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The multiplicative heteroscedastic Von Bertalanffy model

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Abstract. In this work, we propose a heteroscedastic Von Bertalanffy growth model considering a multiplicative heteroscedastic dispersion matrix. All estimates were obtained using a sampling based approach, which allows information to be input beforehand with lower computational effort. Simulations were carried out in order to verify some frequentist properties of the estimation procedure in the presence of small and moderate sample sizes.

The methodology is illustrated on a real Kubbard female chicken corporeal weight dataset.

1 Introduction

Sigmoidal growth models have been widely used for modeling animals and plant growths. Khamis et al. (2005) presented 12 nonlinear growth models for oil palm yield growth. Ersoy et al. (2006), established growth curve parameters of American bronze turkeys. Sengul et al. (2005), used four different nonlinear models to define growth curves of large white turkeys. Among the S-shaped pattern models which are used to explain animal and plant growth, we can mention the Brody, Richards, Gompertz, logistic, Von Bertalanffy, Weibull and Morgan–Mercer–Flodin growth models. Usually, inferences in the parameter models are based on the classical approach, which consists of obtaining estimators via least squares or maximum likelihood methods in a homoscedastic error asymptotic normal distribution.

Although assuming that homoscedasticity leads, at least in principle, to a statistically feasible procedure, the presence of heteroscedasticy in growth datasets is not uncommon in practice. For instance, consider the dataset consisting of measures of corporeal weights of 13 Kubbard female chickens, fed on a comercial diet at the Empresa Brasileira de Pesquisa Agropecuária (Freitas, 2005). In this experiment, the birds were identified by a numbered aluminum ring placed on their right wing. All birds were weighed weekly for a period of seven weeks. The evaluations were always done at the same time and on the same weekday. The individual weights of the birds are shown in Table 1 where the weekly bird average weight

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Table 1 *Corporeal weights (in grams) with the average weekly bird weights and their standard deviations*

	Week						
Chicken	1	2	3	4	5	6	7
1	122	291	500	712	1041	1430	1760
2	129	314	551	830	1096	1485	1820
3	133	308	563	857	1085	1422	1660
4	135	348	584	854	1109	1493	1760
5	110	286	556	782	1105	1538	1870
6	130	302	518	740	1009	1337	1630
7	133	336	630	831	1108	1514	1760
8	138	337	618	937	1144	1570	1820
9	153	352	637	830	1052	1464	1820
10	138	332	484	767	1132	1548	1870
11	137	329	576	844	1127	1391	1660
12	133	298	464	670	988	1387	1720
13	142	345	598	844	1172	1570	1860
Average	133.310	321.380	559.920	807.540	1089.850	1473.000	1770.000
S.D.	2.800	6.290	15.390	19.690	14.880	20.880	22.950

and their respective standard deviations are also found. It can be observed that the weekly standard deviations increase with time. However, fitting one of those models described above by considering the standard classical approach it can be assumed that the error terms are identically distributed which is definitely not the female chicken data case.

Testing for heteroscedasticity in sigmoidal growth models can be conducted using the Goldfeld-Quandt test (Goldfeld et al., 1965). Recently, Lin and Wei (2003, 2004) discussed tests for nonconstant variance and/or correlation in the framework of nonlinear regression models. Cook and Weisberg (1983) discussed a graphic procedure for checking the assumption of homoscedasticity for the usual regression model. This procedure consists of plotting the ordinary least squares residuals against fitted values or an explanatory variable. This procedure can be also used in the case of sigmoidal growth model. In these cases, there is evidence that variance depends on the time if the graph has a megaphone shaped pattern. As we shall see later in the paper, this is the case for the Kubbard female chicken dataset.

In order to accommodate the presence of heteroscedasticy in growth datasets, in this paper we propose a heteroscedastic sigmoidal growth model, in which the deterministic component is given by the Von Bertalanffy model (Von Bertalanffy, 1957). The main idea is to consider a heteroscedastic multiplicative error in the modelling. The choice of the Von Bertalanffy sigmoidal growth model is partly based on its interpretative appeal. This model was proposed as a mechanistic model for animal growth, considering the difference between the metabolic forces of anabolism and catabolism. However, our approach is general and, in principle, may be extended to other sigmoidal growth models.

The paper is organized as follows. Section 2 presents the model formulation. The Inferential procedure and model comparison are presented in Section 3. Section 4 presents the results of a simulation study performed in order to analyze the frequentist properties of the estimation procedure based on our resampling scheme, as well as, to examine the coverage probabilities (CPs) of the asymptotic confidence intervals for the parameters. In Section 5, our methodology is illustrated on the real female chicken dataset presented above. Final comments in Section 6 conclude the paper.

2 Model formulation

The well-known Von Bertalanffy model is given by (Von Bertalanffy, 1957),

$$y_t = \alpha\bigl(1 - \beta \exp(-\gamma t)\bigr)^3 + \varepsilon_t, \tag{2.1}$$

where α is the asymptote of the curve, β determines the intercept, γ determines the growth rate and ε is a vector $n \times 1$ of i.i.d. normal errors with mean zero and specified variance–covariance matrix, n is the number of time observation, t, and y_t is the animal averaged weight in time t. Following Lester, Shute and Abrams (2004) the Von Bertalanffy model is a three parameter sigmoidal growth model which provides a good description of somatic growth after animal maturity. Its parameters are simple functions of age at maturity and reproductive investment.

Usually, the inference in the parameters is based on a homoscedastic error term model. In this case, $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n$ are independent and identically distributed normal random variables with mean zero and unknown variance σ^2. However, when there is a need to explain the phenomenon of growth in the presence of heterogeneity, a heteroscedastic structure for the error terms in the model should be introduced.

In this article, we consider the multiplicative heteroscedasticity model discussed by Harvey (1976). This choice of heteroscedasticity consists of expressing the variance σ^2 in the form

$$\sigma_i^2 = \sigma^2 t^\lambda, \tag{2.2}$$

where λ is an unknown parameter which determines the degree of heteroscedasticity. Although we may express the heteroscedasticity in different ways, the form (2.2) seems to be a natural choice, since it represents a log-linear relationship between $\log(\sigma_i^2)$ and $\log(t)$, with intercept parameter equals to $\log(\sigma^2)$ and slope parameter equals to λ. Moreover, in our case, from the practical point of view, the multiplicative error in the modelling can be empirically justified for the Kubbard female chicken dataset as will be pointed out in the application section.

Under the conditions stated above, the error terms ε_i are assumed to be

$$\varepsilon_i \sim N(0, \sigma^2 t^{\lambda}).$$

3 Inference

Concerning inference, we adopted a full Bayesian approach. The likelihood function, prior distributions for the parameters in the model, details of the MCMC algorithm and the model comparison are described in this section.

The likelihood function of $\boldsymbol{\theta}$ and σ, where $\boldsymbol{\theta} = (\alpha, \beta, \gamma, \lambda)$, given the sample vectors $\mathbf{t} = (1, 2, \ldots, n)'$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)'$ is obtained by the product of the error density functions, that is,

$$\begin{aligned} L(\boldsymbol{\theta}, \sigma | \mathbf{t}, \mathbf{y}) = (2\pi\sigma^2)^{-n/2} \prod_{t=1}^{n} t^{-\lambda/2} \\ \times \exp\left\{ -\frac{1}{2\sigma^2} \sum_{t=1}^{n} t^{-\lambda} \left[y_t - \alpha \left(1 - \beta \exp(-\gamma t)\right)^3 \right]^2 \right\}. \end{aligned} \tag{3.1}$$

The target distribution for inference is the posterior of the parameters of interest $\alpha, \beta, \gamma, \lambda$ and σ. For this, we need to obtain the marginal posterior densities, which are obtained by integrating the joint posterior density with respect to each parameter. The posterior distribution is proper considering proper prior distribution (Ibrahim et al., 2001). However, regardless of the prior distribution chosen, the joint posterior distribution for the proposed model is analytically intractable. As an alternative we used one of Markov chain Monte Carlo methods (MCMC), for example, Gibbs Sampling and the Metropolis–Hastings algorithm (Chib and Greenberg, 1995).

Although not required for our development, since each parameter of the model has a direct interpretation in the context of the recurrent event data, available expert opinions may be expressed in terms of a prior distribution for each parameter separately. Thus, one approach is to encapsulate expert opinions on the model parameters $\alpha, \beta, \gamma, \lambda$ and σ, as a set of independent marginal distributions. We assume a prior density given by $\pi(\alpha, \beta, \gamma, \lambda, \sigma) = \pi(\alpha)\pi(\beta)\pi(\gamma)\pi(\lambda)\pi(\sigma)$. This is by no means the only approach available in this setting, but it is a natural first step which has the advantage of simplifying the computation results.

A gamma distribution can be considered for α, β and γ, an inverse-gamma distribution can be considered for σ^2 and an uniform distribution can be considered for λ such that $\pi(\alpha) \propto \alpha^{a_1 - 1} \exp(-b_1 \alpha)$, $\alpha > 0$, $\pi(\beta) \propto \beta^{a_2 - 1} \exp(-b_2 \beta)$, $\beta > 0$, $\pi(\gamma) \propto \gamma^{a_3 - 1} \exp(-b_3 \gamma)$, $\gamma > 0$, $\pi(\sigma) \propto (\sigma^2)^{-(a_4 + 1)} \exp(-b_4/\sigma^2)$, $\sigma^2 > 0$, and $\pi(\lambda) \propto c$, c constant.

The posterior distribution for the parameter vector, $\boldsymbol{\theta} = (\alpha, \beta, \gamma, \lambda, \sigma)$, considering independence among α, β, γ, λ and σ, is given by

$$\begin{aligned}
&\pi(\alpha, \beta, \gamma, \sigma, \lambda | \mathbf{t}, \mathbf{y}) \\
&\quad \propto \alpha^{a_1-1}\beta^{a_2-1}\gamma^{a_3-1}(\sigma^2)^{-(a_4+1+n/2)} \\
&\quad \times \exp(-b_1\alpha - b_2\beta - b_3\gamma)\prod_{t=1}^{n} t^{-\lambda/2} \\
&\quad \times \exp\left\{-\frac{1}{\sigma^2}\left(b_4 + \frac{1}{2}\sum_{t=1}^{n} t^{-\lambda}[y_t - \alpha(1-\beta\exp(-\gamma t))^3]^2\right)\right\},
\end{aligned} \tag{3.2}$$

where a_1, b_1, a_2, b_2, a_3 and b_3 are the hyperparameters for the gamma prior distributions, and a_4 and b_4 the hyperparameters for the inverse-gamma prior distribution. Integrating the posterior $\pi(\alpha, \beta, \gamma, \sigma, \lambda | \mathbf{t}, \mathbf{y})$ with respect to σ we obtain the joint a posteriori distribution for α, β, γ and λ, given by

$$\begin{aligned}
&\pi(\alpha, \beta, \gamma, \lambda | \mathbf{t}, \mathbf{y}) \\
&\quad \propto \alpha^{a_1-1}\beta^{a_2-1}\gamma^{a_3-1}\prod_{t=1}^{n} t^{-\lambda/2}\exp(-b_1\alpha - b_2\beta - b_3\gamma) \\
&\quad \times \left(b_4 + \frac{1}{2}\sum_{t=1}^{n} t^{-\lambda}[y_t - \alpha(1-\beta\exp(-\gamma t))^3]^2\right)^{-(a_4+n/2)}.
\end{aligned} \tag{3.3}$$

The algorithm needs the complete conditional densities of each parameter. The full conditional distribution of σ^2 is $\mathrm{IG}(a_4 + \frac{n}{2}, b_4 + \frac{1}{2}\sum_{t=1}^{n} t^{-\lambda}[y_t - \alpha(1 - \beta\exp(-\gamma t))^3]^2)$ which is well known and easy to take samples from. We can therefore perform Gibbs updates on this. The full conditionals of the parameters α, β, γ, and λ are given by

$$\begin{aligned}
&\pi(\alpha | \beta, \gamma, \lambda, \mathbf{t}, \mathbf{y}) \\
&\quad \propto \alpha^{a_1-1}e^{-b_1\alpha}\left(b_4 + \frac{1}{2}\sum_{t=1}^{n} t^{-\lambda}[y_t - \alpha(1-\beta\exp(-\gamma t))^3]^2\right)^{-(a_4+n/2)}, \\
&\pi(\beta | \alpha, \gamma, \lambda, \mathbf{t}, \mathbf{y}) \\
&\quad \propto \beta^{a_2-1}e^{-b_2\beta}\left(b_4 + \frac{1}{2}\sum_{t=1}^{n}[y_t - \alpha(1-\beta\exp(-\gamma t))^3]^2\right)^{-(a_4+n/2)}, \\
&\pi(\gamma | \alpha, \beta, \lambda, \mathbf{t}, \mathbf{y}) \\
&\quad \propto \gamma^{a_3-1}e^{-b_3\gamma}\left(b_4 + \frac{1}{2}\sum_{t=1}^{n} t^{-\lambda}[y_t - \alpha(1-\beta\exp(-\gamma t))^3]^2\right)^{-(a_4+n/2)},
\end{aligned}$$

$$\pi(\lambda|\alpha,\beta,\gamma,\mathbf{t},\mathbf{y})$$
$$\propto \prod_{t=1}^{n} t^{-\lambda/2}\left(b_4+\frac{1}{2}\sum_{t=1}^{n} t^{-\lambda}\left[y_t-\alpha\left(1-\beta\exp(-\gamma)\right)^3\right]^2\right)^{-(a_4+n/2)}.$$

These conditional densities do not refer to any known distribution. However, the Metropolis–Hastings algorithm can generate samples for α, β, γ and λ using complete conditional distributions of unknown parameters. The steps are described as follows. We start with $\boldsymbol{\theta}^{(0)} = (\alpha^{(0)}, \beta^{(0)}, \gamma^{(0)}, \lambda^{(0)})$, and generating $\widetilde{\alpha}$ from the prior $\pi(\alpha)$, described previously, and u from uniform distribution $U(0, 1)$. Then, we make the following comparison, if $u \le \min\{1, \pi(\widetilde{\alpha}|\beta^{(0)}, \gamma^{(0)}, \lambda^{(0)}, \mathbf{D})/\pi(\alpha^{(0)}| \beta^{(0)}, \gamma^{(0)}, \lambda^{(0)}, \mathbf{D})\}$ then we update $\alpha^{(1)}$ by $\widetilde{\alpha}$. Otherwise we stay with $\alpha^{(0)}$, that is, $\alpha^{(1)} = \alpha^{(0)}$. Next we do a similar process to obtain $\beta^{(0)}, \gamma^{(0)}$ and $\lambda^{(0)}$, always updating the starting values. We repeat the algorithm steps until a stationary sample is obtained.

In order to verify the Metropolis–Hastings algorithm convergence, Geweke (1992) suggests graphic techniques, while Gelman and Rubin (1992) propose a statistical criterion, the so-called $\sqrt{\widehat{R}}$ statistics, which shall be considered here; $\sqrt{\widehat{R}}$ statistics value close to 1 indicates convergence of the chain.

4 Coverage probability

A small-scale simulation study was performed in order to analyze the frequentist properties of the estimation procedure based on our resampling scheme. To examine the frequentist properties we constructed the credible intervals for all the parameters and calculated their coverage probabilities (CP). We considered different sample sizes, 20, 50 and 100, and different degrees of heteroscedasticy, $\lambda = 0$ (no heteroscedasticity) $\lambda = 0,5$ (weak heteroscedasticity) and $\lambda = 2$ (strong heteroscedasticity). We assumed the following true parameter values $\alpha = 22$, $\beta = 0,4$ and $\gamma = 1$, and without losing generality, the variance σ^2 was assumed to be one.

The hyperparameter values were chosen subjectively, but ensuring non-informativeness. According to the specified priors in Section 3, we considered a gamma distribution G(0.001; 0.001), with a mean and variance equal to 1 and 1000 respectively, and an inverse-gamma distribution IG(3, 60), which has mean and variance equal to 30 and 900 respectively. Thus, the use of these distributions express a very weak knowledge concerning α, β, γ and σ^2.

Overall, nine setups were considered, defined by the different sample sizes and different λ values. For each setup, we generated 300 data sets (a high computational time motivated our choice to keep the simulation size fixed at 300). For each generated sample, we considered two chains of 5500 iterations. The first 500 were ignored to avoid the influence of the first values. The remaining ones were selected with thinning by 20 to avoid series correlation. The convergence of the

Table 2 *Coverage probabilities of the* 95% *credibility intervals for different sample sizes*

λ value	Sample size	20	50	100
$\lambda = 0$	α	0.990	0.977	0.950
	β	0.970	0.963	0.967
	γ	0.980	0.973	0.967
$\lambda = 0.5$	α	0.980	0.970	0.973
	β	0.940	0.967	0.967
	γ	0.957	0.970	0.977
	λ	0.990	0.973	0.973
$\lambda = 2$	α	0.970	0.953	0.970
	β	0.993	0.977	0.963
	γ	0.967	0.970	0.960
	λ	0.990	0.980	0.970

chains were monitored using the method proposed by Gelman and Rubin (1992) and the graphic analysis proposed by Geweke (1992).

In order to obtain the CP of the credibility intervals, for all samples we calculated the parameter 95% credibility intervals and verified if they contained the true parameter values. The empirical CP results for different sample sizes are summarized in Table 2. The results enable us to conclude that small and moderate numbers of observations do not harm the empirical CPs.

For the sake of illustration, from the frequentist point of view, large sample inference for the parameters can be based, in principle, on the maximum likelihood estimates (MLEs) and their estimated standard errors assuming an asymptotic normal distribution for the MLEs (Cox and Hinkley, 1974), with the MLEs having been obtained via direct maximization of (3.1) and the estimate of the asymptotic covariance matrix of $(\widehat{\boldsymbol{\theta}}, \widehat{\sigma})$ obtained through the inverse of the observed Fisher information matrix. However, in animal growth studies, it is common to find small or moderate datasets. In order to check the behavior of the asymptotic theory for small and moderate size samples, we replicated the small-scale simulation study performed above to examine the coverage probabilities of the asymptotical confidence intervals for the parameters. Table 3 presents the empirical CPs. The degree of heteroscedasticy severely affects the CPs by lowering them, particularly in the presence of small samples, which is the case of the Kubbard female chicken data considered here. These findings are evidence for the need of a more adequate procedure for small or moderate sized samples such as the Bayesian approach developed here. The empirical CPs of the credible intervals obtained via our approach (Table 2) are very close to the nominal one even in the presence of a small or moderate number of observations.

Table 3 *Coverage probabilities of the* 95% *confidence intervals for different samples sizes*

λ value	Sample size	20	50	100
$\lambda = 0$	α	0.943	0.953	0.933
	β	0.927	0.943	0.940
	γ	0.927	0.957	0.943
$\lambda = 0.5$	α	0.927	0.930	0.957
	β	0.727	0.890	0.930
	γ	0.830	0.930	0.947
	λ	0.777	0.897	0.930
$\lambda = 2$	α	0.807	0.923	0.940
	β	0.890	0.930	0.937
	γ	0.690	0.937	0.953
	λ	0.737	0.893	0.920

5 Kubbard female chicken data

In this section our methodology is illustrated on the real female chicken dataset presented in Section 1. The Von Bertalanffy model in its homoscedastic and heteroscedastic versions, were fitted to the data.

Prior distributions were equal to the ones specified in Section 4. We considered two chains of 5500 iterations. The first 500 were ignored to avoid the influence of first values. The remaining ones were selected with thinning by 20 to avoid series correlation. The convergence of the chains were monitored using the method proposed by Gelman and Rubin (1992) and the graphic analysis proposed by Geweke (1992). All statistics $\sqrt{\widehat{R}}$ are close to 1, which indicates the convergence of the chains.

Table 4 presents the posterior means, together with their 95% asymptotical credibility intervals, for the asymptote α, the coordinates of the inflection point (X_I, Y_I), the variance σ^2 and the heteroscedasticity parameter λ. The coordinates of the inflection point (X_I, Y_I) have an important biological interpretability (Seber and Wild, 1989). The inflection point is the moment in which the animal switch from the progressive growth phase to the regressive one, that is, the growth rate begins to decrease due to many factors which inhibit the growth progressively. As pointed out in the introduction section we note that the homoscedasticity assumption is not satisfied for this dataset since the credibility intervals for the heteroscedasticity parameter λ do not include the zero value. This result is corroborated by the AIC, BIC and DIC criterion values. These results provide strong evidence in favour of the heteroscedastic Von Bertalanffy model.

The posterior means of the asymptote α and the coordinates (X_I, Y_I) are larger in the model in its homoscedasticity version than in its heteroscedasticity version

Table 4 *The posterior means and* 95% *credibility intervals* (*CI*), *for* α, *the coordinates of the inflection point* (X_I, Y_I), σ^2 *and* λ. *Moreover, the AIC, BIC and DIC criterion values for the model in its homoscedastic and heteroscedastic versions*

λ	Parameter	Mean	95% CI	DIC	AIC	BIC
$\lambda = 0$	α	5940.06	[5939.36; 5940.76]	1007.38	1007.38	1009.64
	X_I	6.95	[6.87; 7.02]			
	Y_I	1760.02	[1759.81; 1760.22]			
	σ^2	3519.61	[2483.17; 4556.06]			
$\lambda \neq 0$	α	4676.25	[3668.43; 5684.06]	970.99	970.99	973.79
	X_I	5.81	[4.90; 6.72]			
	Y_I	1385.56	[1090.91; 1680.20]			
	σ^2	152.87	[34.24; 271.51]			
	λ	2.20	[1.61; 2.79]			

(Table 4). Overall, the model in its heteroscedasticity version seems to be appealing from the practical point of view, while maintaining coherence in the posterior mean obtained values. If the model in its homoscedastic version is considered, the chickens should be slaughtered in 6.9 weeks (the coordinate X_I in Table 4), while considering the model in its heteroscedastic version, which is the adequate one, they may be slaughtered much earlier in 5.8 weeks. This would mean saving time of approximately 16%. Of course, this comparison is crude, since the homoscedastic Von Bertalanffy model is not the appropriate one for the present example. Figure 1 shows the sampling corporeal weights for a period of seven weeks, with the homoscedastic (left panel) and heteroscedastic (right panel) Von Bertalanffy model fitting the 95% lower and upper limit confidence bounds. Denying the presence of heteroscedasticity leads to a false impression of a smaller confidence interval amplitude. Furthermore, Figure 2 shows the residuals for the Kubbard female

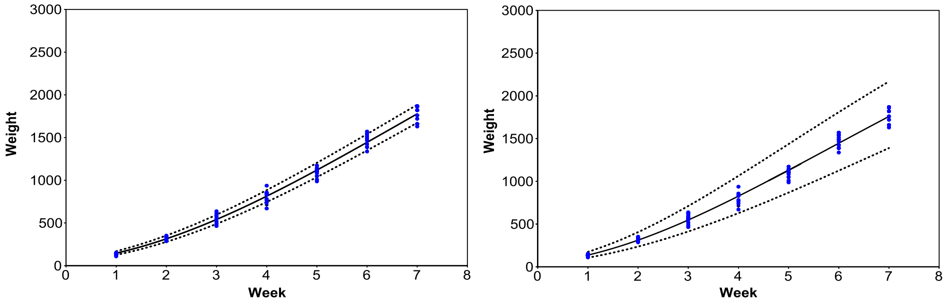

Figure 1 *Left panel*: *Sample corporeal weights for a period of seven weeks*, *the homoscedasticity Von Bertalanffy model fitting* (— — —) *with the* 95% *lower and upper limit* (— — —) *confidence bounds*. *Right panel*: *Sample corporeal weights for a period of seven weeks*, *the heteroscedastic Von Bertalanffy model fitting* (— — —) *with the* 95% *lower and upper limit* (— — —) *confidence bounds*.

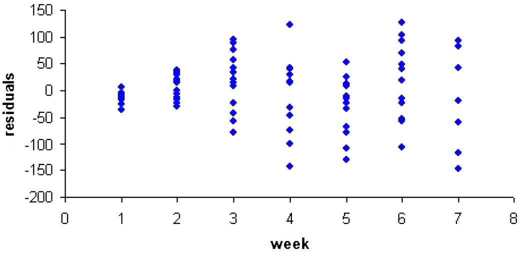

Figure 2 *Kubbard female chicken data—homoscedastic Von Bertalanffy ordinary least squares residuals against time.*

chicken data when the homoscedastic Von Bertalanffy model was fitted to the data. The megaphone-shaped pattern is a characteristic of a heteroscedastic model. In fact, this pattern indicates that the variances of the error terms tend to increase as times $x_i's$ increase, which justify the multiplicative error in the modelling (2.2), which was assumed here. The Goldfeld-Quandt statistic is $F[36,36] = 4.169$ with p-value< 0.000, which is strong evidence in favour of the heteroscedastic hypothesis.

6 Final remarks

In this paper, we presented the known sigmoidal growth model, namely the Von Bertalanffy model, in its heteroscedastic version by considering a multiplicative heteroscedastic structure. Parameter estimates are obtained using a sampling based approach, which allows information to be input beforehand having small computational effort. The simulation results allow us to conclude that small and moderate numbers of observations do not harm the empirical coverage probabilities of the credible intervals. We applied the methodology to a real dataset involving corporeal weights of Kubbard female chickens from which we observed that the amplitude of the chicken weight credible intervals are affected by the presence of heteroscedasticity in the data as the age of the chicken increases. However, an economical advantage comes out by considering it.

Although we focused our study on the Von Bertalanffy model with a multiplicative heteroscedastic structure, our methodology is general and, in principle, may be extended to other sigmoidal growth models with other heteroscedastic structures. This would however introduce extra difficulties in the analysis, but needs further work.

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