**Class 17** – **Basic Curve Fitting (Chp. 14)**

ChE310\_SecB\_S2019 / 3.11.19

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

Announcements:

* April 4 Phase II of project is due.
* Spring break next week! [no office hours, catch on slack]

**Warm Up Group Activity:** submit to Jared by **2:25 pm**.

Solve the following system of equations:

12 = 3\*x\*y + y - z

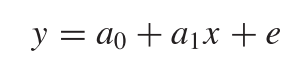
12 = x + y\*x2 + z

- 4 = x - y - z

[Good initial guess, try 1, 1, 1]

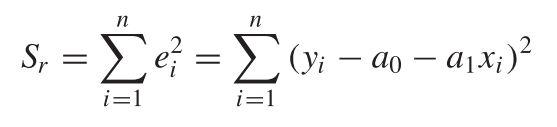
**Outline for Class 16 Lecture**

1. Remember regression vs. interpolation (comic)
2. Example: Pierce 660nm Protein Assay
3. How does it work?
   1. Residual (error)



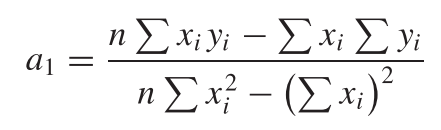


* 1. Minimize sum of squares of residuals



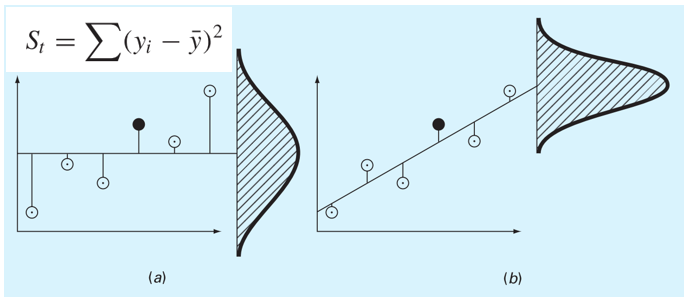
[Find a0 and a1 that minimizes Sr - least squares method]

These can be solved directly for straight line (pg. 338)

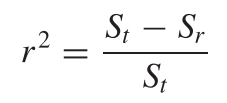


 [See Example 14.4]

1. Quantification of error



* 1. r = correlation coefficient
  2. r2 = coefficient of determination





What does r2 mean?

“Linear model explains \_% of the variability of the data”

1. r2 Adjusted = account for the number of terms (predictors) in your model. Adding more terms, will always make your fit look better, but this adjusted r2 takes this into account. It will ONLY increase if the new term improves the model more than the expected chance.
2. Always plot your answer to double check!
3. Excel vs. Matlab
   1. Excel: Handy if you have one or two vectors to manage
   2. Use Matlab if you:
      1. have a lot of data to fit
      2. you want more than the six stock options
      3. you want to pass the fit parameters as variables
4. Handy tools for Matlab
   1. **polyfit**
      1. Can be interpolation OR regression
      2. Demo with the 660nm data
   2. **fit**
      1. Use to extract goodness of fit
      2. Can also use to plot confidence

[Fit2, GoF] = fit(x,y,'poly1');

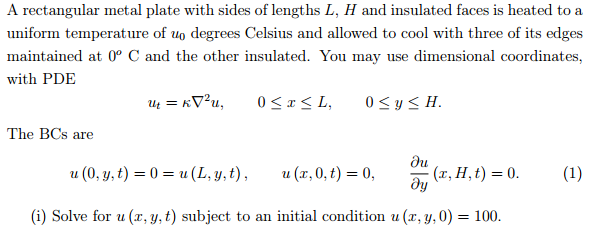
plot(Fit2,x,y,'predobs')

Rsq = GoF.rsquare

* 1. **Confint**
     1. Use to report custom intervals

confint(Fit2,.99)

1. BONUS: How to plot response in 4 dimensions?



Solution:

