Math 251H, Fall 2003

Multivariable Calculus

Matlab Assignment for Chapter 15

The Method of Least Squares

The Method of Least Squares is a method for fitting an analytical function to data. The data may for example be gathered from experiments. As you can imagine, Least Squares is an extremely useful method. In this lab you will learn how to find the (i) linear function $y = mx + b$ and (ii) the quadratic function $y = ax^2 + bx + c$ that are the "best" linear and quadratic fits, respectively, to a set of data points $\{(x_i, y_i) \in \mathbf{R^2}, \quad \text{for}\mathbf{i} = \mathbf{1}, ...\mathbf{N}\}$. To quantify the term "best fit" we minimize the error between the function that is being fitted and the data points. So we have to solve an optimization problem. In general, even if know from theory that the data should be modeled by a linear or quadratic function, noise in the physical process used to generate the data and inevitable errors in the measurement of the data mean that the data points will not exactly lie on a line or a quadratic. In other words, the error between the between the function that is being fitted and the data points will probably not be zero. Nevertheless, for a linear fit, for example, we want to find the values of slope m and y-intercept b that make the error as small as possible.

Fitting a Linear Function to Data

Given a set of data points $\{(x_i, y_i) \in \mathbf{R^2}, \quad \text{for}\mathbf{i} = \mathbf{1}, ...\mathbf{N}\}$ and a function $y = f(x)$, we define the *mean square error,* E, to be the average of the squares of the vertical distances between data and the y-values of the function,

$$E = \frac{1}{N}\sum_{i=1}^{N}[y_i - f(x_i)]^2. \tag{1}$$

In the special case of a linear function $y = f(x) = mx + b$, the error E depends on the values of m and b, and Equation 1 becomes

$$E(m,b) = \frac{1}{N}\sum_{i=1}^{N}[y_i - (mx_i + b)]^2. \tag{2}$$

So it makes sense to define the "best-fit" line to be the one whose parameters (m, b) minimize the error $E(m, b)$.

(1) Your first task is to find the critical points of the function $E(m, b)$ of two variables (m, b). Begin by showing that the equations

$$\frac{\partial E}{\partial b} = 0, \qquad \frac{\partial E}{\partial m} = 0 \tag{3}$$

can be expressed as

$$m \sum_{i=1}^{N} x_i \; + \; bN \; = \; \sum_{i=1}^{N} y_i \tag{4}$$

$$m \sum_{i=1}^{N} x_i^2 \; + \; b \sum_{i=1}^{N} x_i \; = \; \sum_{i=1}^{N} x_i y_i. \tag{5}$$

Notice that this is a system of two linear equations in two unknkowns (m, b). [Remember that the x_i and y_i are numbers!]

(2) Download the data file Data1.dat from the course web page and plot it in Matlab.[1] For this you will need to use the load commands:

```
Data = load('Data1.dat');
x = Data(:,1)
y = Data(:,2)
plot(x,y,'bx');
```

Now write a Matlab program to find the line that best fits the data. This will require you to solve the system of linear equations (4) and (5). To set up the system, you may find the Matlab functions size and sum helpful. If you set it up as a 2×2 matrix system, $Au = v$ where u is the vector of unknowns, then you can solve the equation in Matlab using the command u=A\v, which means $u = A^{-1}v$. For the data in Data1.dat, what are the best values of m and b? Plot the data and the best fit line on the same axes.

Fitting a Quadratic Function to Data

(3) Download the data file Data2.dat from the course web page and plot it in Matlab. As you can see this data looks like it might fit a quadratic function $y = f(x) = ax^2 + bx + c$ quite well.

In analogy with (1) above, write down an error function $E(a, b, c)$ to be minimized and corresponding equations for the critical points. This should give you a 3×3 system of linear equations in unknowns (a, b, c).

Use these equations to write a Matlab program to find the quadratic function that best fits data. Test you program on the data set Data2.dat. What are the best values of (a, b, c)? Plot the data and the best fit quadratic on the same axes.

[1] This synthetic data is courtesy of Prof. Minkoff.