p)$ parameter-effects array and the last $(n-p)$ faces constitute the$(n-p \text{ x } p \text{ x } p)$ intrinsic curvature array (Bates and Watts 1980). The previous and subsequent quantities are computed at the leastsquares parameter estimators.

Curvature measures

Bates and Watts (1980) divide the concept of nonlinearity into two parts: intrinsic nonlinearity (IN) and parameter-effects nonlinearity (PE). Relative intrinsic and parameter-effects curvatures can be used to quantify the global nonlinearity of a nonlinear regression model.

The intrinsic nonlinearity (IN) measures the curvature of the solution locus in sample space. For a linear regression model, IN is zero since the solution locus is straight (a line, plane, or hyperplane). For a nonlinear regression model, the solution locus is curved, with IN measuring the extent of that curvature (Ratkowsky, 1990).

The parameter-effect nonlinearity (PE) is a measure of the lack of parallelism and the inequality of spacing of parameter lines on the solution locus at the least-squares solution. As a result, the parameter-effects curvature can be reduced by reparameterization of the model, whereas intrinsic curvature is an inherent property of the model that cannot be affected by reparameterization (Box, 1971;Ratkowsky, 1990).

The maximum parameter-effects and intrinsic curvatures are defined, in a compact form, as:

$$\mathrm{PE} = \max_{\theta} \|\boldsymbol{\theta}' \mathbf{A}^{\tau} \boldsymbol{\theta}\| \quad (7)$$

$$\mathrm{IN} = \max_{\theta} \|\boldsymbol{\theta}' \mathbf{A}^{\eta} \boldsymbol{\theta}\| (8)$$

[1]Adaptedfrom SAS/STAT 15.1 User'sGuide.

Where PE and IN denote the maximum parameter-effects and intrinsic curvatures, while $\mathbf{A}^{\tau}$ and $\mathbf{A}^{\eta}$ stand for the parameter-effects and intrinsic curvature arrays. The maximization is carried out over a unit-vector of the parameter values (Bates and Watts 1980).

The statistical significance of the intrinsic nonlinearity (IN) and parameter-effects nonlinearity (PE) were evaluated by comparing these values with $1/\sqrt{F}$, where $F = F(\alpha, n-p, p)$ is the inverse of Fisher´s probability distribution obtained at significance level α = 0.05, p is the number of parameters and n is the number of observations. The value $1/\sqrt{F}$ may be regarded as the radius of the curvature of the $100(1-\alpha)\%$ confidence region. Hence, the solution locus may be considered to be sufficiently linear within an approximately 95% confidence regionif $IN < 1/\sqrt{F}$ $(\alpha = 0.05)$. Similarly, if $PE < 1/\sqrt{F}$, the projected parameter lines may be regarded as being sufficiently parallel and uniformly spaced (Ratkowsky, 1990).

Bias and skewness

In practice, only a few of the parameters might dominate the global nonlinearity, in which case these parameters are the reparameterization parameters of interest. Unfortunately, the global nonlinearity measures of Bates and Watts do not differentiate the parameters based on their contribution to the overall curvature. Manifestations of nonlinear behavior include significant bias and skewness. Hence, it is essential to estimate at least these basic statistical properties of the parameter estimates in order to identify the reparameterization parameters of interest (Gebremariam, 2014).

The bias and skewness of the parameter estimates of a nonlinear regression model can be estimated by using the bias measure of Box (1971) and the Hougaard (1985) measure of skewness.

Box's bias

The Box's bias represents the discrepancy between the estimates of the parameters and the true values, and as defined by:

$$\mathrm{Bias}(\hat{\theta}) = \hat{E}[\hat{\theta}i - \theta i] = -\frac{\sigma^2}{2p.\mathrm{mse}} \sum_{j,k=1}^{p} \mathbf{B}_{ij} [\mathbf{A}_j]_{kk} \qquad (9)$$

Where mseis the mean square error.

The Box's bias in the least square estimates of the parameters in nonlinear regression can be expressed as a percentage of the least square estimate:

$$\%\mathrm{Bias}(\hat{\theta}) = 100.\,\mathrm{Bias}(\hat{\theta})/\hat{\theta} \qquad (10)$$

According to Ratkowsky (1983), if the percentage bias is greater than 1% in absolute value, the parameter estimate behavior is considered to be significantly nonlinear. In this case, a reparameterization of the model is necessary.

Hougaard's skewness

The degree to which a parameter estimator exhibits nonlinear behavior can be assessed with Hougaard's measure of skewness $g1i$, because of the close link between the extent of nonlinear behavior of an estimator and the extent of nonnormality in the sampling distribution of this estimator.

Hougaard's skewness measure for the *th* parameter is based on the third central moment:

$$g_{1i} = \hat{E}[\hat{\theta}i - E(\hat{\theta}i)]^3 / (\sigma^2 [\mathbf{L}_{ii}])^{3/2} \qquad (11)$$

Where:

$$\hat{E}[\hat{\theta}i - E(\hat{\theta}i)]^3 = -\sigma^2 \sum_{jkl} [\hat{\mathbf{L}}]_{ij} [\hat{\mathbf{L}}]_{ik} [\hat{\mathbf{L}}]_{il} \left([\hat{\mathbf{V}}_j]_{kl} + [\hat{\mathbf{V}}_k]_{jl} + [\hat{\mathbf{V}}_l]_{jk} \right) \quad (12)$$

$$\mathbf{L} = \left(\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \boldsymbol{\theta}'} \frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right)^{-1} \quad (13) \; ; \quad [\mathbf{V}_j]_{kl} = \sum_{m=1}^{n} \frac{\partial F_m}{\partial \theta_j} \frac{\partial^2 F_m}{\partial \theta_k \partial \theta_l} \quad (14)$$

According to Ratkowsky (1990), if $|g1i| < 0.1$, the estimator of the parameter is very close to linear and, if $0.1 < |g1i| < 0.25$, the estimator is reasonably close to linear. For $|g1i| > 0.25$, the skewness is very apparent, and $|g1i| > 1$ indicates considerable nonlinear behavior.

Example

The following is an application of the measures of nonlinearity in linear regression analysis.

Table I shows the growth of *Saccharomyces cerevisiae*during batch ethanol fermentation from sugarcane molasses.Forfurther details, see Leite (2018).

Table I – Dry mass concentration (X) of *S. cerevisae*during batch ethanol fermentation from sugarcane molasses.

t (h)	X (g/L)
0	17.45
1	17.01
2	17.74
3	18.34
4	19.74
5	21.20
6	22.36
7	23.09
8	23.35
9	23.54
10	23.41

The Weibull growth model (Ratkowsky, 1983) was chosen to be fitted to the experimental data:

$$X = \alpha - \beta \exp(-\gamma t^{\delta}) \quad (15)$$

The parameter estimates and their respective measures of nonlinearity were obtained by using the NLIN procedure of the SAS software. The results are shown in Table II. The intrinsic curvature is less than the critical value $(IN < \rho)$. Therefore, the solution locus may be considered to be sufficiently linear within an approximately 95% confidence region. On the other hand, the model exhibited high parameter-effects curvature $(PE > \rho)$. This indicates that at least one parameter in the model is departing from linear behavior, and the Hougaard's skewness and Box'sbias indicate which parameter or parameters are responsible.

As seen earlier in this paper, parameter estimates that present a percentage bias greater than 1% in absolute value are considered to be significantly nonlinear. Similarly, a value of the standardized Hougaard's skewness measure greater than 0.25 in absolute value indicates nonlinear behavior. As can be seen in Table II, according to these guidelines it is possible to conclude that the estimate of γ is the responsible for the far from linear behavior of the model.This parameter estimate is skewed and biased.

Table II: Statistical results of the least-squares estimation for the Weibull growth model.

IN	PE	ρ	Parameter	Estimate	Standard error	Hougaard's Skewness	% Box's bias
0.141	5.411	0.470	α	23.491	0.078	0.13	0.01
			β	6.421	0.148	0.14	0.09
			γ	0.010	0.003	0.66	2.59
			δ	2.871	0.171	0.18	0.27

ρ = critical curvature value ($\rho = 1/\sqrt{F}$), F (α, n-p, p) is the inverse of Fisher´s probability distribution obtained at significance level α = 0.05, p is the number of parameters and n is the number of observations.

The parameter-effects curvature can be reduced by reparameterization of the model. The goal is to find one that have smaller parameter-effects nonlinearity, whose behavior may thereby more closely approach that of a linear model. The first step in reparameterization is to identify the reparameterization parameters of interest. For the nonlinear regression model at hand, the bias and skewness measures identify γ as the parameter that show strong nonlinear behavior. Consequently, this parameter is the reparameterization parameter of interest. After identifying the parameters of interest, it is possible to use different approaches to re-parameterize a nonlinear regression model (Hougaard 1982). However, reparameterization techniques are beyond the scope of this work and will not be discussed.

Ratkowsky (1990) presents a parameterization of the Weibull model with regard to parameter γ:

$$X = \alpha - \beta \exp(-\exp(-\gamma)\, t^{\delta}) \quad (16)$$

Table III showsthe measures of nonlinearity for the new parameterization. The value of the intrinsic curvature was omitted, because reparameterization does not alter the position of the solution locus.As can be seen below, the new parameterization succeeds in making the nonlinear regression model a close-to-linear model. Unlike the original model (Equation 15), for the reparameterization of the Weibull model (Equation16) the parameter-effects curvatures are less than the critical values. Thus, this reparameterized model can be considered close to linear, that is, the parameter estimates are almost unbiased, normally distributed, and have close-to-minimal variance.

Table III - Statistical results of the least-squares estimation for the reparameterizedWeibull growth model.

PE	ρ	Parameter	Estimate	Std. Error	Skewness	% Box's bias
0.406	0.470	α	23.491	0.078	0.13	0.01
		β	6.421	0.148	0.14	0.09
		γ	4.593	0.278	0.18	0.28
		δ	2.871	0.171	0.18	0.27

ρ = critical curvature value ($\rho = 1/\sqrt{F}$), F (α, n-p, p) is the inverse of Fisher´s probability distribution obtained at significance level $\alpha = 0.05$, p is the number of parameters and n is the number of observations.

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