

VARIOUS MODELS FOR THE FITTING OF A LACTATION CURVE AND ITS CURVATURES

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Abstract

An unbiased estimate of a cow's milk yield plays an important role in monitoring the economics of a dairy farm. A representation of the relationship between milk yield and day after calving is the lactation curve. Estimation of total 305-day lactation from incomplete records (data on monthly measurements) is possible using a suitable regression model for fitting the lactation curve. Various models for description of lactation curves have been developed and tested in the past. The goal of this paper will be the analysis of not only advantages and disadvantages of studied models but also difficulties during linearization and when adjusting the initial solution. Standard estimation practice is to linearize the regression function, and to use algorithms of nonlinear regression. So the problem of choice of the highest quality model is revealed, not only from the view of criterion of approximation but also with respect to individual animal data. Unfortunately, many authors point to a large proportion of not fitted lactations. This proportion may also constitute a criterion for model selection. Problem of not fitted lactations is related to the success of convergence in nonlinear regression. Here, studies of nonlinearity measures of regression functions can help. It is necessary to find criteria in order to recognize whether the linearization is reasonable.

Key words: *lactation curve; estimation of 305-day yield; nonlinear regression; curvature of regression function; Bates-Watts curvature.*

1. Introduction

This contribution deals with problem of a 305-day yield estimation, when the need arises to choose a suitable nonlinear function for approximation of the lactation curve. The booming importance of the fitting a lactation curve is observed in the large number of studies on this topic. If approximation function is nonlinear in parameters, then linearization is used so that the problem can be posed as a linear one, and a well known apparatus of linear statistical models is used. However, these papers are not devoted to provide a view to examining the dependence of quality approximation and the curvature of regression function. Many authors report about a large proportion of not fitted lactation cycles (range from 27 to 50 percent) through all the models. Various functions with a known analytical form for fitting of the lactation curve were formed, but research on the issue of Bates and Watts curvature was not carried yet in any article.

In parameter estimation in nonlinear regression models we need to know initial values of unknown parameters. Thus we must know whether uncertainty in the initial solution is essential in estimation, or whether it can be neglected. If a nonlinear regression model is

linearized in a nonsufficient small neighborhood of the true parameter, then all statistical inferences may be deteriorated.

The subject of our research will be to study the suitability of application of lactation models. So construction of linearization domain for all models will be the main subject to investigation in this paper.

2. 305-day Lactation Approximation

2.1 Models

Various models have been developed and tested in the past (see Golebiewski et al., 1995; Leon-Velarde et al., 1995; Wood, 1985; Silvestre et al., 2006; Marek et al., 2015):

Gaines [in 1927]

$$f(\boldsymbol{\beta}, x) = \beta_1 \exp(-\beta_2 x), \quad (1)$$

Nelder [in 1966]

$$f(\boldsymbol{\beta}, x) = \frac{x}{\beta_1 + \beta_2 x + \beta_3 x^2}, \quad (2)$$

Wood [in 1967]

$$f(\boldsymbol{\beta}, x) = \beta_1 \exp(\beta_2 \ln(x)) \exp(-\beta_3 x), \quad (3)$$

Papajesic and Boder [in 1988]

$$f(\boldsymbol{\beta}, x) = \frac{\beta_1 \exp(\beta_2 \ln(x))}{\cosh(\beta_3 x)}, \quad (4)$$

McMillan [in 1970], Schaeffer [in 1977]

$$f(\boldsymbol{\beta}, x) = \beta_1 \exp(-\beta_2 x) (1 - \exp(-\beta_3 (x - \beta_4))), \quad (5)$$

Ning-Yang [in 1983]

$$f = \beta_1 \exp\left(\frac{-\beta_2 x}{1 - \exp(-\beta_3 (x - \beta_4))}\right), \quad (6)$$

Marek and Zelinková [in 2010]

$$f(\boldsymbol{\beta}, x) = \beta_1 + \frac{2\beta_2\beta_3}{(x - \beta_3)^2 + \beta_4^2}. \quad (7)$$

All nonlinear models f tries to explain dependence of variable Y (daily milk yield) on explaining variable x (time from calving):

$$Y = f(\boldsymbol{\beta}, x) + \varepsilon, \quad (8)$$

where $\boldsymbol{\beta} = (\beta_1, \beta_2, \dots, \beta_k)'$ is unknown vector parameter. Measurements of daily milk yield Y from dataset of monthly measurement are at our disposal. Our problem actually lies in estimating the values of the vector parameter $\boldsymbol{\beta}$ based on nonlinear regression. Cf. (Kubáček, 1995).

2.2 Measurements

In today's cowshed processes daily milk yield measurement is performed only once a month. Therefore, we need an approximation of lactation curve. Based on this approximation the estimate of total 305-day milk yield may be obtained. The study will be conducted for 10 selected cows.

The corresponding pairs of observations at several cows are given in Table 1 and Table 2. Notice that the numbers of daily measurements are different.

On these data we will present the numerical and graphical results of estimation and we will analyze linearization features of all models.

Table 1: The data on monthly measurements of the daily milk yield during particular lactation of several cows (kg)

Cow, order of lactation	Yield Y_1, Y_2, \dots, Y_n [in kilogram]
43539-7	41.2, 42.0, 39.6, 35.2, 26.2, 30.8, 30.6, 28.4, 23.2, 20.6, 23.0
411503-1	35.6 38.9 41.5 41.3 38.0 38.4 39.6 41.4 39.5 37.5 32.0
411572-1	52.4 50.0 43.8 51.1 49.3 45.6 50.9 45.5 44.7 39.8 42.0
411578-1	46.0 39.1 37.1 39.6 44.1 41.6 37.1 39.0 34.2 30.1
411583-1	43.6 36.1 38.7 38.5 39.5 42.1 35.1 36.0 32.3 27.4
411587-1	47.6 52.2 52.4 50.0 43.4 41.0
411605-1	43.8 39.4 37.3 39.6 39.9 38.8 35.8 35.2 26.9 31.2 26.0
411896-1	37.2 45.2 44.2 37.0 39.4 37.6 38.2 34.2 34.9 24.6
411905-1	25.0 42.7 31.0 35.5 35.3 34.2 34.9 33.3 30.0 26.6 23.1
411921-1	31.3 35.7 27.1 26.6 26.9 30.6 28.0 27.4 22.9 20.0 13.7

Source: the author.

Table 2: The order of the day in lactation of several cows

Cow, order of lactation	Day of measurement (the order of the day in lactation) t_1, t_2, \dots, t_n
43539-7	19, 51, 81, 114, 143, 172, 205, 214, 244, 271, 325
411503-1	16 40 72 102 130 166 194 226 254 283 313
411572-1	43 67 99 129 157 193 221 253 281 310 340
411578-1	21 53 88 112 144 174 202 238 266 298
411583-1	28 60 95 119 151 181 209 245 273 305
411587-1	32 63 94 124 155 185
411605-1	11 45 69 100 131 166 193 225 253 283 302 333
411896-1	29 60 91 119 150 180 211 241 272 303
411905-1	17 52 76 108 138 166 202 230 262 290 319
411921-1	43 71 103 131 160 190 222 257 285 314 343

Source: the author.

3. Linearization of Nonlinear Model and Curvature of Nonlinear Model

Estimates of unknown parameters can be computed by method of nonlinear regression. We can estimate the values of unknown parameters occurring in studied nonlinear model by linearization of the model and by ordinary least squares method.

Criterion for estimation is minimization of functional

$$S_e = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2, \hat{Y}_i = f(\hat{\beta}, x_i). \quad (9)$$

3.1 Linearization

If we carry out a Taylor expansion of $f(\beta, x)$ about point β_0 , where β_0 is a vector of suitable initial values, we can transform nonlinear model (8) to linear model

$$\mathbf{Y} - \mathbf{Y}_0 \sim \mathbf{N}[\mathbf{F}\beta, \Sigma], \quad (10)$$

where $\mathbf{Y}_0 = f(\beta_0, x)$ and $\mathbf{F} = (\partial f(\beta_0, x) / \partial \beta')$.

Notation $\mathbf{Y} \sim \mathbf{N}[\mathbf{F}\boldsymbol{\beta}, \boldsymbol{\Sigma}]$ means that observation vector \mathbf{Y} (with elements Y_1, \dots, Y_n) has (symbol \sim) multinomial normal distribution with mean value $\mathbf{F}\boldsymbol{\beta}$ and covariance matrix $\boldsymbol{\Sigma}$. For example, in model (1) the i -th row of matrix \mathbf{F} takes the form of

$$\mathbf{F}_{i.} = \frac{\partial f(\boldsymbol{\beta}_0)}{\partial \boldsymbol{\beta}'} = \left(\frac{\partial f}{\partial \beta_j} \right)_{\beta_0} = \left(\frac{\partial f}{\partial \beta_1}, \frac{\partial f}{\partial \beta_2} \right)_{\beta_0} = \left(e^{-\beta_2^0 x}, -\beta_1 x e^{-\beta_2^0 x} \right).$$

The elements of this matrix can be easily computed through deriving functions f described in (1–6).

In our linearized model $\mathbf{Y} - \mathbf{Y}_0 = \mathbf{F}(\boldsymbol{\beta} - \boldsymbol{\beta}_0)$ a correction $\delta \hat{\boldsymbol{\beta}}$ of initial vector $\boldsymbol{\beta}_0$ is

$$\delta \hat{\boldsymbol{\beta}} = (\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{F}')^{-1} \mathbf{F}'\boldsymbol{\Sigma}^{-1}(\mathbf{Y} - \mathbf{Y}_0). \quad (11)$$

The covariance matrix of the $\hat{\boldsymbol{\beta}}$ estimator is given by

$$\text{var}(\hat{\boldsymbol{\beta}}) = (\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{F}')^{-1}. \quad (12)$$

We can now place the estimate as a new initial vector. The iterative process is continued until fulfillment of the stopping criterion.

A special issue in our calculations is the choice of initial estimate, where values may be gained by information in fitting a similar lactation curve or a using values suggested as “about right” by the experimenter, based on his experience and knowledge. In Table 3 recommended initial vectors are reported according to Leon-Velarde et al. (1985). In the same table, estimates obtained from (10) are presented. Please compare the difference between the initial vectors and estimated vectors.

Table 3: Initial estimates of unknown parameters of regression models for cow No. 43539, lactation No. 7.

Model	$\boldsymbol{\beta}_0$	$\hat{\boldsymbol{\beta}}$
Gaines	(45, 0.002)	(45.19, 0.0024)
Nelder	(0.09, 0.02, 0.05)	(0.0949, 0.0174, 0.0001)
Wood	(5, 0.8, 0.002)	(39.4292, 0.0408, 0.0028)
Papajesic and Boder	(35, 0.06, -0.007)	(52.96, -0.0714, -0.0036)
McMillan	(40, 0.05, -8, 0.005)	(47.02, 0.37, 12.10, 0.0026)
Ning-Yang	(20, -0.03, -0.1, 0.7)	(24.51, -17.13, -0.02, -266.76)
Marek and Zelinková	(14, -1241, -333, 82)	(19.6, -7992.1, -226.9, 34.4)

Source: Marek et al. (2015).

The linearization method has possible drawbacks: the sum of squares may not converge for all cows. So, the sum of squares may oscillate or increase without bound. It is known, that if the model contains strong nonlinearity, this will cause impossibility of linearization and bad statistical properties of estimates. In this context, linearization regions are constructed. (cf. Kubáček, 1995).

3.2 Linearization Domains

The measure of nonlinearity is described by several characteristics. The intrinsic curvature is a key tool in nonlinear regression analysis (Bates and Watts, 1980).

Given a real-valued function $f(\boldsymbol{\beta}, \mathbf{x})$, Bates and Watts intrinsic curvature at point $\boldsymbol{\beta}_0$ is

$$C^{(int)}(\boldsymbol{\beta}_0) = \sup \left\{ \frac{\sqrt{\boldsymbol{\kappa}'(\boldsymbol{\beta}) \boldsymbol{\Sigma}^{-1} \mathbf{M}_F^{\boldsymbol{\Sigma}^{-1}} \boldsymbol{\kappa}(\boldsymbol{\beta})}}{\boldsymbol{\beta}' \mathbf{C} \boldsymbol{\beta}} : \boldsymbol{\beta} \in R^k \right\}, \mathbf{C} = (\mathbf{F}' \mathbf{F})^{-1} \mathbf{F}' \quad (13)$$

The projection matrices are given by formulas $\mathbf{P} = \mathbf{F} (\mathbf{F}' \mathbf{F})^{-1} \mathbf{F}'$ and $\mathbf{M}_F^{\boldsymbol{\Sigma}^{-1}} = \mathbf{I} - \mathbf{P}$. Functional $\boldsymbol{\kappa}(\boldsymbol{\beta})$ is intended by

$$\boldsymbol{\kappa}(\boldsymbol{\beta}) = (\mathbf{H}'_1 \boldsymbol{\Sigma}^{-1} \mathbf{H}_1, \dots, \mathbf{H}'_n \boldsymbol{\Sigma}^{-1} \mathbf{H}_n). \quad (14)$$

So it is necessary to prepare the matrices of second partial derivatives $\mathbf{H}_1, \dots, \mathbf{H}_n$, to which we will gradually substitute individual observations.

For example, in model (1) matrix \mathbf{H}_i take the form of

$$\mathbf{H}_i = \frac{\partial^2 f(\boldsymbol{\beta}_0)}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}'} = (H_{i,j}) = \left(\frac{\partial^2 f}{\partial \beta_i \partial \beta_j} \right) \Big|_{\boldsymbol{\beta}_0} = \begin{pmatrix} 0 & -x_i e^{-\beta_2^0 x_i} \\ -x_i e^{-\beta_2^0 x_i} & \beta_1 x_i^2 e^{-\beta_2^0 x_i} \end{pmatrix}, i = 1, \dots, n.$$

In (Kubáček, 1995) a test of intrinsic linearity of model $H_0: \mathbf{K}^{(int)} = 0$ is considered. This test can be used to derive the following linearization criterion. Set O_b , observes bias of the linear estimator. If $\boldsymbol{\beta}$ in O_b , where

$$O_b = \left\{ \boldsymbol{\beta} : \boldsymbol{\beta}' \mathbf{F}' \boldsymbol{\Sigma}^{-1} \mathbf{F} \boldsymbol{\beta} < \frac{2\sqrt{\delta_{\max}}}{C^{(int)}(\boldsymbol{\beta}_0)} \right\}, \quad (15)$$

then

$$\forall \{\mathbf{h} \in R^k\} |b_h^*(\boldsymbol{\beta})| \leq c \sqrt{\mathbf{h}' \mathbf{C}^{-1} \mathbf{h}}. \quad (16)$$

If the intrinsic curvature of the nonlinear regression model is too big, then the situation may arise that model cannot be linearized. To assess the possibility of linearization, the confidence domain is rendered; that is, it is compared with the confidence domain.

An algorithm published by Kubáček (1995) can be used for calculation of $C^{(int)}$, cf. [6] Remark 5.1. In first step, we choose an arbitrary vector $\boldsymbol{\delta} \mathbf{u} \in R^k$, such that $\mathbf{u}' \mathbf{u} = 1$. After that, we determine the vector $\boldsymbol{\delta} \mathbf{s}$ defined as

$$\boldsymbol{\delta} \mathbf{s} = (\mathbf{F}' \boldsymbol{\Sigma}^{-1} \mathbf{F})^{-1} \cdot (\mathbf{H}_1 \boldsymbol{\delta} \mathbf{u}_1, \mathbf{H}_2 \boldsymbol{\delta} \mathbf{u}_1, \dots, \mathbf{H}_n \boldsymbol{\delta} \mathbf{u}_1) \boldsymbol{\Sigma}^{-1} \mathbf{M}_F^{\boldsymbol{\Sigma}^{-1}} \boldsymbol{\kappa}(\boldsymbol{\delta} \mathbf{u}_1). \quad (17)$$

Then, we identify the vector $\boldsymbol{\delta} \mathbf{u}_2 = \boldsymbol{\delta} \mathbf{s} / \sqrt{\boldsymbol{\delta} \mathbf{s}' \boldsymbol{\delta} \mathbf{s}}$. In the last step, we verify the inequality given as $\boldsymbol{\delta} \mathbf{u}'_2 \boldsymbol{\delta} \mathbf{u}_2 \geq 1 - tol$, where tol is sufficiently small positive number. If the stopping criterion is satisfied, we terminate the iterative process and intrinsic curvature is given after substitution $\boldsymbol{\beta} = \boldsymbol{\delta} \mathbf{u}_2$ into (13). If the inequality is not satisfied, we return to the first step of the algorithm where we update vector $\boldsymbol{\delta} \mathbf{u}$ by $\boldsymbol{\delta} \mathbf{u}_2$.

If the true value of parameter $\boldsymbol{\beta}$ lies in the linearization set, the nonlinear model can be replaced by a linear model. Often it is contemplated that linearization can be used, if confidence domain is covered with linearization domain.

3.3 Confidence Domain

The confidence domain (see Kubáčková, pp. 158-159) for the parameter $\boldsymbol{\beta}$ is a set in parametric space of $\boldsymbol{\beta}$, which covers the true value of $\boldsymbol{\beta}$ with a given probability $1 - \alpha$.

Formula for $(1 - \alpha)$ % -confidence domain is given by

$$\varepsilon_{1-\alpha}(\boldsymbol{\beta}) = \left\{ \mathbf{u} : \mathbf{u} \in \Theta_{\boldsymbol{\beta}}, (\mathbf{u} - \hat{\boldsymbol{\beta}})[\text{var}(\hat{\boldsymbol{\beta}})]^{-1}(\mathbf{u} - \hat{\boldsymbol{\beta}})' \leq \chi_k^2(1 - \alpha) \right\}. \quad (18)$$

The symbol $\chi_k^2(1 - \alpha)$ denotes the $(1 - \alpha)$ -quantile of a χ^2 distribution with k degrees of freedom.

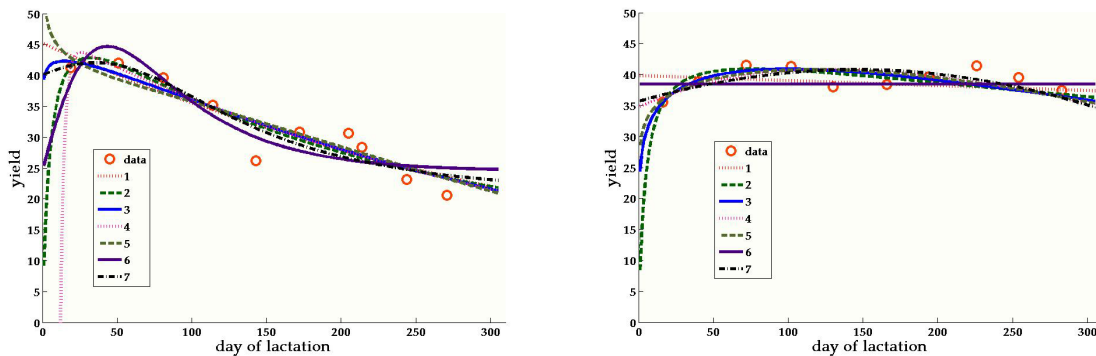
4. Numerical Study

4.1 Quality of Fitting

Firstly, we present graphs and results for several cows. We will particularly comment on whether the parameter estimates are within a reasonable range. This requires, not only evaluating the parameter estimates, but also their residuals. Unusually large standard errors are a sign of convergence problems, even if convergence was apparently achieved in the previous process of estimation.

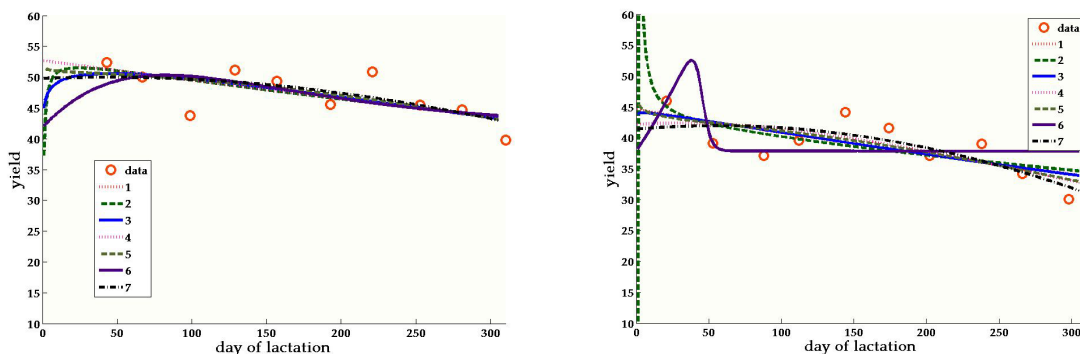
In the next figures, approximations of the lactation curves of all cows and graph of residuals are presented. If a plot of residual versus predictor values, or fitted values shows suspicious behavior, then the assumption of independence of the disturbances may be inappropriate.

Figure 1: Cow No. 43539, 7th lactation — Cow No. 411503, 1st lactation.



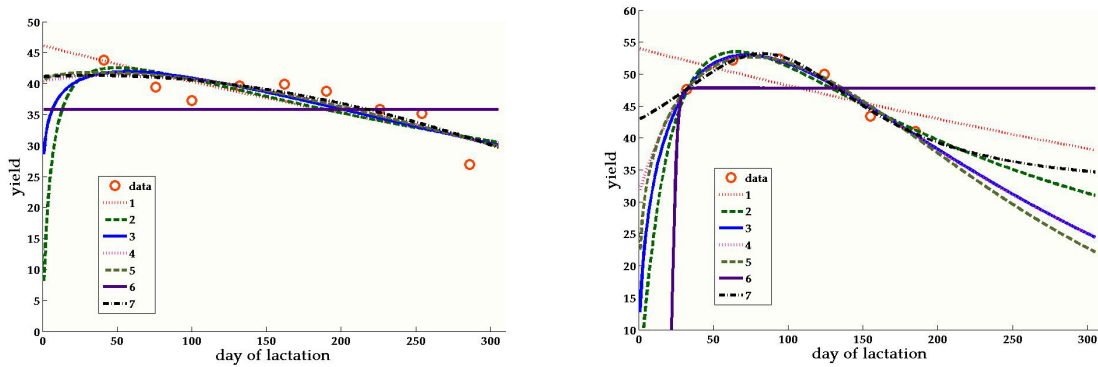
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Figure 2: Cow No. 411572, 1st lactation — Cow No. 411578, 1st lactation.



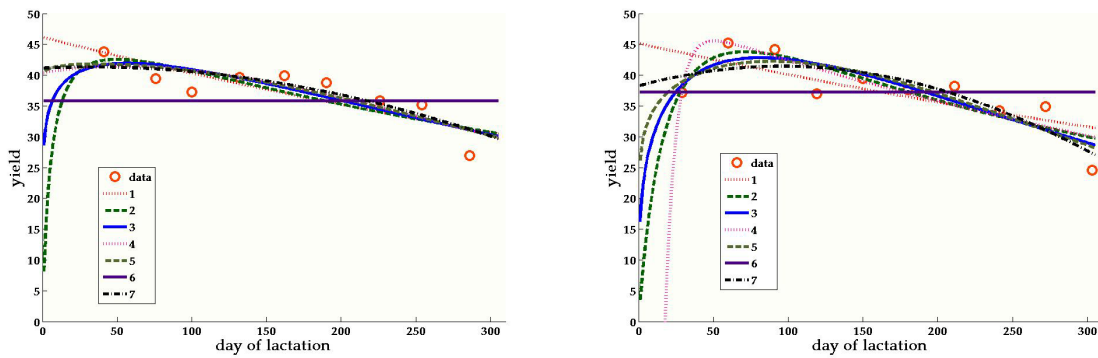
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Figure 3: Cow No. 411583, 1st lactation — Cow No. 411587, 1st lactation.



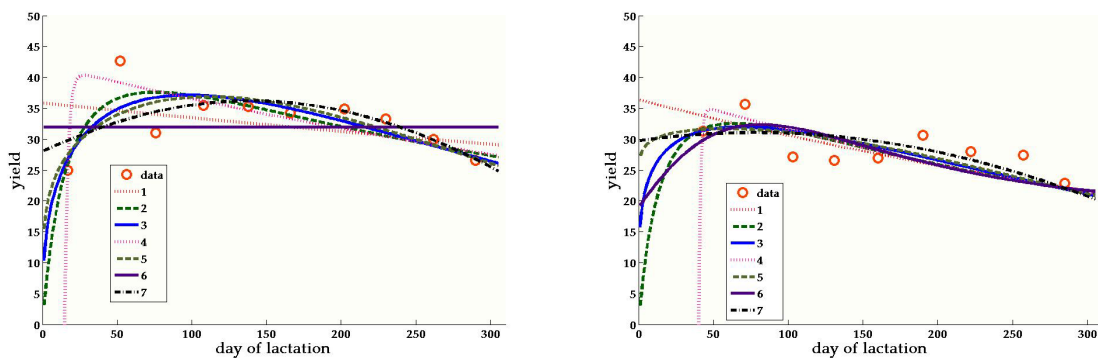
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Figure 4: Cow No. 411605, 1st lactation — Cow No. 411896, 1st lactation.



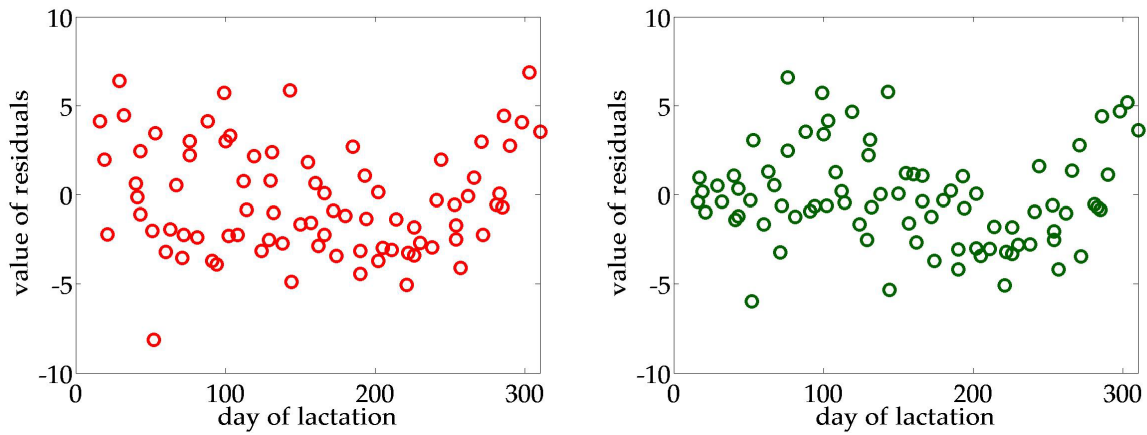
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Figure 5: Cow No. 411905, 1st lactation — Cow No. 411921, 1st lactation.



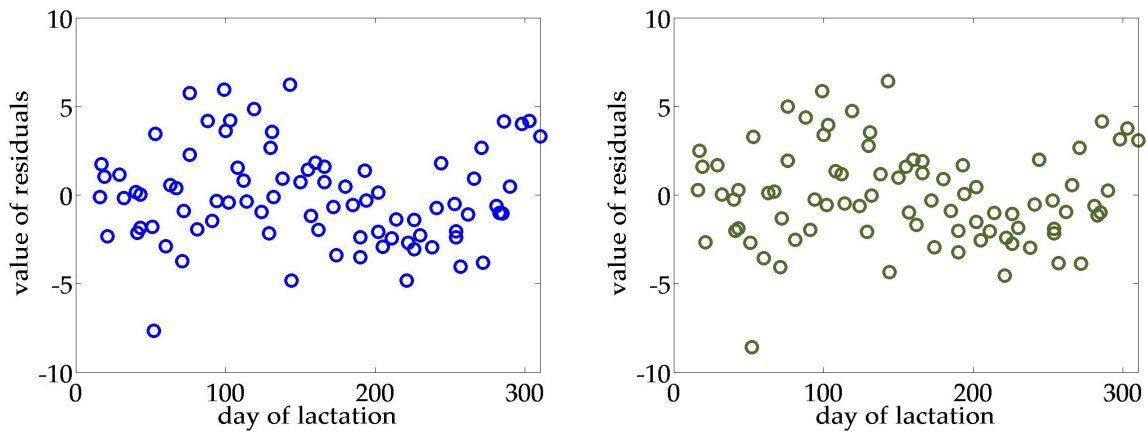
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Figure 6: Graph of residuals: Gaines function — Nelder function.



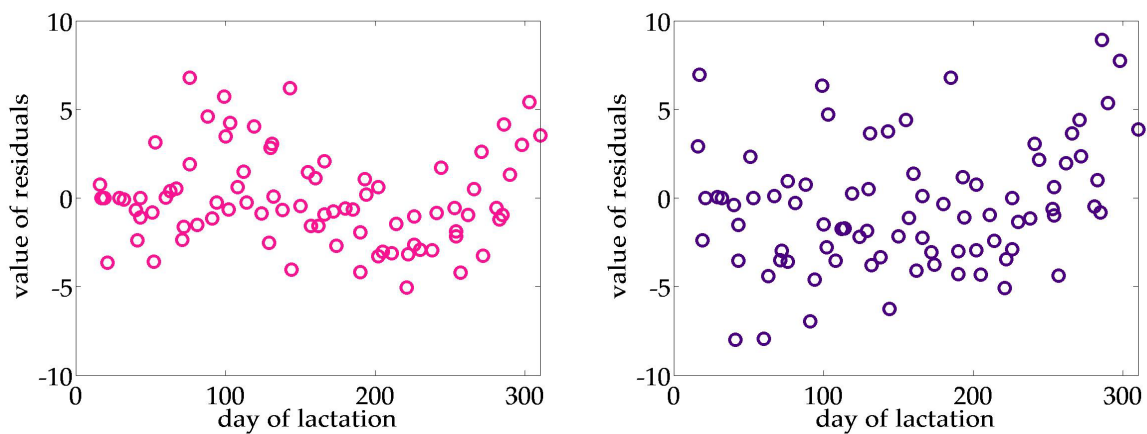
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Figure 7: Graph of residuals: Wood function — Papajesic and Bodero function.



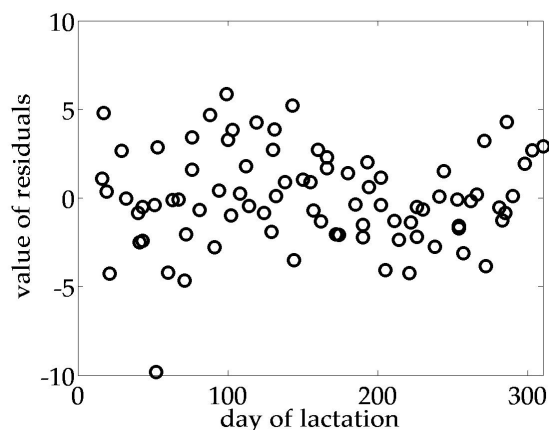
Source: the author.

Figure 8: Graph of residuals: McMillan function — Ning-Yang function.



Source: the author.

Figure 9: Graph of residuals: Marek and Zelinková function.



Source: the author.

Plotting residuals is a simple effective method for checking the adequacy of a model. Unfortunately, most residuals contain graphical formations “sinus” or “small writing omega”.

The largest deviation occurred in our models about the hundredth day. At the beginning of lactation cycle a problem raised in the Nelder model. Large residual occurs at the end of the lactation cycle in the Ning-Yang model.

However, for several cows the McMillan function and the Ning-Yang function take negative values at the beginning of lactation cycle. Several estimates of the Papajesic, Bodero function are convex, so this model is unacceptable.

These facts recommend the use of Wood or Marek, Zelinková model.

The adjusted indexes of determination varied among 0.8 in all models, cf. Table 4.

We can see, that high indexes of determination do not provide a suitable approximation of the lactation curve from the biological point of view.

Table 4: Characteristics of estimate: Cow No 43539

Model	Adjust. R^2	SS	$s = SS/(n-p)$
Gaines	0.8314	8.6863	1.0858
Nelder	0.8370	8.2684	1.1812
Wood	0.8122	9.5232	1.3605
Papajesic and Bodero	0.7837	10.9718	1.5674
McMillan	0.7953	10.1704	1.6951
Ning-Yang	0.7441	12.7121	2.1187
Marek and Zelinková	0.8344	9.5985	1.3712

Source: "the author".

4.2 Lactation models: comparing of curvatures and comparing of linearization domains

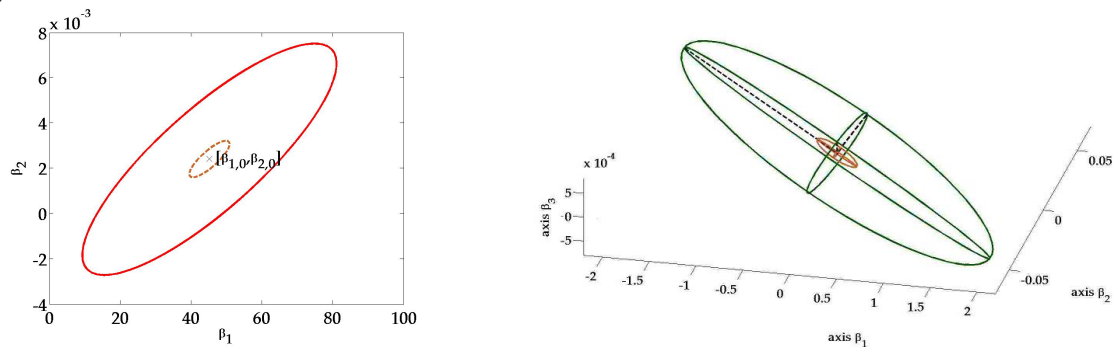
The aim of this section is to compare linearization domain of studied regression model with confidence domain.

Table 5: Curvature of lactation models; $\delta_{\max} = 1.1540$.

Model	$K^{(int)}$
Gaines	0.00887451
Nelder	0.00360315
Wood	0.00046338
Papajesic and Bodero	0.10805379
McMillan	0.00236956
Ning-Yang	0.01718719
Marek and Zelinková	0.00011693

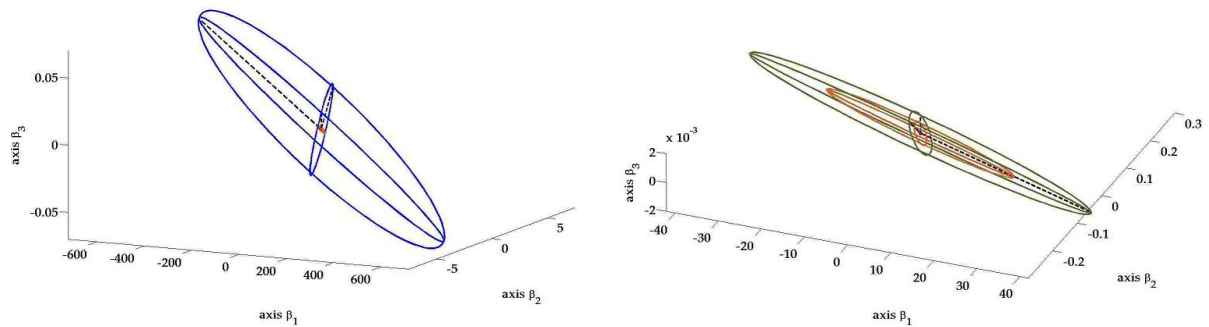
Source: the author.

Figure 10: Linearization and confidence domain: Gaines function — Nelder function.



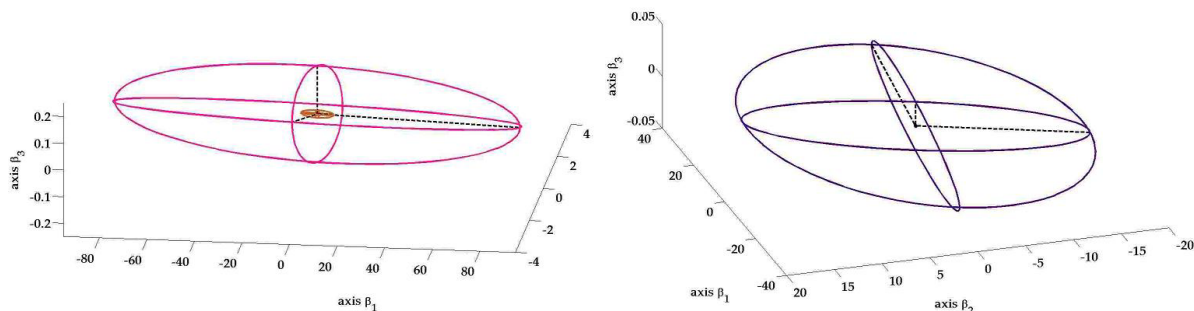
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Figure 11: Linearization and confidence domain: Wood function — Papajesic and Bodero function.



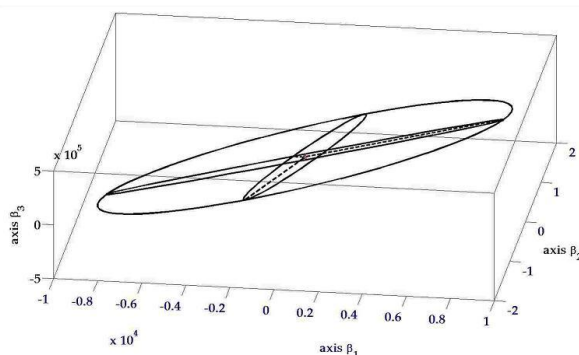
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Figure 12: Linearization and confidence domain: McMillan function — Ning-Yang function.



Source: the author.

Figure 13: Linearization and confidence domain: Marek and Zelinková function.



Source: the author.

The linearization is possible even in the case that we can provide an initial solution lying in this domain. Linearization region of all models is large in comparison with the confidence ellipse. Nonlinear model can be linearized in all situations, where we can choose an initial solution from linearization domain. In practice a small linearization domain brings biased estimates. Criterion was almost not met in the Papajesic model.

Less problems will occur in models with the largest linearization domains and smallest confidence domain (Wood; Ning-Yang; Marek and Zelinková; McMillan as well as Nelder models). But a critical discussion of subsection 4.1 leads to the recognition, that Ning-Yang, McMillan and Nelder model are not suitable.

5. Conclusion

A linearization of nonlinear functions causes an uncertainty in an estimation of unknown parameters of the regression model. Various lactation models are differently sensitive to the quality of the initial solution. On the basis of the Bates Watts curvature, the best models for approximation of lactation curve are Nelder, Wood, McMillan and Marek models. But more facts lead to recommending the use of model Wood or Marek and Zelinková. Great care is also necessary for their use. If the initial solution does not lie in the (very small!) linearization domain, then uncertainty in the initial solution is essential in estimation, and it leads to a completely wrong estimate of the lactation curve. This fact causes a large proportion of not fitted lactation curves in previous studies.

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