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Application and Uses of Four-Parameter Estimates of Nonlinear Growth Analysis

OWAN RAPHAEL A.,
Department of Computing and Sciences, Havilla University Nde-Ikom, Cross River State, Nigeria

CHRIS-CHINEDU, JOY N.,
Department of Mathematics/Statistics, Ignatius Ajuru University, Port Harcourt, Rivers State, Nigeria

ASU ISAAC A.
Department of Electrical Electronics, University of Cross River State, Nigeria

Abstract:
The partial derivatives of the four parameters estimates; Chapman-Richards, von Bertalanffy, Weibull and the Richard's nonlinear growth models are presented and compared. The application of these partial derivatives in estimating the model parameters is illustrated. The parameters are estimated using the Marquardt iterative method of nonlinear regression relating top height to age of Palm tree from the Rhison palm Estate, Rivers State Nigeria. Formulas that provide good initial values of the parameters are specified. Clear definitions of the parameters of the nonlinear models in the context of the system being modeled are found to be critically important in the process of parameter estimation. The Richard's, and the Weibull models have produced a slightly smaller residual standard error (0.13 m) compared to the von Bertalanffy and the Chapman- Richards models (0.14 m). All the models in Table 8 appear to predict reasonable estimates over the entire range of age.

Key words: parameter estimation, nonlinear model, partial derivative, Marquardt iterative

Introduction

Growth studies in many branches of science have demonstrated that more complex nonlinear functions are justified and required if the range of the independent variable encompasses juvenile, adolescent, mature and senescent stages of growth (Philip 1994). Then a function with a sigmoid form, ideally its origin at (0,0), a point of inflection occurring early in the adolescent stage and either approaching a maximum value, an asymptote, or peaking and falling in the senescent stage, is justified. Examples of such models with four parameters include the Chapman-Richards and the von Bertalanffy functions. In contrast to empirical models, e.g., polynomial equations, the above theoretical models have an underlying hypothesis associated with cause or function of the phenomenon described by the response variable and have meaningful parameters from a Rhison palm Estate perspective. Theoretically based equations may also be more reliable for predictions which involve extrapolations beyond the range of data compared to empirical polynomial equations (Martin and Ek 1984). More importantly, theoretical nonlinear mathematical models provide the basis for an objective method of estimating yield class (growth potential) and the sustainable yield of a crop.

Even though there are few theoretical models formulated specifically for forestry applications, many developed in other disciplines have a considerable potential for modelling forest growth and yield parameters. However, the use of theoretical nonlinear mathematical models explicitly formulated to provide consistent growth and yield has not progressed in the field of forestry. This is partly attributed to the fact that the statistical methodology used for fitting nonlinear models to forest growth data is closely related to the mathematics of the models and the importance of this relationship is not well understood in a forestry context (Fekedulegn 1996).

Nonlinear models are more difficult to specify and estimate than linear models and the solutions are determined iteratively (Ratkowsky 1983). The iterative methods used in nonlinear regression include the modified Gauss-Newton method (Taylor series), gradient or steepest-descent method, multivariate secant or false position,
and the Marquardt method (Draper and Smith 1981). If a model, after reparameterization, does not behave in a near-linear fashion, the parameter estimates will not have desirable properties such us unbiasedness, normality, and minimum variance and hence, complex estimation techniques (e.g., the Marquardt (1963) method) may be necessary (Ratkowsky 1983 and 1990). In such cases, the use of partial derivatives rather than computational approximations usually results in more efficient and more precise parameter estimation. Therefore, the purpose of this study was to derive the partial derivatives of nine nonlinear growth models and demonstrate the method of parameter estimation using experimental height growth data.

2: Models and Sample Data

The growth models considered are given in Table 1. Further details, background and historical information can be found in the sources mentioned in Table 1. For all models considered, ω is the dependent growth variable, t is the independent variable (usually age in years), α , β, k, and m are parameters to be estimated, exp is the base of natural logarithms, and ε is the additive error term. The mathematical properties of the models and meaningful forestry interpretation of the parameters are discussed by Fekedulegn (1996). The Rhison palm estate Experiment (1963-2002) was established at the Elele in Ikwerre local government of Rivers State to investigate effects of four thinning treatments on growth and yield of Palm tree. Each treatment was replicated four times and a total of 16 permanent sample plots each with an area of 0.04 hectare were measured at five year intervals up until 2002 and at irregular intervals thereafter. At the time of establishing the experiment in 1963 the stand was 20 years old and the local yield class was 15 cubic meters per hectare per year. Top height growth data from sample plot 3661, that received a B-grade thinning treatment, are used to fit the nonlinear growth models and demonstrate the method of parameter estimation (Table 2). A B grade thinning treatment refers to the removal of dead and dying trees only. These data were made available by the Nigerian Forestry Commission.

Table 1: Nonlinear Mathematical models considered in the study

Model	Intergral form	Source
Chapman-Richard	$w(t)=\alpha(1-\beta\exp(-kt))^{1/(1-m)}+\varepsilon$	Draper & Smith(1981)
Von Bertalanffy	$w(t)=(\alpha^{1-m}-\beta\exp(-kt))^{1/(1-m)}+\varepsilon$	Bertalanffy(1957)Vandy (1994)
Richard	$w(t)=\alpha/(1+\beta\exp(-kt))^{1/m}+\varepsilon$	Richard(1959),Myers(1986)
Weibull	$w(t)=(\alpha-\beta\exp(-kt))+\varepsilon$	Ratkowsky(1983), Myers (1986)

2.1: Aim and objectives

The aim of

1. To derive partial derivatives of the Chapman-Richard, Von Bertalanffy, Richards and Weibull model properties
2. To illustrate the nonlinear least square (NLS) estimation using a modified version of the Levenberg-Marquardt algorithm.

3. To estimate the parameters of the Chapman-Richard, Von Bertalanffy, Richards and Weibull model, using real data and SPSS (23) and MINITAB (16) statistical software.

3: Method of Estimation

Nonlinear regression modelling is similar to linear regression modelling in that both seek to graphically track a particular response from a set of variables. Nonlinear models are more complicated than linear models to develop because the function is created through a series of approximations (iterations) that may stem from trial-and-error. Mathematicians use several established methods, such as the Gauss-Newton method and the Levenberg-Marquardt method. This study used the modified version of the Levenberg-Marquardt method.

For a nonlinear model

$$\omega i = f(t_i, \mathbf{B}) + \varepsilon_i \qquad (1)$$

$i = 1, 2, \ldots n$, where ω is the response variable, t is the independent variable, **B** is the vector of parameters βj to be estimated ($\beta_1, \beta_2, \ldots, \beta_p$), ε_i is a random error term, p is the number of unknown parameters, and n is the number of observation. The estimators of $\beta\, j$'s are found by minimizing the sum of squares residual (SS_{Res}) function

$$SS_{\mathrm{Res}} = \sum_{i=1}^{n} [w_i - f(t_i, B)]^2 \qquad (2)$$

under the assumption that the εi are normal andindependent with mean zero and common variance σ^2. Since ω_i and t_i are fixed observations, the sum of squares residual is a function of **B**.

Least squares estimates of **B** are values which when substituted into Eq. (2) will make the SS_{Res} a minimum and are found by differentiating Eq. (2) with respect to each parameter and setting the result to zero. This provides the p normal equations that must be solved for $\hat{B}$. These normal equations take the form

$$\sum_{i=1}^{n} \{w_i - f(t_i, B)\} \left[\frac{\partial f(t_i, B)}{\partial \beta_j} \right] \qquad (3)$$

for $j = 1, 2, \ldots, p$. When the model is nonlinear in the parameters so are the normal equations. Consequently, for the nonlinear models considered in Table 1, it is impossible to obtain a closed form solution to the least squares estimate of the parameters by solving the p normal equations described in Eq. (3). Hence an iterative method must be employed to minimize the $SS\mathrm{Re}s$ (Draper and Smith 1981, Ratkowsky 1983).

The NLIN (nonlinear regression) procedure in SPSS(23) and MINITAB Statistical software 16 was used to fit the models to the height growth data and estimate the parameters. The Marquardt iterative method was chosen as it represents a compromise between the linearization (Gauss-Newton) method and the steepest descent method and appears to combine the best features of both while avoiding their most serious limitations (Draper and Smith 1981). The Marquardt iterative method requires specification of the names and starting values of the parameters to be estimated, the model using a single dependent variable, and the partial derivatives of the model with respect to each parameter (MINITAB 16/SPSS 23). The usual statistical tests which are appropriate in the general linear model case are, in general, not appropriate when the model is nonlinear and one cannot use the F statistic to obtain conclusions at any stated level of significance (Draper and Smith 1981). Hence the models were compared based on the proportion of the unexplained variation.

4 Results

4.1 Partial Derivatives

For ease of understanding the symbols of the parameters of the nonlinear models given in Table 1, α, β, k, and m, are replaced by new symbols β_0, β_1, β_2, and β_3 respectively. The parameters for all models considered in this paper are defined as follows:

- β_0 is the asymptote or the potential maximum of the response variable;
- β_1 is the biological constant;

- β_2 is the parameter governing the rate at which the response variable approaches its potential maximum; and
- β_3 is the algometric constant. The partial derivatives of the models with respect to each parameter ($\partial\omega / \partial\beta_j$) are given in Tables 3–5. The NLIN procedure in MINITAB(16) and SPSS(23) requires that the integral forms and the partial derivatives of the nonlinear models must be entered in the program using valid MINITAB 16/SPSS 23 syntax.

Table 3: Partial derivatives of Chapman-Richard's growth model

Partial derivative	Model The Chapman-Richards $\omega(t) = \beta_0(1-\beta_1 \exp(-\beta_2 t))^{\frac{1}{1-\beta_3}} + \varepsilon$
$\partial\omega/\partial\beta_0$	$(1-\beta_1 \exp(-\beta_2 t))^{\frac{1}{1-\beta_3}}$
$\partial\omega/\partial\beta_1$	$(-\beta_0 / (1-\beta_3))(1-\beta_1 \exp(-\beta_2 t))^{\frac{1}{1-\beta_3}-1} (\exp(-\beta_2 t))$
$\partial\omega/\partial\beta_2$	$(\beta_0\beta_1 t / (1-\beta_3))(1-\beta_1 \exp(-\beta_2 t))^{\frac{1}{1-\beta_3}-1} (\exp(-\beta_2 t))$
$\partial\omega/\partial\beta_3$	$(\beta_0 / (1-\beta_3)^2)(1-\beta_1 \exp(-\beta_2 t))^{\frac{1}{1-\beta_3}} \ln(1-\beta_1 \exp(-\beta_2 t))$

Table 4: Partial derivatives of Von Bertalanffy's growth model

Partial derivative	Model The von Bertalanffy $\omega(t) = \left(\beta_0{}^{(1-\beta_3)} - \beta_1 \exp(-\beta_2 t)\right)^{\frac{1}{1-\beta_3}} + \varepsilon$
$\partial\omega/\partial\beta_0$	$\left(\beta_0^{-\beta_3}\right)\left(\beta_0^{(1-\beta_3)} - \beta_1 \exp(-\beta_2 t)\right)^{\frac{1}{1-\beta_3}-1}$
$\partial\omega/\partial\beta_1$	$(-\exp(-\beta_2 t) / (1-\beta_3))\left(\beta_0{}^{(1-\beta_3)} - \beta_1 \exp(-\beta_2 t)\right)^{\frac{1}{1-\beta_3}-1}$
$\partial\omega/\partial\beta_2$	$(\beta_1 t / (1-\beta_3))(\exp(-\beta_2 t))\left(\beta_0{}^{(1-\beta_3)} - \beta_1 \exp(-\beta_2 t)\right)^{\frac{1}{1-\beta_3}-1}$
$\partial\omega/\partial\beta_3$	$\left(\exp\left((1/(1-\beta_3))\ln\left(\beta_0^{(1-\beta_3)} - \beta_1 \exp(-\beta_2 t)\right)^{\frac{1}{1-\beta_3}-1}\right)\Big/(1-\beta_3)\right) \bullet$ $\left[\left(\ln\left(\beta_0^{(1-\beta_3)} - \beta_1 \exp(-\beta_2 t)\right)\Big/(1-\beta_3)\right) - \left(\ln(\beta_0)\left(\beta_0^{(1-\beta_3)}\right)\Big/\left(\beta_0^{(1-\beta_3)} - \beta_1 \exp(-\beta_2 t)\right)\right)\right]$

Table 5: Partial derivatives of Richard's and Weibull's growth model

Partial derivative	Model: The Richard's $\omega(t)=\beta_0\Big/\left(1+\beta_1\exp(-\beta_2 t)\right)^{\frac{1}{\beta_3}}+\varepsilon$	The Weibull $\omega(t)=\left(\beta_0-\beta_1\exp(-\beta_2 t^{\beta_3})\right)+\varepsilon$
$\partial\omega/\partial\beta_0$	$\left(1+\beta_1\exp(-\beta_2 t)\right)^{\frac{-1}{\beta_3}}$	1.0
$\partial\omega/\partial\beta_1$	$\left(-\beta_0/\beta_3\right)\left(1+\beta_1\exp(-\beta_2 t)\right)^{\frac{-1}{\beta_3}-1}\left(\exp(-\beta_2 t)\right)$	$-\exp(-\beta_2 t^{\beta_3})$
$\partial\omega/\partial\beta_2$	$\left(\beta_0\beta_1 t/\beta_3\right)\left(1+\beta_1\exp(-\beta_2 t)\right)^{\frac{-1}{\beta_3}-1}\left(\exp(-\beta_2 t)\right)$	$\exp(-\beta_2 t^{\beta_3})\ \beta_1 t^{\beta_3}$
$\partial\omega/\partial\beta_3$	$\beta_0\left(1+\beta_1\exp(-\beta_2 t)\right)^{\frac{-1}{\beta_3}}\ln\left(1+\beta_1\exp(-\beta_2 t)\right)\beta_3^{-2}$	$\exp(-\beta_2 t^{\beta_3})\ \beta_1\beta_2\ \ln(t)t^{\beta_3}$

4.2 Starting Value Specification

The Marquardt iterative method requires that an initial or starting value for each parameter be estimated. Starting value specification is one of the most difficult problems encountered in estimating parameters of nonlinear models (Draper and Smith 1981). However, the problem of specifying initial values of parameters can be solved with proper understanding of the definition of the parameters in the context of the phenomenon being modelled. Wrong starting values result in longer iteration, greater execution time, non-convergence of the iteration, and possibly convergence to unwanted local minimum sum of squares residual (MINITAB 16). Hence expressions that provide good starting values for some of the parameters were developed. The most efficient order for determining starting values is β_0, β_2, β_3, and finally β_1.

The only parameter that is simple to specify is β_0. This is attributed to the clarity of its definition. The parameter β_0 is defined in the literature (Bertalanffy 1957, Richard 1959) as maximum possible value of the dependent variable determined by the productive capacity of the site. Therefore, in modelling the top height-age relationship β_0 was specified as the maximum value of the response variable in the data. For all nonlinear models given in Table 1 the β_2 parameter is defined as the rate constant at which the response variable approaches its maximum possible value β_0. On the basis of this definition it was found that the expression

$$\frac{(w_2-w_1)/(t_2-t_1)}{\beta_{0s}} \qquad (4)$$

where ω_1 and ω_2 are values of the response variable corresponding to a wide range of the predictor variable t_1 and t_2, and β_{0s} is the starting value specified for the β0 parameter, gave good starting values for the β_2 parameters. For modeling biological growth variables the algometric constant, β_3, lies between zero and one ($0 < \beta_3 < 1$) for the Chapman-Richards growth model and is positive ($\beta_3 > 0$) for the von Bertalanffy and Weibull growth models. The starting value for the biological constant, β_1, was specified by evaluating the models at the start of growth when the predictor variable is zero. Table 6 gives expressions used to specify starting values of the β_1 parameter for each model. $\omega(0)$ is the magnitude of the response variable at the start of growth, which ideally is zero, but one should choose a relatively small positive number.

Table 6: Expression used to specify the starting value for the biological constant (β_1).

Model	Expression
Chapman-Richard	$w(0) = (\beta_{0s}^{1-\beta_3} - \beta_1)^{\frac{1}{1-\beta_3}}$
Von Bertalanffy	$w(0) = \beta_{0s}(1-\beta_1)^{\frac{1}{1-\beta_3}}$
Richard	$w(0) = \beta_{0s}/(1+\beta_1)^{\frac{1}{\beta_3}}$
Weibull	$w(0) = (\beta_{0s} - \beta_1)$

The least squares estimates of the parameters of the nonlinear models for top height-age relationship are given in Tables 7. The parameter estimates for Richard's growth functions is statistically significant at the 5% level. Estimates of β_1, β_2, and β_3 for Chapman- Richards and the von Bertalanffy growth models are not statistically significant at the 5% level.

Parameter estimates of the Weibull growth model except β_2 are statistically significant at the 5% level. However, the Marquardt iteration procedure did not converge for the negative exponential model and hence, no parameter estimates of this model are presented.

Statistical significance of the parameters of the nonlinear models was determined by evaluating the 95% asymptotic confidence intervals of the estimated parameters. The null hypothesis $H_0 : \beta_j = 0$ was rejected when the 95% asymptotic confidence interval of β_j does not include zero.

Table 7: Parameters Estimates for the four –parameter models for Top-Age relationship

Parameter	Model			
	Chapman-Richards	von Bertelanffy	Richard's	Weibull
β_0	28.347774	28.345941	25.484602	27.222914
β_1	0.8301844	4.5621873	0.00008673	26.243522
β_2	0.0253696	0.0253749	0.0367779	0.0051663
β_3	0.4902212	0.4904567	0.00003342	1.3263582

Table 8 provides predicted values of top height over the range of age using the least squares parameter estimates derived from the Marquardt algorithm. The Richard's, and the Weibull models have produced a slightly smaller residual standard error (0.13 *m*) compared to the von Bertalanffy and the Chapman- Richards models (0.14 *m*). All the models in Table 8 appear to predict reasonable estimates over the entire range of age. When nonlinear models are fitted to a biological growth data set statistical non-significance of the estimated parameters might imply one of the following:

(a) one or more parameters in the model may not be useful, or more accurately, a reparameterized model involving fewer parameters might be more appropriate;

(b) the biological growth data used for fitting the model are not adequate for estimating all the parameters; or

(c) the model assumptions do not conform with the biological system being modelled. The argument in (b) was the case with the Chapman-Richards and the von Bertelanffy growth models. Investigation of the differential forms and second derivatives of the Chapman-Richards and the von Bertalanffy models indicate that the functions are suitable to model a system that encompasses the entire range of the life cycle (i.e., juvenile, adolescent, mature and senescent stages) of a biological response variable. However, the top height growth measurements considered in this study (Table 1) lacks data on juvenile and senescent stages of growth. Hence, non-significance of three of the parameters of the two models might be attributed to this cause. To support this argument we have included an initial data point (age = 0, top height = 0) to the data in Table 2 and refitted the Chapman-Richards and the von Bertalanffy models. Table 8 shows the parameter estimates, asymptotic standard error (ASE) and asymptotic 95% confidence intervals (95% ACI) for each parameter of these two models. Without inclusion of the initial data point three of the parameters (β_1, β_2, and β_3) are not statistically significant (see Table 8). However, inclusion of the initial data point has resulted in statistically significant estimates of the three parameters. Inclusion of any additional data point from an early or juvenile stage of growth will result innsignificant improvement in the estimates of the parameters of these two models. This clearly illustrates that significance of the parameters of the Chapman-Richards and the von Bertalanffy growth models depends on the range of the growth data.

The Chapman-Richards, Richard's, and the von Bertalnffy growth models have points of inflection and are sigmoid. These models are suitable for quantifying a growth phenomenon that exhibit a sigmoid pattern over time.

Table 8: Actual and predicted values of top height and the associated residual standard error for each fitted model.

Age(yrs)	Top height(m)	Chapman-Richard	Von-Bertalanffy	Richard's	Weibull
20	7.3	6.78	6.79	7.30	6.78
25	9.0	8.58	8.58	8.55	8.58
30	10.9	10.33	10.33	10.27	10.33
35	12.6	11.99	11.99	12.40	11.99
40	13.9	13.55	13.55	13.54	13.54
45	15.4	14.99	14.99	15.02	14.99
50	16.9	16.33	16.33	16.37	16.33
55	18.2	17.54	17.54	17.58	17.55
60	19.0	18.65	18.65	18.65	18.65
64	20.0	19.46	19.46	19.41	19.46
RSE[1](m)		0.14	0.14	0.13	0.13

Table: Comparison of parameter estimates for Von Bertalanffy and Chapman-Richard's modes when an initial growth response data is added.

	Von-Bertalanffy							
	Without Initial point 1				With initial point 2			
	βi	ASE 3	95% ACI 4		βi	ASE 3	95% ACI 4	
Parameter			Lower	Upper			Lower	Upper
β0	28.35	4.443	17.48	39.22	30.92	2.156	25.82	36.02
β2	4.574	11.46	-23.47	32.62	14.48	4.509	3.827	25.15
β2	0.025	0.012	-0.005	0.056	0.019	0.003	0.012	0.026
β3	0.409	0.551	-0.859	1.839	0.22	0.073	0.048	0.392

Chapman-Richard							
Without Initial point 1				With initial point 2			
βi	ASE 3	95% ACI 4		βi	ASE 3	95% ACI 4	
		Lower	Upper			Lower	Upper
28.35	4.443	17.48	39.22	30.92	2.156	25.82	36.02
4.574	11.46	-23.47	32.62	14.48	4.509	3.827	25.15
0.025	0.012	-0.005	0.056	0.019	0.003	0.012	0.026
0.409	0.551	-0.859	1.839	0.22	0.073	0.048	0.392

Note: [1] Parameter estimates when no juvenile top height is available (data from table 2)
[2] Parameter estimates when one juvenile top height data point (0,0) is added.
[3] ASE: Asymptotic standard error
[4] ACI: Asymptotic Confidence Interval

5: Discussion

Provided that one has knowledge of the meaning of the parameters of the model and the phenomena being modeled, it may be possible to identify when an iteration procedure has converted to a local minimum sum of squares residual. One recognizes this non-optimal solution by reviewing the magnitude and sign of the estimated parameters, and the size of the asymptotic correlation matrix of the estimated parameters. Large asymptotic correlation matrices for the estimated parameters of the nonlinear models may indicate that some of the parameters are not important or the model is over parameterized. However, Draper and Smith (1981) explain that large correlations of the estimated parameters do not necessarily mean that the original model is inappropriate for the physical situation under study. For example, in a linear model, when a particular β (a coefficient) does not appear to be different from zero, it does not always imply that the corresponding x (independent variable) is ineffective; it may be that, in the particular set of data under study, x does not change enough for its effect to be discernible. In general, efficient parameter estimation can best be achieved through a good understanding of the meaning of the parameters, the mathematics of the models, including the partial derivatives, and the system being modeled.

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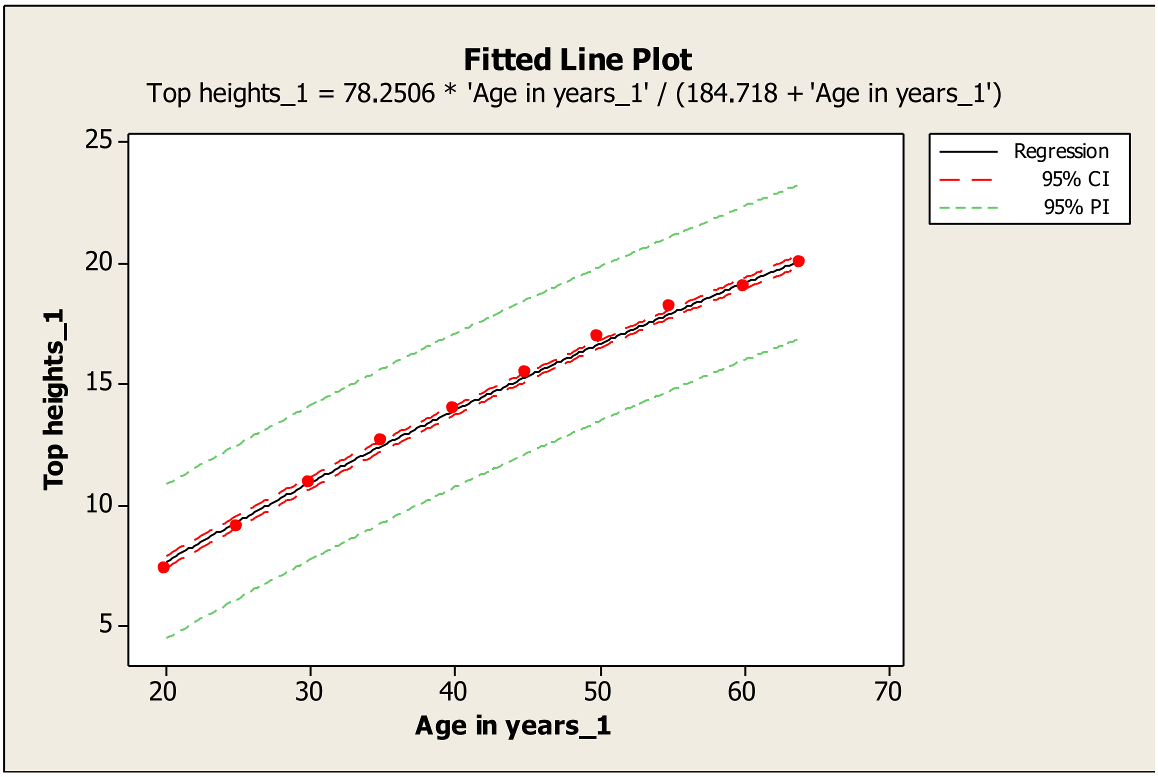
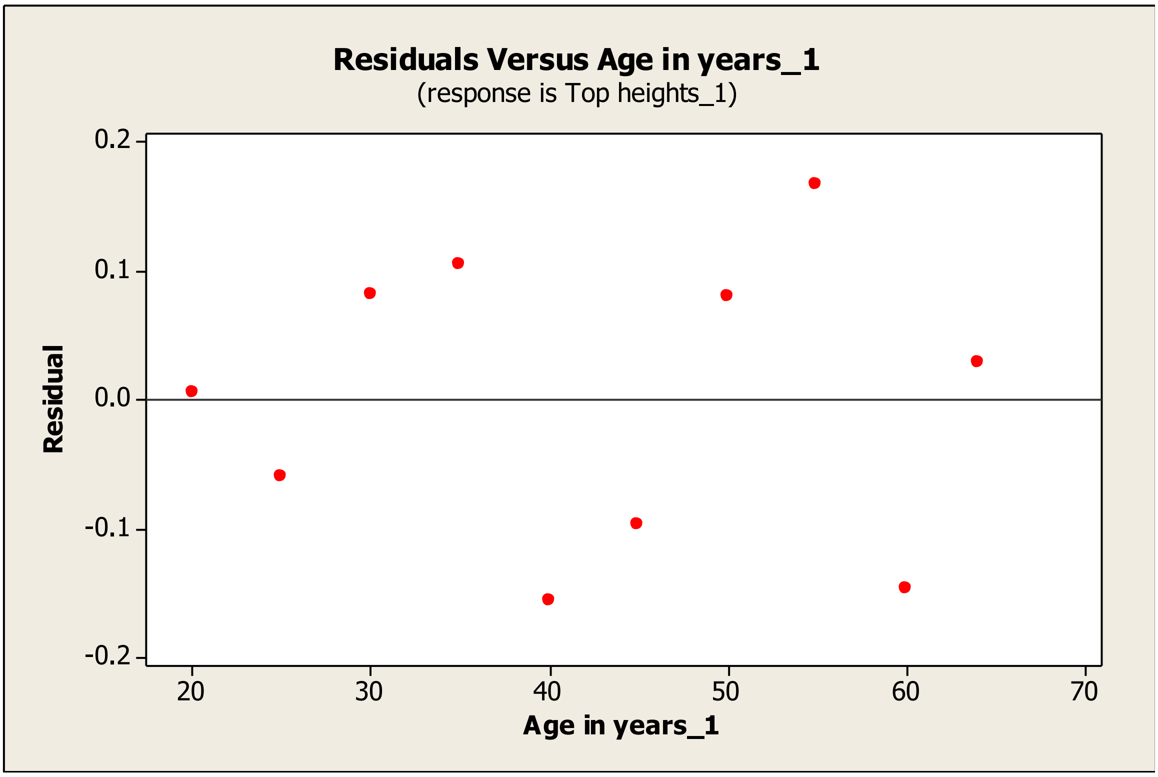
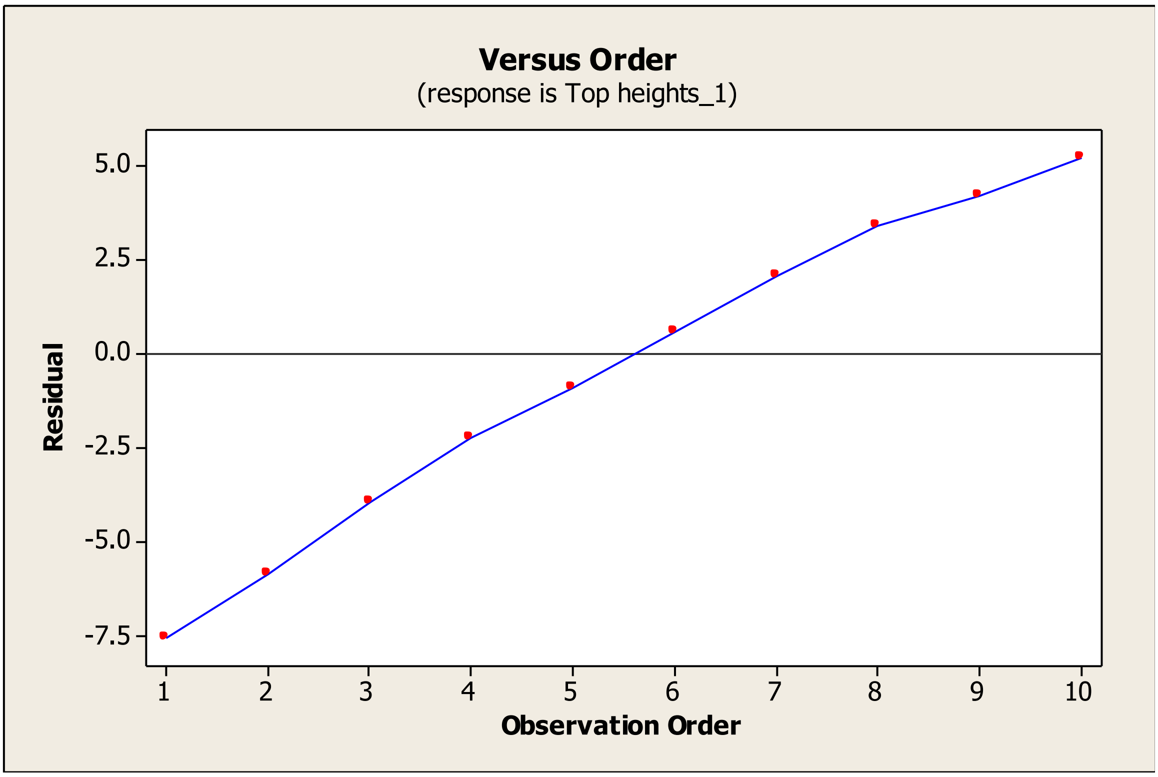
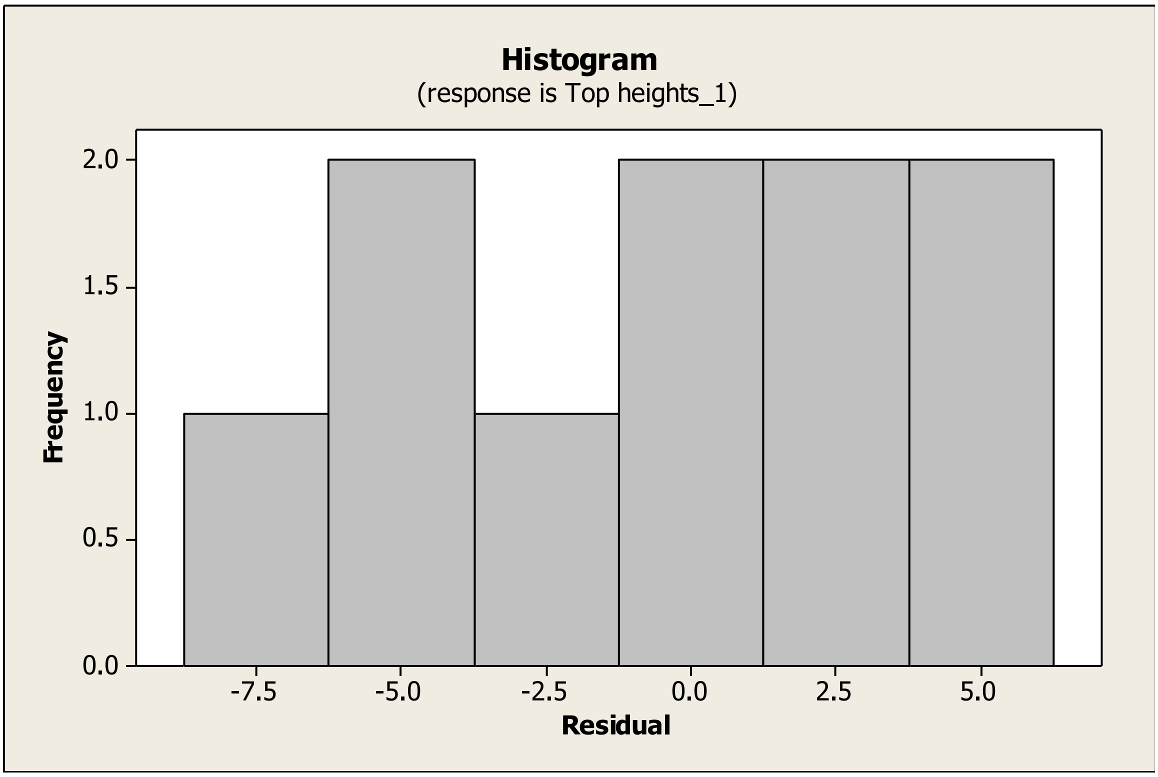
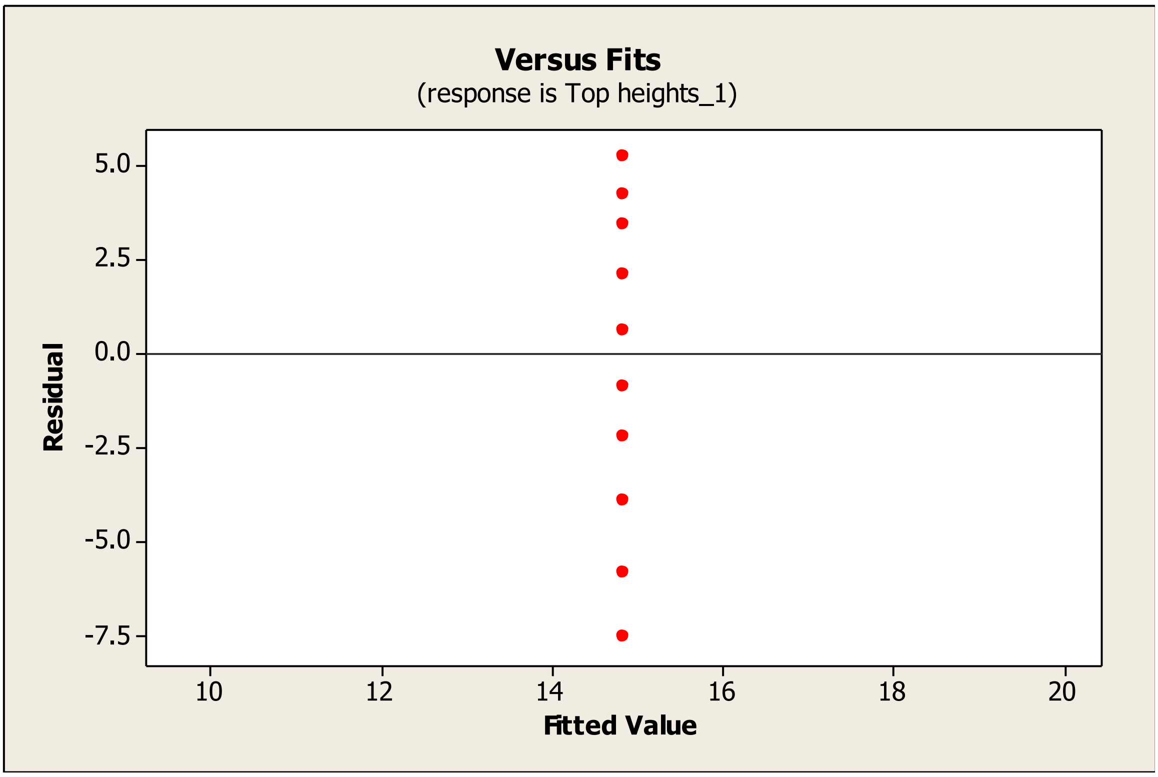
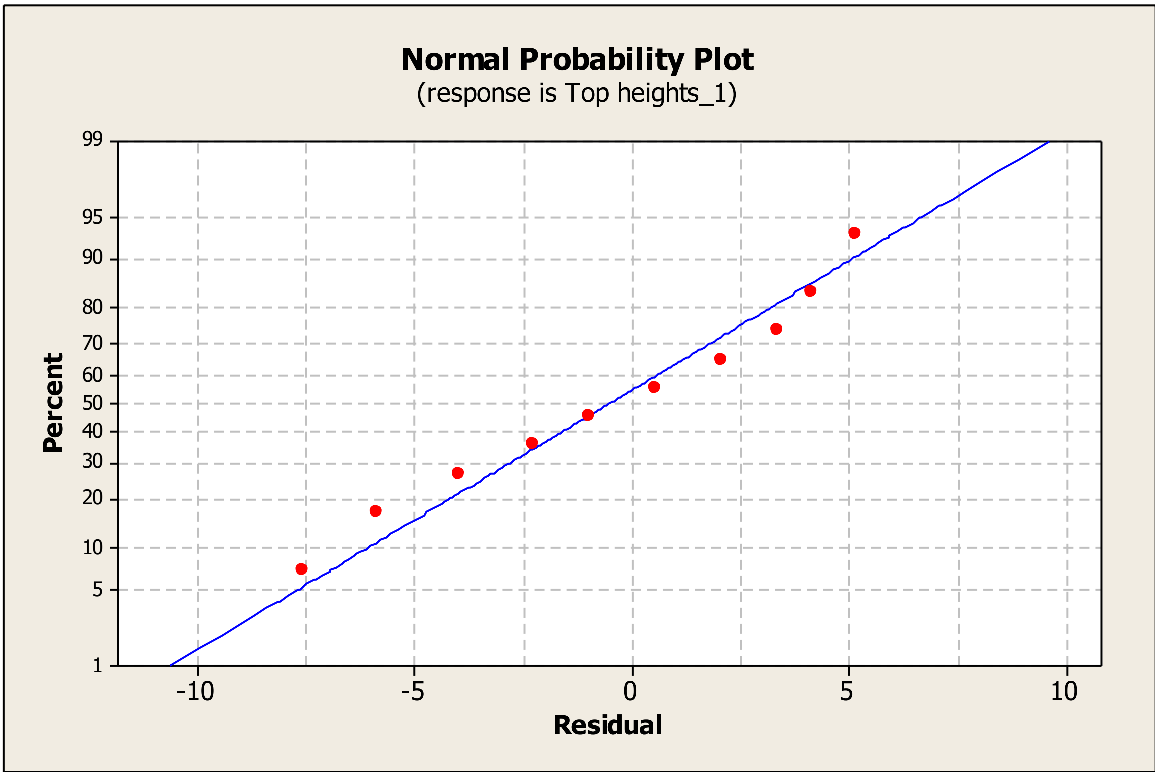

Fitted Line Plot
Top heights_1 = 78.2506 * 'Age in years_1' / (184.718 + 'Age in years_1')
Regression
95% CI
95% PI
Top heights_1
Age in years_1
25
20
15
10
5
20
30
40
50
60
70

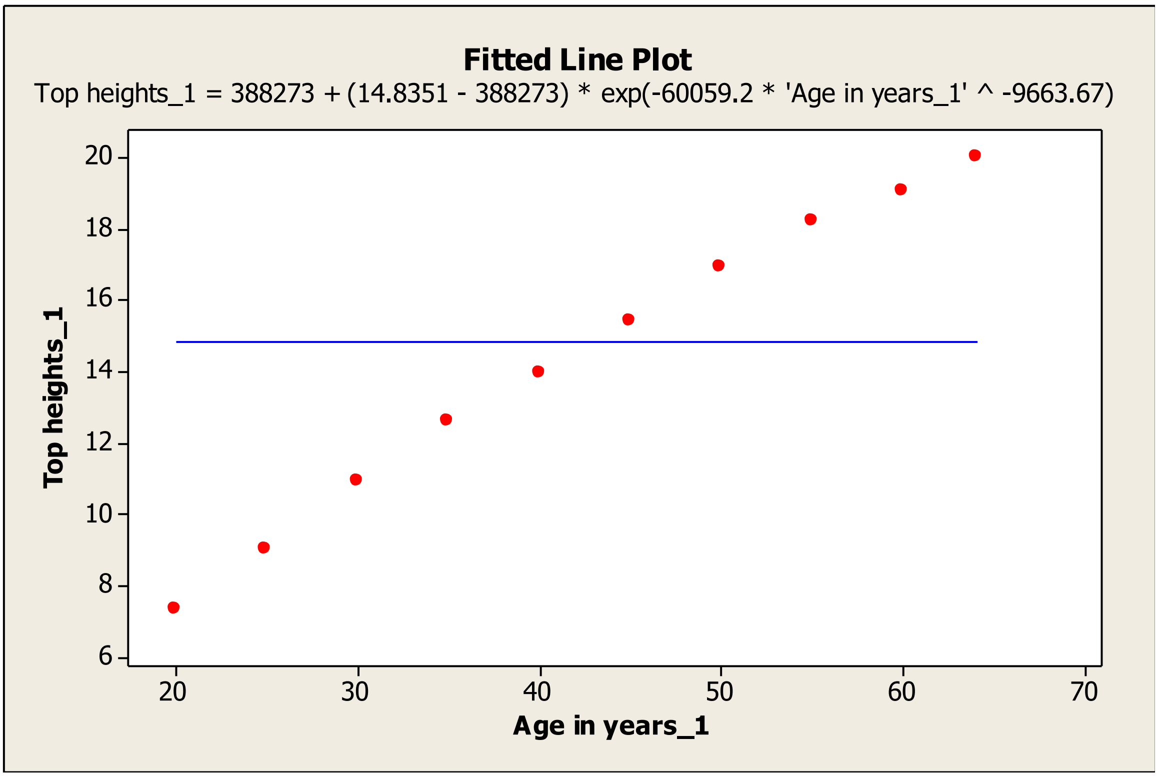

Residuals Versus Age in years_1
(response is Top heights_1)
Residual
Age in years_1
0.2
0.1
0.0
-0.1
-0.2
20
30
40
50
60
70

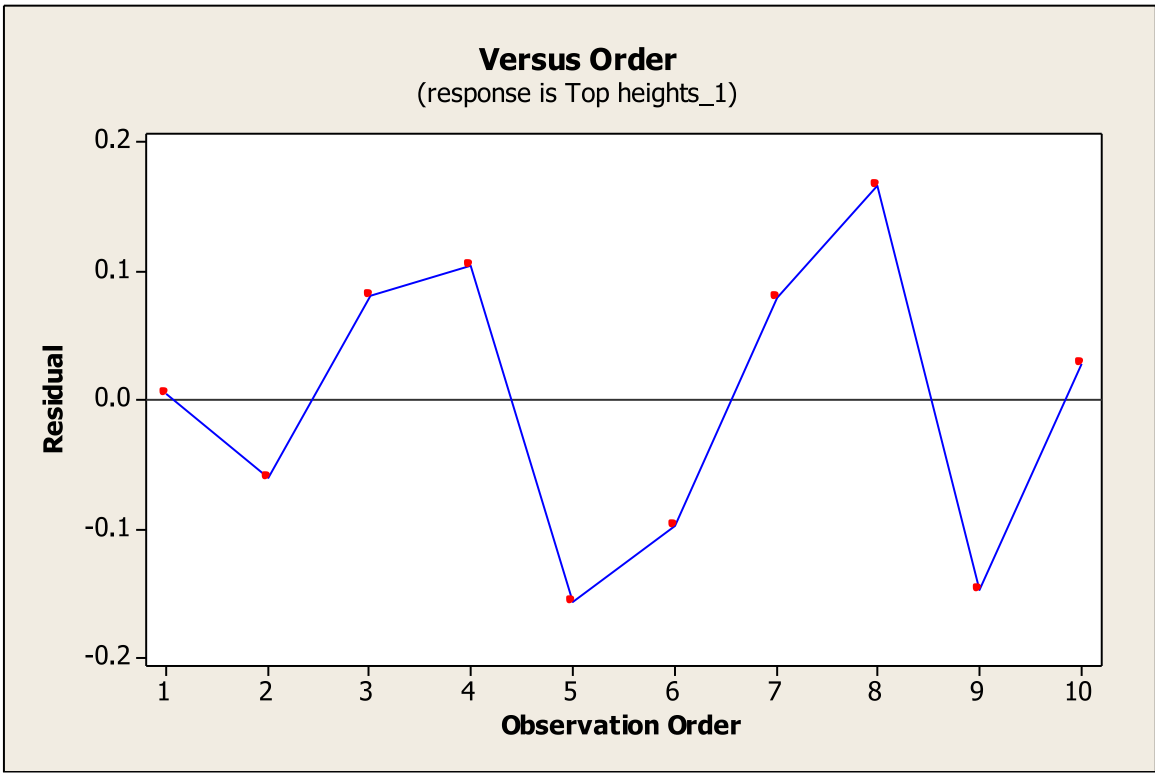

Versus Order
(response is Top heights_1)
Residual
5.0
2.5
0.0
-2.5
-5.0
-7.5
1
2
3
4
5
6
7
8
9
10
Observation Order


Histogram
(response is Top heights_1)
Frequency
2.0
1.5
1.0
0.5
0.0
-7.5
-5.0
-2.5
0.0
2.5
5.0
Residual


Versus Fits
(response is Top heights_1)
Residual
Fitted Value
5.0
2.5
0.0
-2.5
-5.0
-7.5
10
12
14
16
18
20


Normal Probability Plot
(response is Top heights_1)
Percent
Residual
99
95
90
80
70
60
50
40
30
20
10
5
1
-10
-5
0
5
10


Fitted Line Plot
Top heights_1 = 388273 + (14.8351 - 388273) * exp(-60059.2 * 'Age in years_1' ^ -9663.67)
Top heights_1
Age in years_1
20
18
16
14
12
10
8
6
20
30
40
50
60
70


Versus Order
(response is Top heights_1)
Residual
Observation Order
0.2
0.1
0.0
-0.1
-0.2
1
2
3
4
5
6
7
8
9
10