Nonlinear Regression Models without Data Linearization

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NOTE: This worksheet demonstrates the use of Maple to illustrate finding the constants of nonlinear regression models without data linearization.

Introduction

This worksheet illustrates finding the constants of a nonlinear regression model without data linearization. Three common nonlinear models are illustrated - 1) Exponential 2) Power 3) Saturation Growth.

Exponential: $y=ae^{bx}$ **Power:** $y=ax^b$ **Saturation:** y=(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) ,...., (x_n, y_n) , you can best fit one of the above nonlinear

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, S_r .

2) Minimize S_r 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*.

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

Section 1: Input Data

Below are the input parameters to begin the simulation. This is the only section that requires user input.

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 <u>nonlinear model with</u> data linearization worksheet. For convergence, use initial guesses for *a* and *b* close to the values of *a* and *b* obtained by using data linearization.

Input Parameters:

n = number of data points **X** = array of x values **Y**= array of y values **model_type** = type of nonlinear regression model the user wishes to evaluate **Ainit** = initial guess values for a **Binit** = initial guess values for b

```
> restart;
  n:=3;
  X:=[0.5,1,3];
  Y:=[2*exp(0.5), 2*exp(1.), 2*exp(3.)];
  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 "saturation"
  model_type:="exponential";
  Ainit:=7.3;
  Binit:=1.39;
                                      n := 3
                                  X := [0.5, 1, 3]
                   Y := [3.297442542, 5.436563656, 40.17107384]
                            model_type := "exponential"
                                    Ainit := 7.3
                                   Binit := 1.39
                                                                                    (2.1)
```

V Section 2: Finding the constants of the model

```
> Assigning the proper regression model
if (model_type="exponential") then
f:=x->a*exp(b*x);
end if;
if (model_type="power") then
f:=x->a*x^b;
end if;
if (model_type="saturation") then
f:=x->a*x/(b+x);
end if;
Calculating the sum of the square of the residuals
Sr:=0:
for i from 1 by 1 to n do
Sr:=Sr+(Y[i]-f(X[i]))^2:
end do:
```

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(diff(Sr,a)=0):
eqn2:=expand(diff(Sr,b)=0):
```

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

```
soln:=fsolve({eqn1,eqn2},{a=Ainit,b=Binit}):
assign(soln):
print(`The constants of the `,model_type,` model are a= `,a,`
and b= `,b);
```

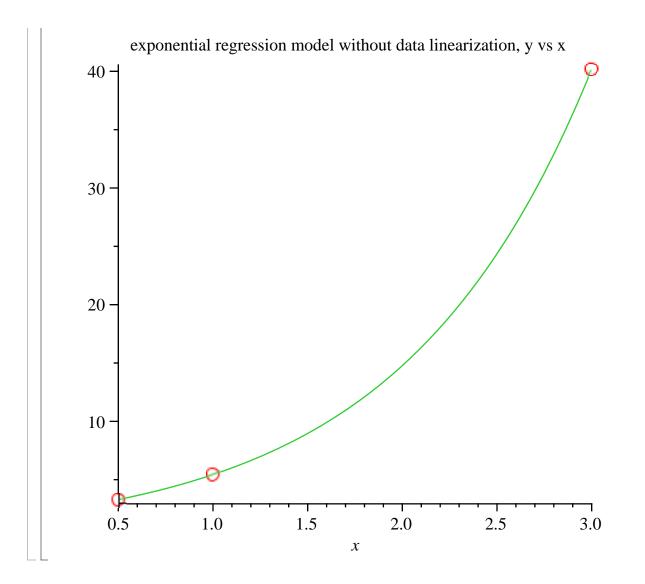
>

```
f := x \rightarrow a e^{bx}
```

The constants of the, "exponential", *model are a = , 2.00000026, and b = , 0.9999999956*(3.1)

```
> Plotting the observed values and the predicted curve
predicted:=f(x);
observed:=[seq([X[i],Y[i]],i=1..n)];
ttl:=cat(model_type, ~ regression model without data
linearization, y vs x`):
plot([observed,predicted],x=X[1]..X[n],style=[POINT,LINE],
symbol=CIRCLE,symbolsize=20,title=ttl);
```

predicted := 2.000000026 e^{0.9999999956x} *observed* := [[0.5, 3.297442542], [1, 5.436563656], [3, 40.17107384]]



References

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

Conclusion

Maple 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.

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