Criteria of goodness of fit test in the selection of non-linear models for the description of biological performances

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A study was undertaken to analyze the goodness of fit of non-linear models, for describing the live weight performance during growth of crossbred Bufalypsos animals under grazing conditions through the utilization of fourteen statistical criteria. The non-linear models in the logistic, Gompertz, von Bertalanffy and Brody parameters were adjusted to the data corresponding to 43 weighings carried out during two lactations (1064). The best criteria to select non-linear models are: coefficient of determination R^2, mean square of the prediction error (MSPE), standard error of estimation, standard error of each parameter, analysis of residuals, mean absolute error (MAE) and percentage of mean absolute error (PMAE). Estimations of parameters, as the analysis of residuals, are inefficient when working with the average of observations. In particular, for buffalo females the logistic was the best fitting model.

Key words: *non-linear models, goodness of fit test, statistical criteria*

Presently, studies using non-linear models in the parameters (commonly known as non-linear models) to formulate inferences and biological interpretations have notably increased.

The description and prediction of animal growth are the main objectives of the fitting of mathematical models to growth studies. The purpose of fitting mathematical models to growth is mainly directed at summarizing, in three or four parameters the productive characteristics to attain its biological interpretation, in the case of non-linear models. Similarly they are indicated for evaluating the response profile of the treatment as time goes by, studying response interactions of sub-populations or treatments with time, identifying in a population the heaviest animals at younger ages, obtaining the variance between and in individuals of great interest in studies of growth curves.

Non-linear mathematical models, empirically developed to relate weight to age, in the description of the growth curve in different species (Freitas 2005) have been very useful to predict growth rates, to estimate nutritional requirements, to evaluate the selection and other aspects of interest for animal management.

Colmenares and Cermeño (1997) have conducted research studies to fit data to different models. These authors have found coefficients of determination (R^2) between 0.688 and 0.93, using the Gamma, Logarithmic, Inverse Polynomial and Parabolic Exponential models, among others. However, the most commonly used models for describing performance and growth of animals and plants are Brody functions (Brody 1945), von Bertalanffy (Bertalanffy 1957), Richards (Richards 1959), Logistics (Nelder 1961) and Gompertz (Laird 1965). More recently the studies of Torres *et al*. (2007), Malhado *et al*. (2008) and Noguera *et al*. (2008) can be cited.

Depending on the species or animal breed, the number of observations or the characteristics observed, the results could vary in respect to the model of best fit to the animal curve (Mazzini *et al*. 2003, McManus *et al*. 2003 and Santoro *et al*. 2005). In Cuba, Fundora *et al*. (2006) worked in the characterization of the growth curve of river buffaloes through a linear model and a logistic non-linear model. Torres *et al*. (2007) developed a stochastic model for predicting the live weight performance in this species. Also Fraga *et al*. (2003) published a study using four linear and non-linear mathematical models for estimating the standard lactation curve of this same species.

In the majority of the investigations two or three statistical criteria were employed to analyze the goodness of fit test of the models, among them, the significance of the model (α) and the coefficient of determination (R^2). Some studies refer to the mean square of the error. However, there are other criteria defined in the statistical literature and that should be considered in studies of model selection, particularly when working with non-linear models.

This study was aimed to analyze the goodness of fit test of non-linear models for describing the live weight performance during growth of crossbred Bufalypso animals under grazing conditions, through the use of twelve statistical criteria.

Materials and Methods

The non-linear models used were:

Logistic model

$$W(t) = \frac{A}{1 + \exp^{-Bt+C}} + \varepsilon$$

Gompertz model

$$W(t) = A\exp^{B\exp(-Ct)} + \varepsilon$$

von Bertalanffy model

$$W(t) = (A - B\exp(-Ct))^3 + \varepsilon$$

Brody model

$W(t) = A(1 - B\exp^{-CT}) + \varepsilon$

Where:

W is the independent variable

A, B and C are parameters of the models

T is the variable measured in the time (month)

ε is random error, normally distributed with mean zero and constant variance

The iterative procedure of estimation of the parameters of Levenberg-Marquardt was applied to carry out the fitting of the models. The convergence of the square sum of the error and of the parameters as Ixe-8 was prefixed by the SPSS regression command for Windows (2002).

For the analysis of the goodness of fit test and the selection of the best models, the statistical criteria published by Chacin (1998), Guerra (2003), Torres and Ortiz (2005) and Malhado (2008), were used, namely:

1. Coefficient of determination R^2 and R^2 fitted by the degrees of freedom
2. MSPE statistics (mean square of the prediction error)
3. SSPE statistics (square sum of the prediction error)
4. Mean square, corresponding to the fitted model
5. Standard error of the estimation
6. Standard error of the parameter estimators
7. Coefficient of variation of the estimators
8. Confidence limits of the parameters
9. Redundancy test of the parameters
10. Diagnosis of the multicolinearity (Durbin-Watson)
11. Coefficients of correlation between predicted and real results
12. Analysis of residuals through:

Medium absolute error (MAE)

Percentage of medium absolute error (PMAE)

Medium error (ME)

Percentage of medium error (PME)

In order to show the usefulness of the statistics selected, the information corresponding to the live weights (LW) of 15 Bufalypso females, born in the Institute of Animal Science (province of Mayabeque, Cuba), were used. Animals were fed under a free suckling system until 10 d. of age and later they had until weaning, restricted suckling and rotational grazing.

Live weights were controlled monthly from birth until 42 months of age. In that moment they were incorporated to reproduction with approximately 370 kg.

For the statistical processing the statistical packages SPSS (V 15.0), Infostat (2001) and Statgrafic (2000) all on Windows, were employed.

Results

In figure 1 are shown the LW obtained and the estimations by the four models tested. Although LW performances were similar, it is confirmed that there are differences in the estimated values, mainly in performance at birth (t = 0) and at the end (t = 42). In this regard, the three phases pointed out by Noguera *et al*. (2008) were identified: 1) acceleration phase, that ideally must have its origin in point (0,0) with very fast and positive growth speed, reaching a maximum value at the inflection point of the curve; 2) deceleration phase from the point of inflection, with growth speed starting to decrease due to physiological factors that restrain growth; 3) linear phase occurring when the animal stops growth or when growth can be considered only for tissue

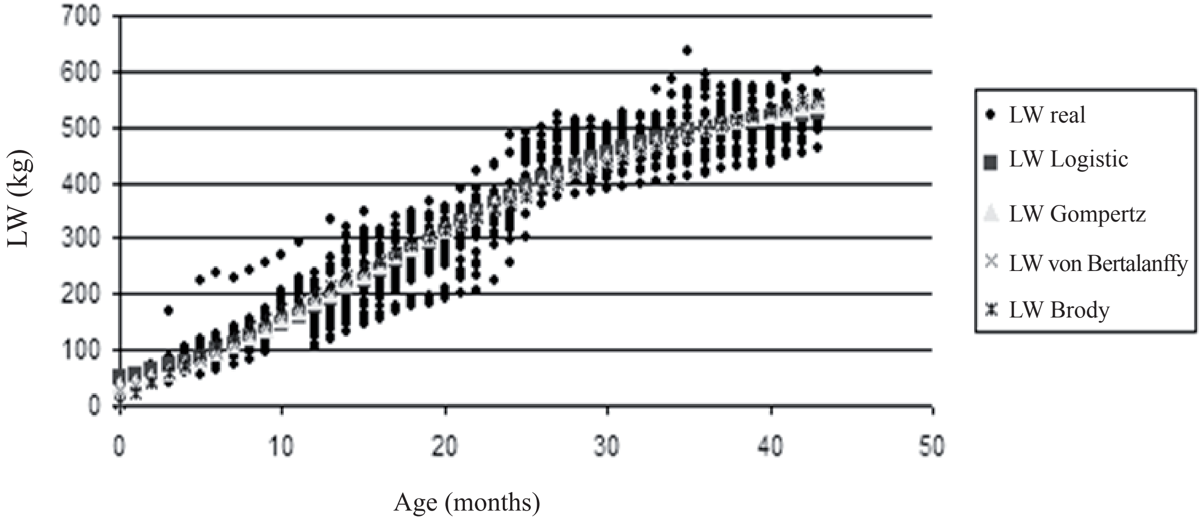

Figure 1. LW performance from birth to 43 months of age, observed and estimated by the fitted models

replacement.

In the four non-linear models tested (Logistic, Gompertz, von Bertalanffy and Brody), the A parameter represented the asymptotic weight of the animal (table 1). It was not necessarily the heaviest weight the animal reached but the asymptotic weight to which it tends at maturity, regardless of the variations. On comparing the estimations obtained through the four models, the highest value corresponded to Brody's model (1053.33 kg) and the lowest, to the logistic (546.34 kg). Similar results were obtained by Malhado *et al*. (2008) in Murrah buffaloes, but in a closer range. The highest value was also for Brody's model (688.0 kg), and the lowest for the logistic curve (601.9 kg). For the A parameter there was overestimation in Brody's model.

According to Abreu *et al*. (2004), the B parameter is the integration factor that fits the initial weight values. Generally, it is associated to the birth weight (degree of animal development at birth to reach the asymptotic weight). However, Noguera *et al*. (2008) stated that this parameter does not have biological significance. Nonetheless, its importance is considered for modeling the sigmoid curve, from birth to the adult age, at 42 months of age.

The C parameter, maturity rate of the animals, is a function between the maximum growth rate and the adult weight of the animal (growth speed). Animals with high C values represent an early maturity regarding to those of similar initial weight. In the estimation of this parameter the opposite of the asymptotic weight occurred, with the estimations of the models considered (0.02 to 0.13). Oliveira *et al*. (2000) in bovines reported a similar performance in the estimations of this parameter.

Results for the twelve statistical criteria are shown in table 2. The first of them, the coefficient of determination R2, is a statistics widely used as indicator of the goodness of fit test and had a higher value for the logistic model. The coefficient of determination, fitted for the degrees of freedom of the model, showed very similar values to that of the unfitted coefficient, since the studied models only have an independent variable, though it turned out redundant to report the two coefficients of determination in cases like these.

The lower medium square of the prediction error (MSPE) also corresponded to the logistic model, increasing in an important way for the other three models tested. The square sum of the prediction error (SSPE) showed the same performance than the mean square of the prediction error. The mean square of the fitted model had inverse performance to the two previous criteria, since it explains the variability of the model. It is concluded that the application of these three criteria in non-linear models with only one independent (dynamic) variable is redundant, though the use of the first is recommended. This offers more information on the variance of errors.

The standard error of the estimation refers to the normal deviation of the residuals. This was also lower for the logistic model, and increased for the remaining ones. The importance of learning the standard error of each parameter is related to the possibility of estimating their confidence intervals and make probability inferences of the range in which they move.

The criteria coefficient of variation of the estimators (%) and redundancy test of the parameters do not supplied information allowing to establish differences between the models tested.

The statistics of Durbin-Watson, of Durban *et al*. (1971), is used to find the serial correlation between the errors, and it is approximately 2 -ρ, where:

ρ is the sampling correlation between e_i, and e_{i-1}

The similarity between the values found for this statistics in the four models tested showed that there was serial correlation (P < 0.05). This was to be expected in models where the independent variable (LW) is measured in time in the same animal. Thus, this criterion did not provide differences, although its determination is necessary to evaluate the risks in the non-compliance of the errors assumed.

The coefficients of correlation between predicted and real results are high and significant (P < 0.001) for all the models. Thus, this criterion did not allow either to differentiate the goodness of fit tests of the models evaluated.

Regarding the criteria for the analysis of the precision of the estimations (analysis of residuals), figure 2 shows the graphic performance of the residuals. The range of variation of the residuals was between -150 and 150. Extreme values corresponded, mainly to the models of Brody and von Bertalanffy (-50 to -100 and of 100 to 150). This graph is indispensable for learning the general performance of the residuals.

With respect to the precision of the estimations, each of the statistics presented (MEA, PMAE, ME and PME)

Table 1. Parameters for each one of the fitted models

Parameters	Logistic	Gompertz	von Bertalanffy	Brody
A	546.34	607.12	8.68	1053.33
B	9.73	2.86	5.70	1.00
C	0.13	0.07	0.06	0.02

Table 2. Statistical criteria for the four models analyzed

Criteria	Logistic	Gompertz	von Bertalanffy	Brody
R2 coefficient of determination	0.936	0.932	0.930	0.922
R2 adjusted by the degrees of freedom	0.935	0.932	0.929	0.922
Statistics MSPE (Mean square of the prediction error)	1748.86	1850.58	1911.86	2120.16
Validation of the predictions of the model				
Statistics SSPE (Square sum of the prediction error	1853797.19	1961612.35	2026577.16	2247364.76
Mean square of the prediction model	47370297.60	47334359.22	4 7312704.28	47239108.41
Standard error of estimation	41.78	42.97	43.68	46.00
Standard error parameters	A ± 4.854 B ± 0.375 C ± 0.003	A ± 9.081 B ± 0.059 C ± 0.002	A ± 0.058 B ± 0.072 C ± 0.002	A ± 68.735 B ± 0.004 C ± 0.002
Confidence limits of parameters	A 536.82 : 555.87 B 8.99:10.46 C 0.13: 0.12	A 589.30: 624.94 B 2.75: 2.98 C 0.07: 0.08	A 8.57: 8.80 B 5.84: 5.56 C 0.06: 0.05	A 918.45: 1188.20 B 0.99: 1.01 C 0.01: 0.02
Coeficiente de variación de los estimadores , %	0.486	0.487	0.486	0.480
Redundancy test of parameters	Without zero value	Without zero value	Without zero value	Without zero value
Durbin Watson (independence of errors)	0.223	0.213	0.224	0.252
Lack of fitting test of the model				
Coefficients of correlation between predicted and real results.	0.967	0.965	0.964	0.960
Analysis of the precision of the estimations (Analysis of residuals)				
MAE (Mean absolute error)	31.95	32.74	33.57	36.15
PMAE (Percentage of the mean absolute error)	12.92	12.60	13.49	16.09
ME (Mean error)	0.221	-1.54	0.551	0.00
PME (Percentage of the mean error)	-3.00	0.524	-1.05	-0.97
Number of interactions	11.0	8.0	4.0	26.0

is based on the prediction errors, that is, in the differences between the values of the data in time t and the prediction of this value made at time t-1. The first two, MEA and PMAE, measure the magnitude of the errors, and the last two, ME and PEM, the bias. The logistic and Gompertz models were those showing the lowest values for the magnitudes of MEA and PMAE errors. However, the ME of the logistic and Brody showed lower values. In regard to PME of Gompertz, was the best and the logistic, the worst. Results obtained for ME and PME are contradictory, therefore, they do not help definitively to the selection of the model with best goodness of fit.

There are other goodness of fit test criteria that could be considered and which take into account the basis hypotheses corresponding to the analysis of regression. These are based on testing statistics for the normality, autocorrelation and homocedasticity hypotheses (Cook and Weisber 1982 and Guerra *et al*. 2003). Figure 3 shows the graphic performance of the normality test in the four models tested. The residuals fulfill this hypothesis and only in the first and last months of measurement these values move away being, therefore, the predictions less accurate.

It is concluded that best criteria for selecting non-

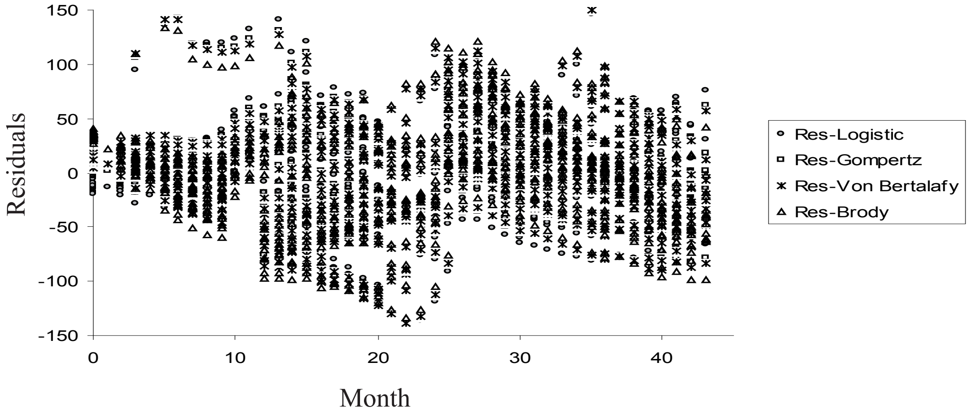

Figure 2. Residual representation for the fitted models

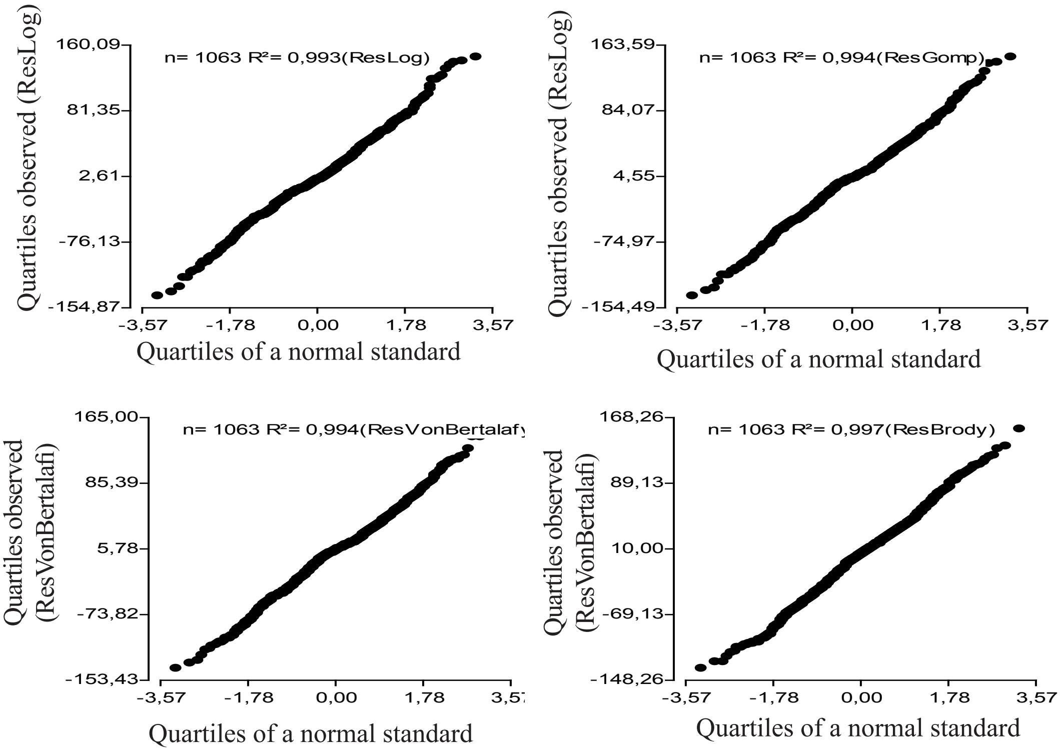

Figure 3. Normality test performance for the residuals in the four models tested

linear models are: coefficient of determination R^2, mean square of the prediction error (MSPE), standard error of the estimation, standard error of each parameter, residuals analysis, mean absolute error (MAE) and percentage of mean absolute error (PMAE). In the case of growth, for Bufalypsa female the best fit was attained with the logistic model.

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