
Numerical Analysis

Math 370 Fall 2004
©2004 Ron Buckmire

MWF 2:30 - 3:25pm
Fowler North 5

Worksheet 20

SUMMARY Discrete Least Squares Approximation

READING Recktenwald, Sec 9.1, pp 455–468

Linear Algebra Approach To Discrete Least Squares Approximation

What is the system of equations we are trying to solve when finding a line of best fit $y = ax + b$ for m data points (x_k, y_k) ?

$$\begin{aligned} ax_1 + b &= y_1 \\ ax_2 + b &= y_2 \\ &\vdots \\ ax_m + b &= y_m \end{aligned}$$

1. What are the known parameters here and what are the unknown variables ?
2. Write the system as a linear system $A\vec{c} = \vec{y}$

3. What are the dimensions of the matrix A and the vectors \vec{c} and \vec{y} ?

We define a vector called \vec{r} known as the residual vector and try to minimize the size (norm) of this vector since an exact solution to the matrix equation above is extremely unlikely.

$$\|\vec{r}\|_2^2 = \vec{r}^T \vec{r} = (\vec{y} - A\vec{c})^T (\vec{y} - A\vec{c})$$

4. If we consider this norm to be $\rho = \rho(\vec{c})$ we can think of our problem as finding the value of \vec{c} which minimizes the size of $\rho(\vec{c})$. (Sound familiar?). Let's simplify the function first, and then minimize. Make sure you understand each step.

$$\begin{aligned} \rho(c) &= y^T y - y^T A c - (A c)^T y + (A c)^T A c \\ &= y^T y - y^T A c - c^T A^T y + c^T A^T A c \\ &= y^T y - 2y^T A c + c^T A^T A c \end{aligned}$$

Thus, the general form of the Normal Equations can be written:

Least Squares Fit Using Other Functions

There is no reason why one has to pick the linear function $P(x) = ax + b$ to fit the data to. That is, one does not have to do the fit to a linear function (or even transform the data so that a linear relationship can be established between input and output variables).

Suppose

$$y = P(x) = c_1 f_1(x) + c_2 f_2(x) + \dots + c_k f_k(x) = \sum_{i=1}^k c_i f_i(x)$$

Thus the best fit problem will become one of finding the k c_i values which cause the least square error to be minimized.

Note: If k , the number of basis functions, is equal to the number of data points, m , then one is really doing **interpolation** instead of polynomial best fit.

Exercise

1. Write down the expression $E(\vec{c}) = E(c_1, c_2, \dots, c_n)$ which must be minimised:

Polynomial Of Best Fit

To simplify things, let's assume that the basis functions are monomials and we have m data points

$$P(x) = \sum_{k=0}^n a_k x^k, \quad \text{where } n + 1 < m$$

2. Why does $n + 1$ have to be less than m ?

EXAMPLE

Let's find the normal equations whose solution is the a_k values. (HINT: write it in Matrix Form.)

The above represents the $n + 1$ **normal equations** in the $n + 1$ unknowns a_0, a_1, \dots, a_n

Using polyfit in MATLAB

Let's try and find a second degree polynomial which fits the data $(0, 1)$, $(0.25, 1.2840)$, $(0.5, 1.6487)$, $(0.75, 2.1170)$ and $(1.00, 2.7183)$

3. What will the dimensions of the matrix equation to be solved look like? (i.e. what is n and what is m ?)

4. Find the coefficients of the polynomial using `polyfit`
(Write down what commands you use)

5. Plot the data and the polynomial of best fit on the same graph.
(Write down what commands you use)