Lab 5, Calc Lab: Curve Fitting

April 7, 2004

1 Matlab Info

In general, Matlab has made it easy to fit a line to data, with some other types of functions. In this lab, we'll explore some modeling problems that will first require a transformation of the data before we can use Matlab.

In Matlab, we'll plot the data, then use the "Basic Fitting" tools. We'll save the coefficients for later use.

2 Chemistry: Enzyme Kinetics

There is some theory in chemistry that proposes the following model for the rate of an enzymatic reaction:

$$v = \frac{K_{\max} c}{k_n + c}$$

where c is the concentration of substrate and v is the reaction speed. The model parameters are the constants $K_{\max}$ and k_n.

1. Before doing any work, are there vertical and/or horizontal asymptotes for v? In Matlab, choose some random coefficients for $K_{\max}$ and $k_n > 0$, and plot the function so that you get a feeling for what this is doing.

   ```
   Kmax=1;  kn=56;
   c=linspace(0, 100);
   v=(Kmax*c)./(kn+c);
   plot(c,v);
   ```

2. The function is not linear in its parameters. The main problem is that we cannot simplify the denominator of the fraction. However, notice that:

$$\frac{1}{v} = \frac{k_n + c}{K_{\max} c} = \frac{k_n}{K_{\max} c} + \frac{1}{K_{\max}} = \frac{k_n}{K_{\max}} \cdot \frac{1}{c} + \frac{1}{K_{\max}}$$

Now by letting $y = \frac{1}{v}$ and $x = \frac{1}{c}$, we have a line, $y = mx + b$. To get back to the model function,

$$K_{\max} = \frac{1}{b} \quad \text{and} \quad k_n = \frac{m}{b}$$

Some data is given next. We will proceed in our analysis by:

- Plot $1/c$ versus $1/v$.
- Use the basic fitting tools to determine the line of best fit- we want the slope and intercept.
- Use the slope and intercept to find the values of $K_{\max}$ and k_n.
- Plot the original data together with the "best fitting" original curve.

You might want to do these steps as a script file so that you have your example typed up.

3. The data is given as:

c	5	10	20	40	50	100
v	0.068	0.126	0.218	0.345	0.39	0.529

You may either type in the data directly or go to the class website and download `Enzyme Data Set 1`.

2.1 Homework Problem

We'll change the model slightly to a *sigmoidal* function,

$$v = K_{\max} \frac{c^2}{k^2 + c^2}$$

- Change the model into a linear form.
- Download the data set `Enzyme Homework Data Set` from the class website.
- Find the best fitting parameters.
- Plot the original data (as points) and the model function.
- Turn in your plot and your script file.

3 Population Modeling

A population model with an environmental limit on the growth of the population can be done via the following differential equation:

$$\frac{dy}{dt} = ay(b - y)$$

This is called a separable differential equation, and can be solved by partial fractions. In this case, we can write that:

$$y(t) = \frac{b}{1 + c\mathrm{e}^{-kt}}$$

where $c = \mathrm{e}^{Cb}$ and $k = ab$. We want to model the population of the United States with this function, but it is not in linear form. However,

$$\frac{b}{y} = 1 + c\mathrm{e}^{-kt} \quad \Rightarrow \quad \ln\left(\frac{b}{y} - 1\right) = \ln\left(c\mathrm{e}^{-kt}\right) = \ln(c) - kt$$

This will partially solve our problem- c and k are now linear- but b must be estimated. Here is some data (population is in millions):

Year	1900	1920	1940	1960	1980
Pop	76.1	106.5	132.6	180.7	226.5

We'll estimate $b = 500$.

3.1 Homework:

Estimate our model parameters using the data above. The final graph you'll produce will plot:

- The original data (as red circles).
- The estimated data for all years between 1900-1999.
- Estimated data from the Census Bureau from 1900-1999 (download this from the class website).

Comment on the accuracy of this plot. Does changing b have much effect on the plot- why did we choose 500 instead of 150 or 1500?

4 Biological Modeling

Are the weight of a mammal and its heart rate related? Use the (nonlinear) model:

$$W = AR^n$$

where W is weight, R is heart rate (beats per minute), and A, n are the parameters we need to find.

Homework:

- Download the data from the class website.
- Linearize the model.
- Find the parameters giving the line of best fit, and comment on the results. Plot the result (as the line and also as $W = AR^n$

Turn in a plot of the linear relationship, together with the values of