

Nonlinear Regression Models without Data Linearization

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```
ClearAll;  
Off[General::spell1]
```

Introduction

This worksheet illustrates finding the constants of a nonlinear regression model without data linearization. Three common nonlinear models are illustrated.

Exponential: $y = ae^{bx}$

Power: $y = ax^b$

Saturation: $y = \frac{ax}{b+x}$

where a and b are the constants of the above regression models.

Given n data points $(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots, (x_n, y_n)$, you can best fit one of the above models to the data. In this worksheet, the constants a and b are calculated in the following steps:

- 1) Find the sum of the squares of the residuals, Sr .
- 2) Minimize Sr by differentiating with respect to a and b and setting the resulting two equations equal to zero.
- 3) Solve the two nonlinear equations simultaneously for a and b .

Mathematica will then return the real solutions of a and b . To learn more about nonlinear regression models see the Nonlinear Regression model worksheet.

Section 1: Input Data

Below are the input parameters to begin the simulation. This is the only section that requires user input. Once the values are entered, *Mathematica* will return the constants of the nonlinear regression model that is specified by the user with the *modeltype* variable.

NOTE: Before evaluating the worksheet, the user must enter initial guesses of the constants of the model a and b . For reasonable initial guesses, use the solution from the Nonlinear Model with data linearization worksheet. For convergence, use initial guesses a and b close to the values of a and b obtained by using data linearization.

Input Parameters:

- Number of data points, n

```
n = 5  
5
```

- Array of x values, X

```
x = {10, 16, 25, 40, 60}  
{10, 16, 25, 40, 60}
```

- Array of y values, Y

```
Y = {94, 118, 147, 180, 230}  
{94, 118, 147, 180, 230}
```

- For *exponential* model call model type to be "exponential"
For *power* model assign the model type variable as "power"
For *saturation growth* model, assign the model type variable to be "growth"

```
modeltype = "power"  
power
```

- Insert your initial guesses for a and b here. Reasonable initial guesses for a and b can be obtained from data linearization models.

Initial Guess values for a

```
Ainit = 30.199  
30.199
```

Initial Guess values for b

```

Binit = 0.489

0.489

Clear[a];
Clear[b];
Clear[Sr];

```

Section 2: Finding the constants of the model

Assigning the proper regression model

```

If[modeltype == "exponential", f[x_] = a * E^(b * x)];
If[modeltype == "power", f[x_] = a * x^b];
If[modeltype == "growth", f[x_] = (a * x) / (b + x)];

```

Calculating the sum of the square of the residuals

```

Sr = 0;
For[i = 1, i ≤ n, i++, Sr = Sr + ((Y[[i]] - f[X[[i]]]) ^ 2)];

Sr

(94 - 10b a)2 + (118 - 16b a)2 + (147 - 25b a)2 + (180 - 40b a)2 + (230 - 60b a)2

```

Differentiating the sum of the square of the residuals with respect to the constants of the model, a and b , to setup two simultaneous nonlinear equations and two unknowns.

```

eqn1 = Expand[D[Sr, a] == 0];
eqn2 = Expand[D[Sr, b] == 0];

```

Solving the two simultaneous nonlinear equations. We are using *FindRoot* since we are looking for real solutions.

```

soln = FindRoot[{eqn1, eqn2}, {{a, Ainit}, {b, Binit}}, MaxIterations → 1000];
a /. soln[[1]];
a = %;
b /. soln[[2]];
b = %;
Print["The constants of the ", modeltype, " model are a = ", a, " and b = ", b]

The constants of the power model are a = 29.335 and b = 0.499663

```

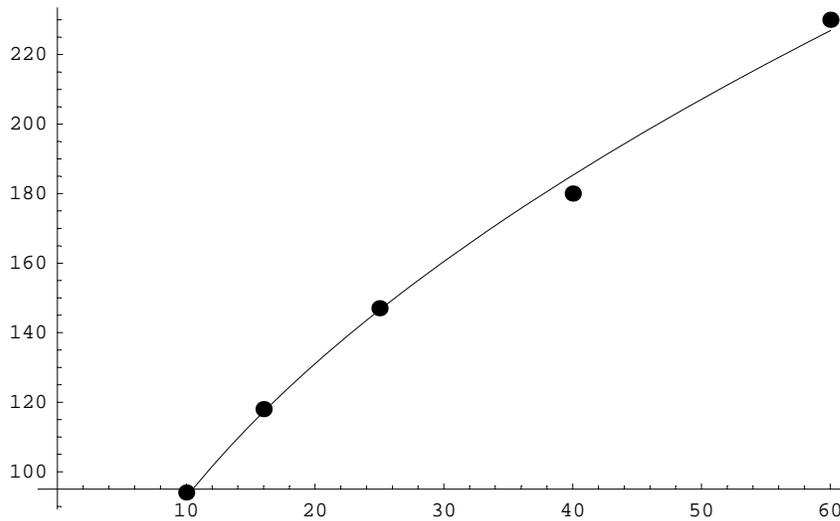
Plotting the observed values and the predicted curve

```

predicted = f[x];
observed = Table[{X[[i]], Y[[i]]}, {i, 1, n}];
ttl = Print[modeltype, " regression model, y vs x"];
points = ListPlot[observed, PlotStyle -> PointSize[.02], DisplayFunction -> Identity];
lin = Plot[predicted, {x, Min[X], Max[X]}, DisplayFunction -> Identity];
Show[points, lin, DisplayFunction -> $DisplayFunction]

```

power regression model, y vs x



- Graphics -

Conclusion

Mathematica helped us in illustrating three common nonlinear models of regression. Answer the following questions using the worksheet

- 1) Verify each of the models by using data that exactly follows the regression model.
- 2.) What is the difference in the solution between nonlinear models obtained via data that is linearized and data that is not linearized.

References

[1] Autar Kaw, *Holistic Numerical Methods Institute*, <http://numericalmethods.eng.usf.edu/nbm>, See How does Nonlinear Regression Work?