



Estimation of Nonlinear Regression Parameters Precision

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Abstract: The aim of this paper is to estimate the parameter precision values in nonlinear regression using Microsoft Excel. In case of simple linear regression, these values can be obtained from regression analysis in Excel. Commercially available programs output these values, but the main limitation is that they force the users to adopt a black box approach. The procedure described here can be adopted to any nonlinear dataset assuming that parameters obtained from solver accurately describe the nonlinear regression model. For one of the nonlinear datasets from NIST Statistical reference datasets, the parameters are initially estimated by using Solver and then by using Finite differences method parameter precision values are calculated. The results obtained were found to be comparable with the reported values.

Key Words: Nonlinear regression, solver, least squares, perturbation

1. Introduction

Regression analysis deals with the relationship between one or more independent variables and a dependent variable. Regression analysis is performed by selecting a suitable function which accurately describes the relationship between the two and estimator to calculate the parameter values. These regression parameters are calculated by least squares method. In linear regression [1], either the parameters are linear or the function describing the model is linear. Nonlinear regression methods are applied when the relationship between dependent and

independent variables is not linear. Nonlinear regression relies on iterative procedure to find the best fit. The process [2] starts with initial values for each parameter, and then by using least squares fitting, the best fit parameter values which minimize the sum of squared residuals are estimated. Microsoft Excel Solver Add-in estimates parameters for nonlinear regression by least squares method, but it doesn't estimate their precision. The paper aims to use finite difference method to estimate these values.

2. Nonlinear Regression

A model is considered to be nonlinear if any of the partial derivatives with respect to any of the model parameters are dependent on any other model parameters, any of the

derivatives do not exist or are discontinuous. A nonlinear model can be expressed as (equation 1):

$$y = f(\theta; t) + \epsilon \quad (1)$$

where y is the vector of responses, f is the function used to describe the model, θ is vector of model parameters, t is the predictor variable and ϵ is the vector of residuals [3].

Rat43 dataset from National Institute of Standards and Technology (NIST) website

[4], was selected to estimate the parameter precision by finite difference method. This dataset was selected, as the data can be fitted by using nonlinear regression method and is included in the higher level of difficulty group.

$$y = \frac{\beta_1}{((1 + e^{[\beta_2 - \beta_3 * t]})^{1/\beta_4})} \quad (2)$$

The nonlinear regression model described by equation 2 was used to fit the data, where response variable (y) is the dry weight of onion bulbs, whereas predictor variable (t) is

growing time [4]. The model parameters were estimated by using both starting values and the results are given in Table 1.

Table 1. Rat43 Dataset Values

t (growing time)	y (onion bulb dry weight)
1	16.08
2	33.83
3	65.80
4	97.20
5	191.55
6	326.20
7	386.87
8	520.53
9	590.03

10	651.92
11	724.93
12	699.56
13	689.96
14	637.56
15	717.41

Solver Implementation to Estimate Parameter Values (Table 2)

a) Data is entered in Excel, growing time (t) in column A and onion bulb dry weight (y) in column B.

b) Initial values for β_1 , β_2 , β_3 and β_4 given in NIST website were used [4].

c) By substituting different values of t , initial values of β_1 , β_2 , β_3 and β_4 in equation (2) different calculated y values were obtained.

d) Sum of squared errors (SSE) was obtained by adding the squared differences between y and y calculated value. SUMXMY2 function in Microsoft Excel was used to calculate the SSE value. In the parameters worksheet, cells B2 to B16 contains y values, cells C2 to C16

contains y calculated values which were obtained by using start 1 initial estimates. SSE value was obtained by using the formula “SUMXMY2 (C2:C16, B2:B16)”.

e) Best fitted parameter values were obtained by minimizing the SSE value using generalized reduced gradient (GRG) nonlinear method.

f) The process was also repeated by using second set of start values as given in the NIST website [4].

g) Results obtained from both start values were in agreement with the reported values [4].

Table 2. Model Parameter Results Obtained After Least Square Fitting Using Excel Solver

Parameter	Start 1	Values obtained	Start 2	Values obtained	Certified values
β_1	100	699.6415127	700	699.6415126	699.6415127000
β_2	10	5.27712531	5	5.277125383	5.2771253025
β_3	1	0.759629383	0.75	0.759629391	0.75962938329
β_4	1	1.279248389	1.3	1.279248414	1.2792483859

3. Finite Difference Method

For a function with two or more independent variables, the partial derivative of that function with respect to a particular variable is the derivative of that function with respect to that variable, while holding the other variables constant [5]. The partial derivative term of each data point can be calculated by numer-

ical differentiation. The parameter term (β_1) is varied by a small amount from its optimized value while the other parameters terms are held constant. This variation of a parameter by a small amount is called perturbation. The partial derivatives are calculated by using the formula in Equation 7

[6] for all data points. Then the process is repeated for all the parameter terms in the model [6]. The Jacobian matrix (J) is constructed from all these partial derivative

terms and is given by the following equation (3) [7], where m is the number of nonlinear parameters.

$$J = \begin{bmatrix} \left(\frac{\partial y_1}{\partial \beta_1}\right) & \left(\frac{\partial y_1}{\partial \beta_2}\right) & \dots & \left(\frac{\partial y_1}{\partial \beta_m}\right) \\ \left(\frac{\partial y_2}{\partial \beta_1}\right) & \left(\frac{\partial y_2}{\partial \beta_2}\right) & \dots & \left(\frac{\partial y_2}{\partial \beta_m}\right) \\ \vdots & \vdots & \ddots & \vdots \\ \left(\frac{\partial y_n}{\partial \beta_1}\right) & \left(\frac{\partial y_n}{\partial \beta_2}\right) & \dots & \left(\frac{\partial y_n}{\partial \beta_m}\right) \end{bmatrix} \quad (3)$$

The parameter precision can be estimated from the matrix of partial derivatives (E), which is obtained by multiplying transpose of

J with itself ($E = J^T * J$) [7] and is given in equation 4.

$$E = \begin{bmatrix} \Sigma \left(\frac{\partial y_1}{\partial \beta_1}\right)^2 & \Sigma \left(\frac{\partial y_1}{\partial \beta_1} * \frac{\partial y_2}{\partial \beta_2}\right) & \dots & \Sigma \left(\frac{\partial y_1}{\partial \beta_1} * \frac{\partial y_m}{\partial \beta_m}\right) \\ \Sigma \left(\frac{\partial y_1}{\partial \beta_1} * \frac{\partial y_2}{\partial \beta_2}\right) & \Sigma \left(\frac{\partial y_2}{\partial \beta_2}\right)^2 & \dots & \Sigma \left(\frac{\partial y_2}{\partial \beta_2} * \frac{\partial y_m}{\partial \beta_m}\right) \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma \left(\frac{\partial y_1}{\partial \beta_1} * \frac{\partial y_m}{\partial \beta_m}\right) & \Sigma \left(\frac{\partial y_2}{\partial \beta_2} * \frac{\partial y_m}{\partial \beta_m}\right) & \dots & \Sigma \left(\frac{\partial y_m}{\partial \beta_m}\right)^2 \end{bmatrix} \quad (4)$$

The square roots of the diagonal elements of the above E matrix inverse when multiplied by root residual standard deviation (RSD) yields the precision for the respective parameter (equations 5 and 6) [7], where SSE value

was obtained from solver implementation and df is the degrees of freedom (difference between number of observation and number of parameters in the model).

$$\beta_{i,\text{precision}} = \text{RSD} * \sqrt{E^{-1}_{ii}}, i = 1, 2, 3, \dots m \quad (5)$$

$$\text{RSD} = \sqrt{\frac{\text{SSE}}{\text{df}}} \quad (6)$$

The individual partial derivatives for the J matrix can be calculated from the following equations (7) [7], where δ (perturbation) can

be 10^{-6} or 10^{-7} [7]. The above calculations are performed in Microsoft Excel to obtain the parameter precision values for all the parameters.

$$\begin{aligned}
 \left(\frac{\partial y_i}{\partial \beta_1}\right)_{\beta_2, \dots, \beta_4, t_i} &\approx \frac{y[\beta_1(1 + \delta), \beta_2, \beta_3, \beta_4, t_i] - y[\beta_1, \beta_2, \beta_3, \beta_4, t_i]}{\beta_1(1 + \delta) - \beta_1} \\
 \left(\frac{\partial y_i}{\partial \beta_2}\right)_{\beta_1, \beta_3, \beta_4, t_i} &\approx \frac{y[\beta_1, \beta_2(1 + \delta), \beta_3, \beta_4, t_i] - y[\beta_1, \beta_2, \beta_3, \beta_4, t_i]}{\beta_2(1 + \delta) - \beta_2} \\
 \left(\frac{\partial y_i}{\partial \beta_3}\right)_{\beta_1, \beta_2, \beta_4, t_i} &\approx \frac{y[\beta_1, \beta_2, \beta_3(1 + \delta), \beta_4, t_i] - y[\beta_1, \beta_2, \beta_3, \beta_4, t_i]}{\beta_3(1 + \delta) - \beta_3} \\
 \left(\frac{\partial y_i}{\partial \beta_4}\right)_{\beta_1, \beta_2, \beta_3, t_i} &\approx \frac{y[\beta_1, \beta_2, \beta_3, \beta_4(1 + \delta), t_i] - y[\beta_1, \beta_2, \beta_3, \beta_4, t_i]}{\beta_4(1 + \delta) - \beta_4}
 \end{aligned} \tag{7}$$

4. Results and Discussion

The partial derivative calculations for the first parameter using parameter values obtained from Start 1 values are shown in Figure 1. Values in Column A9 to B23 corresponds to the raw data, values in C9 to C23 correspond to calculated values obtained after solver optimization. For values in D9 to

D23, to the first parameter (β_1) δ (10^{-6}) was added and then its corresponding y (independent variable) values are calculated. The values in E9 to E23 are calculated as per equation 7. The calculations are repeated for all the parameters to obtain the partial derivative matrix (J), as given in equation 3.

	A	B	C	D	E	F	G	H	I	J
6										
7	1. For paramter β_1									
8	t	y	cal (y) - 1	cal ($y(\beta_1[1+\delta],$ $\beta_2, \beta_3, \beta_4, t_i)$)	$\left(\frac{\partial y_t}{\partial \beta_1}\right)$ $\beta_2, \dots, \beta_4, t_i$					Start 1
9	1	16.08	20.30188	20.3019031	2.9E-02				β_1	699.6415
10	2	33.83	36.41495	36.4149893	5.2E-02				β_2	5.277125
11	3	65.80	64.63606	64.6361257	9.2E-02				β_3	0.759629
12	4	97.20	112.3302	112.330263	1.6E-01				β_4	1.279248
13	5	191.55	187.5353	187.535493	2.7E-01				SSE	8786.405
14	6	326.20	292.3813	292.381567	4.2E-01				δ	1.0E-06
15	7	386.87	413.3579	413.358358	5.9E-01					
16	8	520.53	523.4563	523.456782	7.5E-01					
17	9	590.03	602.693	602.693607	8.6E-01					
18	10	651.92	650.1694	650.170022	9.3E-01					
19	11	724.93	675.4649	675.465532	9.7E-01					
20	12	699.56	688.0892	688.089879	9.8E-01					
21	13	689.96	694.1823	694.182966	9.9E-01					
22	14	637.56	697.0753	697.076022	1.0E+00					
23	15	717.41	698.4383	698.438971	1.0E+00					
24										

Figure 1. Excel Sheet Showing Partial Derivative Calculation One Parameter (β_1)

[Click here to view/download complete Excel file](#)

[or click here go to Appendix](#)

The Jacobian matrix in cells N9 to N23 are obtained by pasting the values of E9 to E23 for first parameter. The values O9 to Q23 in

the matrix are obtained similarly from the other three parameters, and the resulting matrix is shown in Figure 2.

	M	N	O	P	Q
7					
8		Jacobian matrix			
9		2.9E-02	-1.6E+01	1.6E+01	-5.6E+01
10		5.2E-02	-2.8E+01	5.6E+01	-8.4E+01
11		9.2E-02	-4.8E+01	1.4E+02	-1.2E+02
12		1.6E-01	-7.9E+01	3.2E+02	-1.6E+02
13		2.7E-01	-1.2E+02	6.0E+02	-1.9E+02
14		4.2E-01	-1.5E+02	9.2E+02	-2.0E+02
15		5.9E-01	-1.6E+02	1.1E+03	-1.7E+02
16		7.5E-01	-1.3E+02	1.0E+03	-1.2E+02
17		8.6E-01	-8.2E+01	7.4E+02	-7.0E+01
18		9.3E-01	-4.6E+01	4.6E+02	-3.7E+01
19		9.7E-01	-2.3E+01	2.6E+02	-1.9E+01
20		9.8E-01	-1.1E+01	1.4E+02	-9.0E+00
21		9.9E-01	-5.4E+00	7.0E+01	-4.3E+00
22		1.0E+00	-2.6E+00	3.6E+01	-2.0E+00
23		1.0E+00	-1.2E+00	1.8E+01	-9.4E-01

Figure 2. Jacobian Matrix

The result in Figure 3 is obtained by taking inverse of matrix E. The first parameter precision is obtained by multiplying the

square root of value in N28 and RSD value (equation 8) [7].

	M	N	O	P	Q
26					
27		Inverse of matrix E			
28		0.332721	-0.02439	-0.00254	0.007355
29		-0.02439	0.005432	0.000504	-0.00176
30		-0.00254	0.000504	4.79E-05	-0.00016
31		0.007355	-0.00176	-0.00016	0.000592

Figure 3. Inverse of Matrix E

$$\begin{aligned}
 \text{RSD} &= \sqrt{\frac{8786.404908}{(15 - 4)}} = 28.26241466 \\
 \beta_{1,\text{precision}} &= \text{RSD} * \sqrt{\text{N28 cell value}} \\
 \beta_{2,\text{precision}} &= \text{RSD} * \sqrt{\text{O 29 cell value}} \\
 \beta_{3,\text{precision}} &= \text{RSD} * \sqrt{\text{P 30 cell value}} \\
 \beta_{4,\text{precision}} &= \text{RSD} * \sqrt{\text{Q 31 cell value}}
 \end{aligned}
 \tag{8}$$

The results obtained were comparable with the reported values [4] and are given in Table 3.

Table 3. Comparison Standard Deviation of Parameter Estimate Values

Parameter	Values obtained	Reported values
β_1	16.3023271498	16.3022978170
β_2	2.0829153607	2.0828735829
β_3	0.19566584176	0.19566123451
β_4	0.68762926694	0.68761936385

5. Conclusions

The parameter precision results obtained from the finite difference method were comparable to the reported values. Finite difference method offers a convenient approach to estimate nonlinear regression parameter precision values. Even though the method is robust in calculating precision values, limitations due to solver, like lack of

convergence during optimization or parameter values inaccurately describing the model, can be encountered. For example, in the case of MGH10 dataset (which is available in the NIST website), the parameter values obtained after solver optimization are incorrect, which in turn leads to inaccurate parameter precision values.

6. References

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$$\left(\frac{\partial y_i}{\partial \beta_1}\right)_{\beta_2, \dots, \beta_4, x_i} \approx \frac{y[\beta_1(1 + \delta), \beta_2, \beta_3, \beta_4, x_i] - y[\beta_1, \beta_2, \beta_3, \beta_4, x_i]}{\beta_1(1 + \delta) - \beta_1}$$

1. For paramter β_1

x	y	cal (y) - 1	cal (y($\beta_1[1+\delta]$, $\beta_2, \beta_3, \beta_4, x_i$))	$\left(\frac{\partial y_i}{\partial \beta_1}\right)_{\beta_2, \beta_3, \beta_4, x_i}$
1	16.08	20.30188	20.301903	2.9E-02
2	33.83	36.41495	36.414989	5.2E-02
3	65.80	64.63606	64.636126	9.2E-02
4	97.20	112.3302	112.33026	1.6E-01
5	191.55	187.5353	187.53549	2.7E-01
6	326.20	292.3813	292.38157	4.2E-01
7	386.87	413.3579	413.35836	5.9E-01
8	520.53	523.4563	523.45678	7.5E-01
9	590.03	602.693	602.69361	8.6E-01
10	651.92	650.1694	650.17002	9.3E-01
11	724.93	675.4649	675.46553	9.7E-01
12	699.56	688.0892	688.08988	9.8E-01
13	689.96	694.1823	694.18297	9.9E-01
14	637.56	697.0753	697.07602	1.0E+00
15	717.41	698.4383	698.43897	1.0E+00

	Start 1
β_1	699.6415
β_2	5.277125
β_3	0.759629
β_4	1.279248
SSE	8786.405
δ	1.0E-06

Parital derivative matrix

2.9E-02	-1.6E+01	1.6E+01	-5.6E+01
5.2E-02	-2.8E+01	5.6E+01	-8.4E+01
9.2E-02	-4.8E+01	1.4E+02	-1.2E+02
1.6E-01	-7.9E+01	3.2E+02	-1.6E+02
2.7E-01	-1.2E+02	6.0E+02	-1.9E+02
4.2E-01	-1.5E+02	9.2E+02	-2.0E+02
5.9E-01	-1.6E+02	1.1E+03	-1.7E+02
7.5E-01	-1.3E+02	1.0E+03	-1.2E+02
8.6E-01	-8.2E+01	7.4E+02	-7.0E+01
9.3E-01	-4.6E+01	4.6E+02	-3.7E+01
9.7E-01	-2.3E+01	2.6E+02	-1.9E+01
9.8E-01	-1.1E+01	1.4E+02	-9.0E+00
9.9E-01	-5.4E+00	7.0E+01	-4.3E+00
1.0E+00	-2.6E+00	3.6E+01	-2.0E+00
1.0E+00	-1.2E+00	1.8E+01	-9.4E-01

2. For parameter β_2

x	y	cal (y) - 1	cal ($y(\beta_1, \beta_2[1+\delta], \beta_3, \beta_4, x_i)$)	$\left(\frac{\partial y_i}{\partial \beta_2}\right)_{\beta_1, \beta_3, \beta_4, x_i}$
1	16.08	20.30188	20.3018	-1.6E+01
2	33.83	36.41495	36.414806	-2.8E+01
3	65.80	64.63606	64.635807	-4.8E+01
4	97.20	112.3302	112.32973	-7.9E+01
5	191.55	187.5353	187.53468	-1.2E+02
6	326.20	292.3813	292.38046	-1.5E+02
7	386.87	413.3579	413.35711	-1.6E+02
8	520.53	523.4563	523.45559	-1.3E+02
9	590.03	602.693	602.69257	-8.2E+01
10	651.92	650.1694	650.16913	-4.6E+01
11	724.93	675.4649	675.46473	-2.3E+01
12	699.56	688.0892	688.08913	-1.1E+01
13	689.96	694.1823	694.18224	-5.4E+00
14	637.56	697.0753	697.07531	-2.6E+00
15	717.41	698.4383	698.43827	-1.2E+00

	Start 1
β_1	699.6415
β_2	5.277125
β_3	0.759629
β_4	1.279248
SSE	8786.405
δ	1.0E-06

Inverse of matrix E			
0.332721	-0.02439	-0.00254	0.007355
-0.02439	0.005432	0.000504	-0.00176
-0.00254	0.000504	4.79E-05	-0.00016
0.007355	-0.00176	-0.00016	0.000592

RSD	28.26241
β_1	16.30233
β_2	2.082915
β_3	0.195666
β_4	0.687629

3. For parameter β_3

x	y	cal (y) - 1	cal ($y(\beta_1, \beta_2, \beta_3[1+\delta], \beta_4, x_i)$)	$\left(\frac{\partial y_i}{\partial \beta_3}\right)_{\beta_1, \beta_2, \beta_4, x_i}$
1	16.08	20.30188	20.301895	1.6E+01
2	33.83	36.41495	36.414995	5.6E+01
3	65.80	64.63606	64.636171	1.4E+02
4	97.20	112.3302	112.33039	3.2E+02
5	191.55	187.5353	187.53576	6.0E+02
6	326.20	292.3813	292.38198	9.2E+02
7	386.87	413.3579	413.35879	1.1E+03
8	520.53	523.4563	523.45703	1.0E+03
9	590.03	602.693	602.69356	7.4E+02
10	651.92	650.1694	650.16972	4.6E+02
11	724.93	675.4649	675.46505	2.6E+02
12	699.56	688.0892	688.08929	1.4E+02
13	689.96	694.1823	694.18232	7.0E+01
14	637.56	697.0753	697.07535	3.6E+01
15	717.41	698.4383	698.43829	1.8E+01

	Start 1
β_1	699.6415
β_2	5.277125
β_3	0.759629
β_4	1.279248
SSE	8786.405
δ	1.0E-06

4. For parameter β_4

	y	cal (y) - 1	cal ($y(\beta_1, \beta_2, \beta_3, \beta_4[1+\delta], x_i)$)	$\left(\frac{\partial y_i}{\partial \beta_4}\right)_{\beta_1, \beta_2, \beta_3, x_i}$
1	16.08	20.30188	20.30181	-5.6E+01
2	33.83	36.41495	36.41485	-8.4E+01
3	65.80	64.63606	64.63591	-1.2E+02
4	97.20	112.3302	112.32995	-1.6E+02
5	191.55	187.5353	187.53506	-1.9E+02
6	326.20	292.3813	292.38102	-2.0E+02
7	386.87	413.3579	413.35773	-1.7E+02
8	520.53	523.4563	523.45611	-1.2E+02
9	590.03	602.693	602.69291	-7.0E+01
10	651.92	650.1694	650.16932	-3.7E+01
11	724.93	675.4649	675.46483	-1.9E+01
12	699.56	688.0892	688.08918	-9.0E+00
13	689.96	694.1823	694.18227	-4.3E+00
14	637.56	697.0753	697.07532	-2.0E+00
15	717.41	698.4383	698.43827	-9.4E-01

	Start 1
β_1	699.6415
β_2	5.277125
β_3	0.759629
β_4	1.279248
SSE	8786.405
δ	1.0E-06