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Bootstrap study of parameter estimates for nonlinear Richards growth model through genetic algorithm

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Richards nonlinear growth model, which is a generalization of the well-known logistic and Gompertz models, generally provides a realistic description of many phenomena. However, this model is very rarely used as it is extremely difficult to fit it by employing nonlinear estimation procedures. To this end, utility of using a very powerful optimization technique of genetic algorithm is advocated. Parametric bootstrap methodology is then used to obtain standard errors of the estimates. Subsequently, bootstrap confidence-intervals are constructed by two methods, viz. the Percentile method, and Bias-corrected and accelerated method. The methodology is illustrated by applying it to India's total annual foodgrain production time-series data.

Keywords: Richards growth model; genetic algorithm; simulated binary crossover; mutation operator; bootstrap

1. Introduction

Nonlinear growth models play a very important role in getting an insight into the underlying mechanism. These models are generally 'mechanistic' and the parameters have meaningful biological interpretation [10]. Richards four-parameter nonlinear growth model, which is a generalization of the well-known logistic and Gompertz models, generally provides a realistic description of many phenomena. In respect of Richards model in discrete time, Loibel *et al.* [8] tackled the identifiability problem by employing the Box–Cox transformation. In order to ensure better interval estimation for the parameters, the approach is complemented with the profile maximum likelihood estimate combined with bootstrap technique. For fitting nonlinear growth models in continuous time, nonlinear estimation procedures, like Levenberg–Marquardt procedure are generally employed. Recently, Iquebal *et al.* [7] made attempts to apply Richards model to describe

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India's annual foodgrain production time-series data. The SAS, Ver. 9.0 software package was used for data analysis. Several initial values for the parameters were tried. However, global convergence did not take place. Thus, Richards model could not be fitted to given data by employing 'Nonlinear estimation procedures'.

Fortunately, during the last few years, a very powerful and versatile stochastic search and optimization technique of genetic algorithm (GA), which is based on the principles of genetics and natural selection, has been proposed [1–3]. Ghosh *et al.* [6] used this methodology to develop GA-based estimators of ordinary least squares (OLS) variance–covariance matrix for the linear regression model under heteroscedasticity and showed that the proposed estimators perform better than the corresponding existing estimators in terms of their capability to reduce the total relative bias and the total root mean square error. In order to fit Richards nonlinear growth model, Iqbal *et al.* [7] demonstrated that, for the data under consideration, the GA-methodology was successful, despite failure of nonlinear estimation procedures. However, authors obtained only the parameter estimates and, in the absence of computation of corresponding standard errors, it was not possible to assess the efficiency of the parameter estimates. The present paper is an extension of this work in the sense that, not only standard errors of estimates are computed by Parametric bootstrap technique, but bootstrap confidence-interval of the parameters are also constructed by two methods, viz. Percentile method and Bias-corrected and accelerated (BC_a) method.

The organization of the present paper is as follows. In Section 2, a brief description of Richards nonlinear growth model is provided. Section 3 is concerned with the bootstrap study of standard errors of parameter estimates along with construction of bootstrap confidence-intervals by percentile and BC_a methods. Finally, an illustration of the methodology for India's foodgrain production time-series data is discussed in Section 4.

2. Richards nonlinear growth model

The model is defined as

$$\frac{dX}{dt} = \frac{r X (K^m - X^m)}{m K^m}, \quad (1)$$

where $X(t)$ is the population-size or biomass at time t , r is intrinsic growth rate, K is the carrying capacity, and m is an additional parameter. The ranges of all the parameters are positive except $m \geq -1$, because $m < -1$ is non-physiological, giving infinite growth rate as $t \rightarrow 0$. To solve Equation (1), let $y = X^{-m}$, then

$$\frac{dy}{dt} + ry = rK^{-m} \quad (2)$$

which is a linear differential equation. Solving it, we get

$$X(t) = \frac{K X_0}{[X_0^m + (K^m - X_0^m)e^{-rt}]^{1/m}} \quad (3)$$

2.1 Some particular cases

(i) When $m = -1$, Equation (1) reduces to

$$\frac{dX}{dt} = r(K - X) \quad (4)$$

which is a monomolecular model.

(ii) When $m = 1$, Equation (1) reduces to the following logistic growth rate form:

$$\frac{dX}{dt} = rX \left(1 - \frac{X}{K} \right) \tag{5}$$

(iii) When $m = 0$, Equation (1) becomes an indeterminate form and the following Gompertz growth rate form is obtained by applying the L' Hospital rule:

$$\frac{dX}{dt} = rX \log \left(\frac{K}{X} \right) \tag{6}$$

2.2 Point of inflexion

The point of inflexion of Richards model, obtained by solving $d^2X/dt^2 = 0$, for which $d^3X/dt^3 \neq 0$, is given by

$$X = \frac{K}{(m + 1)^{1/m}}, \quad m \neq -1 \tag{7}$$

and it occurs at time

$$t = \frac{1}{r} \log \left(\frac{K^m - X_0^m}{m X_0^m} \right), \quad m \neq -1 \tag{8}$$

It may be noted that the point of inflexion for Richards model is very flexible as it is not fixed, but can occur at any fraction of carrying capacity, K .

3. Bootstrap study

As mentioned in the Introduction section, the estimation of parameters for nonlinear Richards growth model may be carried out by applying the GA optimization technique with a view to minimizing the fitness value, which is the residual sum of squares [7]. The efficiency of the parameter estimates is now studied by the Bootstrap methodology [5]. It consists of generating samples from the estimated Richards model $F(X, \hat{\theta})$ along with bootstrapped residuals from the population of empirical errors. The bootstrapped generated samples (1000, in our case) are denoted by $X^*(b)$, $b = 1, 2, \dots, B$. Parameter estimate of each component of $\hat{\theta}$, denoted as $\hat{\theta}$, from each sample is computed using GA and is denoted by $\hat{\theta}^*(b)$, $b = 1, 2, \dots, B$. The estimated bias of $\hat{\theta}$, denoted by \hat{B}_B , is obtained as

$$\hat{B}_B = \text{bias}(\hat{\theta}^*) = \hat{\theta}^*(\cdot) - \hat{\theta}$$

where

$$\hat{\theta}^*(\cdot) = \frac{\sum_{b=1}^B \hat{\theta}^*(b)}{B} \tag{9}$$

The estimated standard error (\hat{s}_B) of $\hat{\theta}$ is obtained as

$$\hat{s}_B = \left[\frac{\sum_{b=1}^B \{ \hat{\theta}^*(b) - \hat{\theta}^*(\cdot) \}^2}{(B - 1)} \right]^{1/2} \tag{10}$$

The point and interval estimates taken together give an idea about the error in estimating true parameter θ . The bootstrap confidence-interval is based on bootstrap standard error estimate. The ideal bootstrap estimate $\lim_{B \rightarrow \infty} \hat{s}_B = s_{\hat{F}} = s_{\hat{F}}(\hat{\theta}^*)$ considers $B = \infty$, in which case, the

plug-in estimate \hat{s}_∞ equals $s_{\hat{F}}(\hat{\theta}^*)$. The rule of thumb, as mentioned in Efron and Tibshirani [5], is to take $B = 200$ for estimating the standard error, while a much larger value of B is required for computation of bootstrap confidence intervals. The bootstrap standard errors for parameter estimates may be used to assign approximate confidence intervals to parameter θ . Most commonly used confidence interval, i.e. standard confidence interval under large sample size is

$$[\hat{\theta} - z^{(1-\alpha)}s_{\hat{F}}, \hat{\theta} - z^{(\alpha)}s_{\hat{F}}], \tag{11}$$

where $z^{(\alpha)}$ is the 100α th percentile point of the $N(0, 1)$ distribution.

3.1 Percentile-method

Let $\hat{\theta}$ be the usual plug-in estimate of a parameter θ and $s_{\hat{F}}$ be its estimated standard error. The end points of standard confidence interval $[\hat{\theta} - z^{(1-\alpha)}s_{\hat{F}}, \hat{\theta} - z^{(\alpha)}s_{\hat{F}}]$ can be described in a way that is particularly convenient for bootstrap calculations. Particularly, if we assume that $\hat{\theta}^*$ indicates a random variable drawn from the normal distribution $N(\hat{\theta}, s_{\hat{F}}^2)$, then $\hat{\theta}_{lo} = \hat{\theta} - z^{(1-\alpha)}s_{\hat{F}}$ and $\hat{\theta}_{up} = \hat{\theta} - z^{(\alpha)}s_{\hat{F}}$ are the 100α th and $100(1 - \alpha)$ th percentiles of $\hat{\theta}^*$. This suggests use of the percentiles of bootstrap histogram to define confidence-limits. A bootstrap dataset X^* is generated from $F(X, \hat{\theta})$ and bootstrap replications $\hat{\theta}^* = s(X^*)$ are computed. Let \hat{G} be the cdf of $\hat{\theta}^*$. The $(1 - 2\alpha)$ percentile interval is defined by the α and $(1 - \alpha)$ percentiles of \hat{G} :

$$(\hat{\theta}_{\%,lo}, \hat{\theta}_{\%,up}) = (\hat{G}^{-1}(\alpha), \hat{G}^{-1}(1 - \alpha)) \tag{12}$$

The percentile interval is connected with the bootstrap t -interval if we approximate the distribution of $(\hat{\theta} - \theta)$ by $(\hat{\theta}^* - \hat{\theta})$ and it can be shown that the resulting interval is

$$(2\hat{\theta} - \hat{G}^{-1}(1 - \alpha), 2\hat{\theta} - \hat{G}^{-1}(\alpha)) \tag{13}$$

The percentile method can be thought of as an algorithm for automatically incorporating transformation so that the transformed statistic follows normal distribution without any need to know the correct transformation. Also the percentile interval is the transformation respecting in the sense that, for any (monotone) parameter transformation $\phi = g(\theta)$, it is simply the percentile interval for θ mapped by $g(\theta)$, i.e.

$$(\hat{\phi}_{\%,lo}, \hat{\phi}_{\%,up}) = (g(\hat{\theta}_{\%,lo}), g(\hat{\theta}_{\%,up})) \tag{14}$$

3.2 Bias-corrected with acceleration constant (BC_a)-method

The percentile method can be thought of as a straightforward computational algorithm for extending the effectiveness of standard confidence intervals. The Bias-corrected (BC) approach of interval estimation, although more complicated to define than the percentile method, is almost as easy to use as the percentile method. The BC method, introduced by Efron [4], assumes normality and constancy of the standard error for construction of confidence intervals. It can be achieved by some transformation $\hat{\phi} = g(\hat{\theta})$, $\phi = g(\theta)$, say, where

$$\frac{\hat{\phi} - \phi}{\tau} \sim N(-z_0, 1) \tag{15}$$

τ being the standard error of $\hat{\phi}$. Allowing the bias constant z_0 considerably improves the approximation in many cases. The confidence interval $(\hat{\phi} + \tau z_0) \pm \tau z^{(\alpha)}$ for ϕ can be converted back to a confidence interval for θ by the inverse transformation $\theta = g^{-1}(\phi)$. The advantage of BC method

is that all of these are done automatically from bootstrap calculation, without requiring to know the correct transformation g . The improved bootstrap method, called BC with the acceleration constant (BC_a) method [5], makes one further generalization of the BC method. It can be demonstrated that the BC_a interval gives the second-order correct interval of θ under reasonable condition and takes care of major adjustments of exact confidence limit, which is typically of the form [4]:

$$\hat{\theta} + \hat{\sigma} \left(z^{(\alpha)} + \frac{A_n^{(\alpha)}}{\sqrt{n}} + \frac{B_n^{(\alpha)}}{n} + \dots \right), \tag{16}$$

where n is sample size. The asymptotic property of the BC_a interval adheres to the asymptotic property of the confidence interval based on the maximum likelihood estimator. Let $\hat{\theta}^{*(\alpha)}$ indicate the 100 α th percentile of B bootstrap replications $\hat{\theta}^*(1), \hat{\theta}^*(2), \dots, \hat{\theta}^*(B)$. The BC_a interval endpoints are also given by percentiles of the bootstrap distribution, but are not necessarily the same as the percentiles of bootstrap t -distribution. It is assumed that for some monotone transformation g , the bias constant z_0 , and acceleration constant a , the transformation $\hat{\phi} = g(\hat{\theta})$, results in $\hat{\phi} - \phi = \sigma_\phi(Z - z_0)$, where $\phi = g(\theta)$, and $\sigma_\phi = 1 + a\phi$. It is not difficult to find the correct interval for ϕ which has α -level endpoints:

$$\phi[\alpha] = \hat{\phi} + \sigma_{\hat{\phi}} \frac{z_0 + z^{(\alpha)}}{1 - a(z_0 + z^{(\alpha)})} \tag{17}$$

In terms of the inverse of bootstrap cdf \hat{H} of $\hat{\phi}^*$, it is easy to show that

$$\phi[\alpha] = \hat{H}^{-1}(\Phi(z[\alpha])), \tag{18}$$

where

$$z[\alpha] = z_0 + \frac{z_0 + z^{(\alpha)}}{1 - a(z_0 + z^{(\alpha)})}. \tag{19}$$

Using the relationship $\hat{H}^{-1}(\alpha) = g(\hat{G}^{-1}(\alpha))$, where \hat{G} is the bootstrap cdf of $\hat{\theta}^*$, it can be shown that the correct central BC_a confidence interval of level $(1 - 2\alpha)$ for θ is

$$(\hat{G}^{-1}(\Phi(z[\alpha])), \hat{G}^{-1}(\Phi(z[1 - \alpha]))). \tag{20}$$

The percentiles $\Phi(z[\alpha]), \Phi(z[1 - \alpha])$ depend on two vectors a and z_0 , which are to be estimated. The value of the bias-correction z_0 is obtained from the proportion of bootstrap replications less than the original estimate $\hat{\theta}$ by the equation

$$z_0 = \Phi^{-1} \left(\frac{\#\{\hat{\theta}^*(b) < \hat{\theta}\}}{B} \right) \tag{21}$$

The estimate of a , given by Miller [9], is in terms of the jackknife values of a statistic $\hat{\theta} = s(x_1, x_2, \dots, x_n)$. To this end, let $x_{(i)} = (x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_n)'$ be the original data with

observation at the i th time point deleted and let $\hat{\theta}_{(i)} = s(x_i)$. Defining

$$\hat{\theta}_{(\cdot)} = \sum_{i=1}^n \frac{\hat{\theta}_{(i)}}{n}, \tag{22}$$

a simple expression for the acceleration is

$$\hat{a} = \frac{\sum_{i=1}^n (\hat{\theta}_{(\cdot)} - \hat{\theta}_i)^3}{6 \left\{ \sum_{i=1}^n (\hat{\theta}_{(\cdot)} - \hat{\theta}_i)^2 \right\}^{3/2}} \tag{23}$$

It is to be noted that the parameter θ is vector valued for the underlying probability set up guided by the Richards model. Subsequently, the bias and acceleration estimates are also vector valued with four components each and Equations (22) and (23) should be read accordingly.

The confidence interval $(\hat{\theta}_{lo}, \hat{\theta}_{up})$, based on the percentile and BC_a methods, for each parameter is described by its ‘Length’ and ‘Shape’, where

$$\text{Length} = \hat{\theta}_{up} - \hat{\theta}_{lo} \text{ and Shape} = \frac{\hat{\theta}_{up} - \hat{\theta}}{\hat{\theta}_{lo} - \hat{\theta}} \tag{24}$$

When these exist, exact confidence intervals, are often quite asymmetric. Shapes of the BC_a intervals usually come out to be greater than one, implying thereby that these are asymmetric. Thus, the condition of exact intervals by the bootstrap methodology is satisfied. On the contrary, a serious error in terms of good theoretical coverage properties is committed by the percentile method, whose shape being close to unity, reflects the symmetric nature of confidence intervals.

4. An illustration

India’s annual foodgrain production data for the post-Green revolution era, viz. 1966–1967 to 2004–2005 obtained from various issues of ‘Agricultural Statistics at a Glance’, published by the Directorate of Economics and Statistics, Ministry of Agriculture, India, are considered for the present study. The same are reproduced in the second column of Table 1 for ready reference. After reparameterization, Equation (3) becomes

$$X(t) = \frac{a}{[1 + \exp(b - ct)]^{1/d}} + \varepsilon(t) \tag{25}$$

where $a = K$, $b = \log(K^m / X_0^m - 1)$, $c = r$, $d = m$, and $\varepsilon(t)$ is a random error term assumed to be independently and identically distributed. In order to fit Equation (3) to data through GA, the objective function to be minimized is

$$\sum_{t=1}^T \left[X(t) - \frac{a}{[1 + \exp(b - ct)]^{1/d}} \right]^2 \tag{26}$$

Computer programs for data analysis were developed using C-language in Microsoft visual C++ compiler. The GA parameters, viz. population size, crossover probability, and mutation probability for minimization of Equation (26) are, respectively, 40, 0.9, 0.01 with number of generations as 100. Using above parameter set up, GA has terminated with accuracy level ($\eta = 10^{-3}$) in 99 out of 100 runs, in general [7]. The parameter estimates along with estimated bias and standard error obtained through GA are reported in Table 2. It may be noted that the percentage standard errors throughout are generally quite low, indicating thereby that the parameters are estimated efficiently. The fitted values along with residuals are then computed and reported respectively in third and fourth columns of Table 1.

Table 1. Fitting of Richards nonlinear growth model to India's foodgrain production data (million tonnes) using GA.

Year	Observed	Fitted	Residuals
1966–1967	74.23	94.72	–20.49
1967–1968	95.05	97.00	–1.95
1968–1969	94.01	99.32	–5.31
1969–1970	99.50	101.70	–2.20
1970–1971	108.42	104.13	4.29
1971–1972	105.17	106.62	–1.45
1972–1973	97.03	109.16	–12.13
1973–1974	104.67	111.76	–7.09
1974–1975	99.83	114.42	–14.59
1975–1976	121.03	117.13	3.90
1976–1977	111.17	119.90	–8.73
1977–1978	126.41	122.73	3.68
1978–1979	131.90	125.62	6.28
1979–1980	109.70	128.57	–18.87
1980–1981	129.59	131.57	–1.98
1981–1982	133.30	134.64	–1.34
1982–1983	129.52	137.76	–8.24
1983–1984	152.37	140.94	11.43
1984–1985	145.54	144.18	1.36
1985–1986	150.44	147.48	2.96
1986–1987	143.42	150.83	–7.41
1987–1988	140.35	154.23	–13.88
1988–1989	169.92	157.69	12.23
1989–1990	171.04	161.19	9.85
1990–1991	176.39	164.74	11.65
1991–1992	168.38	168.34	0.04
1992–1993	179.48	171.97	7.51
1993–1994	184.26	175.65	8.61
1994–1995	191.50	179.35	12.15
1995–1996	180.42	183.09	–2.67
1996–1997	199.44	186.84	12.60
1997–1998	192.26	190.61	1.65
1998–1999	203.61	194.39	9.22
1999–2000	209.80	198.17	11.63
2000–2001	196.81	201.95	–5.14
2001–2002	212.85	205.71	7.14
2002–2003	174.77	209.46	–34.69
2003–2004	213.19	213.17	0.02
2004–2005	198.36	216.85	–18.49

Table 2. Parameter estimates along with bias and % standard error.

Parameter	Estimate	Bias	% Standard error
<i>a</i>	290.26281	0.793	4.17
<i>b</i>	4.76365	0.013	7.14
<i>c</i>	0.09995	–0.007	11.11
<i>d</i>	4.17308	0.084	6.95

4.1 Residual analysis

In order to assess as to whether or not the Richards model is fitted properly, it is important to carry out the 'Residual analysis'. The main assumption regarding independence of error terms is first examined through the 'Run test' on residuals. The calculated value of $|Z|$ is obtained as 0.970, which being less than 1.96, indicates that the assumption of independence of errors is not

violated at 5% level. Subsequently, the Durbin–Watson test, which is more efficient than the Run test, is applied on residuals $\{e_t\}$. To this end, in the first instance, the assumption of normality of errors is examined. The Shapiro–Wilk test statistic value of 0.961 indicates that the assumption of normally distributed errors is not violated at 5% level. The Durbin–Watson test statistic given by

$$d = \frac{\sum_{t=2}^n (e_t - e_{t-1})^2}{\sum_{t=1}^n e_t^2}.$$

is computed as 1.805. The tabulated values for $n = 39$ at 5% level are $d_L = 1.435$ and $d_U = 1.540$. As $d > d_U$, there is no statistical evidence that the error terms are positively autocorrelated. Further, $4 - d > d_U$, thus there is no statistical evidence that the error terms are negatively autocorrelated. Thus, by the Durbin–Watson test also, the assumption of independence of error terms is not violated at 5% level. For visual inspection, the graph of residuals is exhibited in Figure 1.

4.2 Goodness-of-fit

Goodness-of-fit measures, viz. mean absolute error (MAE), root mean squared error (RMSE), percentage forecast error (PCFE) are computed and are reported in Table 3, which indicate that the Richards model provides a good fit to data.

From the fitted model, the point of inflexion is calculated as $t = 33$. Thus, the maximum growth rate is achieved in 1999, implying thereby that India’s foodgrain production for subsequent years would take place at a retarded pace; this result may have serious implications from the policy point of view.

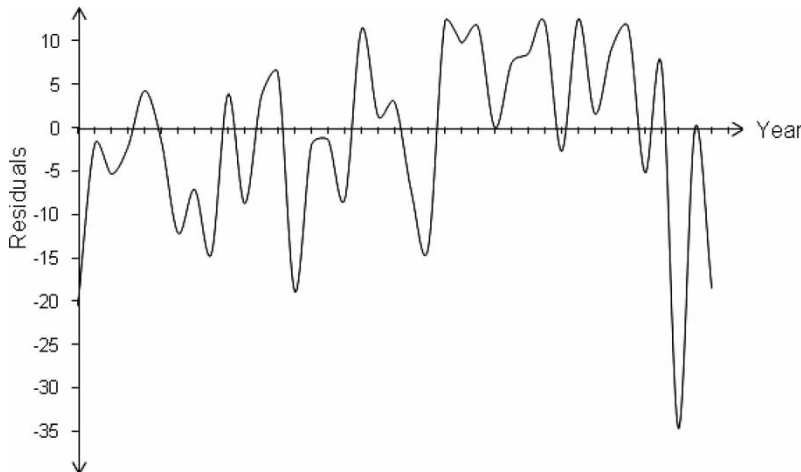


Figure 1. Graph of residuals.

Table 3. Various measures of goodness of fit.

Measures	Calculated values
MAE	8.32
RMSE	10.77
PCFE	5.69

4.3 Lengths and shapes of confidence-intervals

Lengths and shapes of confidence intervals constructed by percentile and BC_a methods are exhibited in Table 4. A perusal shows that lengths of the BC_a intervals are shorter for parameters *a* and *b* compared with those for percentile intervals whereas for the other two parameters, viz. *c* and *d*, these are only slightly longer. Further, in view of their shape values around one, the percentile intervals are generally symmetric in nature, which does not guarantee the existence of exact 95% confidence intervals. On the other hand, the BC_a intervals have shape values greater than one for all the parameter estimates, indicating thereby that these give exact 95% confidence intervals. To sum up, it may be concluded that, for present data, the BC_a method has performed better than the percentile method.

4.4 Forecast performance

The forecast performance of the fitted Richards model is studied by computing the bootstrap estimate of the mean square prediction error (MSPE). To this end, we generate 1000 samples each of size 41 using the Richards model, where the estimated parameters from outset data are taken as true parameter values. The errors are independently and identically distributed random variables from the population of observed errors due to fitting the Richards model to data. In each of the 1000 samples, GA was performed to estimate the parameters as well as to find the one-step ahead forecast error. The MSPE, computed by the formula

$$\frac{\sum_{i=1}^{1001} R_i^2}{1001}, \tag{27}$$

where R_i^2 denote the one-step ahead squared forecast error in the *i*th bootstrap sample, is merely 4.35. Further, forecasting of India’s foodgrain production on the basis of fitted Richards nonlinear growth model is carried out from 2005–2006 till 2008–2009 and the results are reported in Table 5. A perusal shows that the observed and fitted values are quite close to each other.

Hence, it may be concluded that the Richards model is successful in modelling and forecasting of India’s annual foodgrain production data.

Table 4. Lengths and shapes of confidence-intervals.

Parameter	Percentile method			BC _a -method		
	Interval	Length	Shape	Interval	Length	Shape
<i>a</i>	[278.45, 302.16]	23.71	1.01	[280.34, 301.24]	20.90	1.11
<i>b</i>	[4.39, 5.28]	0.89	1.41	[4.57, 5.13]	0.56	1.95
<i>c</i>	[0.07, 0.11]	0.04	1.00	[0.07, 0.12]	0.05	1.50
<i>d</i>	[3.84, 4.41]	0.57	0.73	[3.90, 4.50]	0.60	1.22

Table 5. Forecasting of India’s foodgrain production (million tonnes).

Year	Observed	Fitted	Difference
2005–2006	208.60	220.48	–11.88
2006–2007	217.28	224.05	–6.77
2007–2008	230.78	227.57	3.21
2008–2009	233.88	231.00	2.88

5. Conclusion

In this paper, utility of GA for fitting of Richards nonlinear growth model is highlighted. The proposed procedure is successfully applied for modelling and forecasting of India's annual foodgrain production data. The importance of this work is that this methodology is applicable even in those cases in which 'Nonlinear estimation procedures' fail to converge. The methodology has been put on a sound statistical footing by computation of confidence intervals through two methods. This, in turn, would go a long way in building of various scenarios for forecasting purposes. It is hoped that, applied statisticians would also start employing the GA for fitting other similar nonlinear growth models. Work is in progress to extend the methodology applicable when the errors are not independent but follow AR(1) errors and shall be reported separately in due course of time.

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