**Class 18** – **Advanced Curve Fitting (Chp. 15)**

ChE310\_Sec1\_F2019 / 10.24.19

<http://www.reuelgroup.org/numerical-methods-che-310.html>

Announcements:

* Nov 12 Phase II of project is due.
* Email Dr. Reuel if you want to join Friday supplement

**Warm Up Group Activity:** submit to Slack by **2:20 pm**.

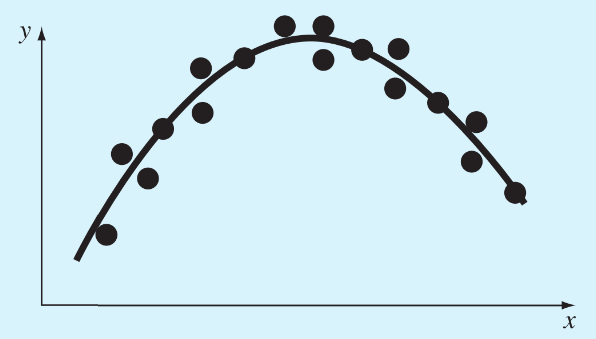
With Matlab, provide linear fit coefficients and the coefficient of determination for the following data. Also plot the data, with the fit and 95% confidence intervals.

x =[1 2 3 4 5 6 7 8 9 10];

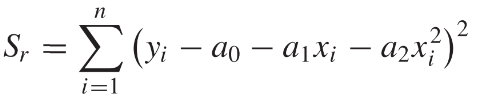
y =[5.0 9.6 11.7 15.5 19.4 21.0 25.9 27.2 30.8 34.1];

**Outline for Class 18 Lecture**

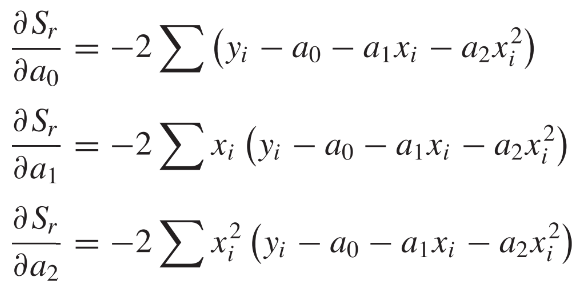
1. Polynomial regression (Least squares method)



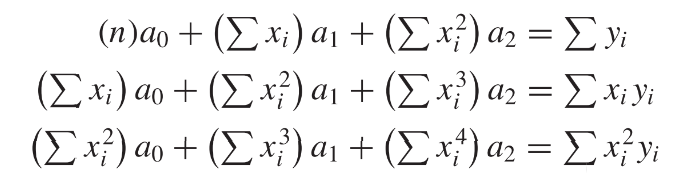
* 1. Sum of squares of residuals (same as linear)



* 1. Minimize this quantity by taking partial derivative wrt each of the coefficients and setting this equation equal to zero

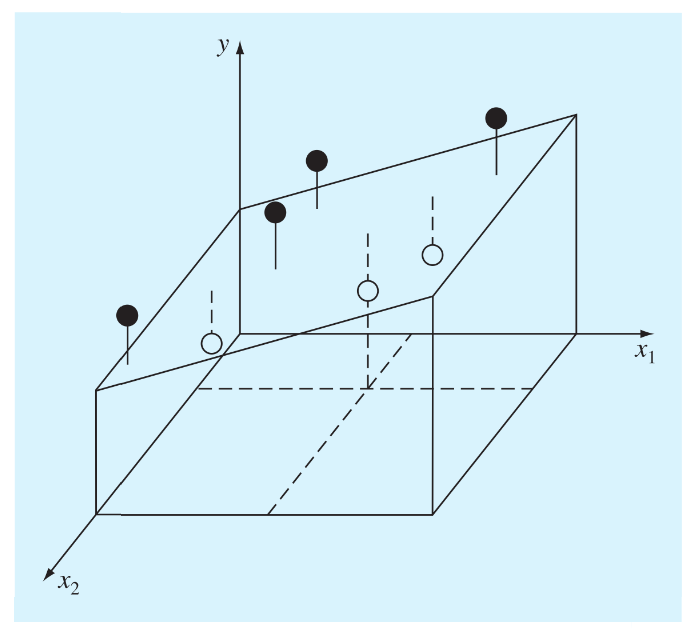
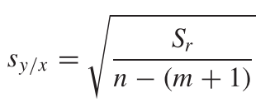


* 1. Rearrange to find normal eqns



* 1. Solve as system of linear eqns ( **\** )
  2. Example 15.1 good walk through (pg. 363)

1. Multiple linear regression (fitting a plane)

Similar to above (Ex. 15. 2)

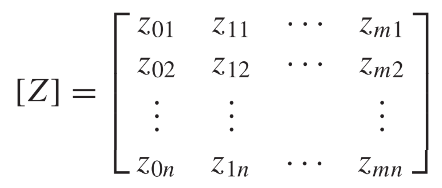
Standard error

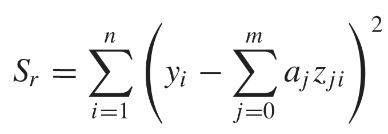
n = # points, m = order polynomial

1. General matrix solution - linear least squares









Take partial derivative, set equal to zero:



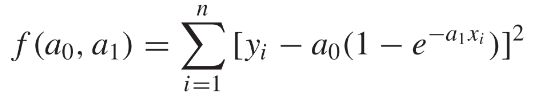
Again, use ( **\** ) to solve this system of equations.

Example 15.3

1. **polyfit** which uses QR decomposition (lin. Alg.)
2. Nonlinear regression.

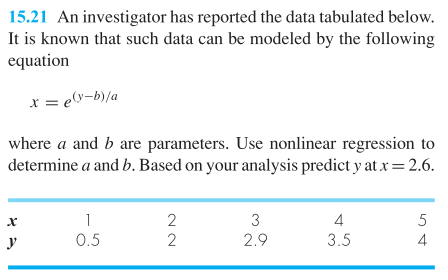


Convert to an objective function for optimization

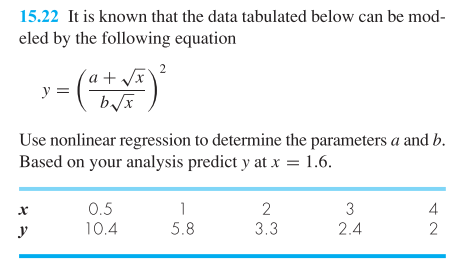


Can use **fminsearch** as we did before, or…

1. **fit** and **fittype**



1. **cftool** , powerful GUI



1. Practice loops – use Matlab to loop through data and extract parameters

* Let’s say you have run a batch reactor 20 times, and you want to determine how the fill rate varies to appropriately size your pumps.
* ‘Slopes.xls’ contains data.
* Columns = independent trials
* Rows = measurements taken at 10 min intervals
* What is the mean and stdev of the fill rate?
* What are the r2 values?
* What tool to use? Matlab or Excel?