Least Squares Fitting

Aim

To demonstrate how to use the least squares approximation method to fit a curve to a set of data.

Learning Outcomes

At the end of this section you will be able to:

- Understand what least squares approximation is,
- Use least squares approximation to find the best fit linear curve for a given set of data points.

Least squares approximation is a method for calculating the **best fit** linear curve to a given set of data. Using the method of *least squares approximation* guarantees that we find the best fit curve for the data, but it also guarantees that everyone has the same linear curve fitted to the data.

A linear curve is represented by the equation

$$y = mx + c.$$

Let $\mathbf{x}$ and $\mathbf{y}$ be $n \times 1$ column matrices. We are trying to solve the set of linear equations:

$$\begin{array}{rcl} y_1 & = & mx_1 + c \\ y_2 & = & mx_2 + c \\ \vdots & = & \vdots \;\; + \vdots \\ y_n & = & mx_n + c \end{array}$$

for the two unknowns m and c. When written as a matrix equation, we get:

$$\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \begin{pmatrix} c \\ m \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

or just

$$\mathbf{Ma} = \mathbf{y}$$

Unfortunately here we have an overdetermined linear system - a system with more equations than there are unknowns. This results in you being unable to find an exact solution to satisfy all the equations - instead we approximate the best solution for all the equations.

One approach is to multiply both sides of the matrix equation by $\mathbf{M^T}$ (the transpose of $\mathbf{M}$) - yielding two equations in two unknowns.

$$\mathbf{M^TMa} = \mathbf{M^Ty}$$

It is easy to see that

$$\mathbf{M^TM} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_2 \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} = \begin{pmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{pmatrix}$$

and

$$\mathbf{M^Ty} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{pmatrix}.$$

Therefore the equation becomes

$$\begin{pmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{pmatrix} \begin{pmatrix} c \\ m \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{pmatrix}.$$

Example

Use the least squares method to fit the best fit curve to the following set of data.

x	-4.5	-3.2	-1.4	0.8	2.5	4.1
y	0.7	2.3	3.8	5.0	5.5	6.6

It is clear to see that

$$\mathbf{M} = \begin{pmatrix} 1 & -4.5 \\ 1 & -3.2 \\ 1 & -1.4 \\ 1 & 0.8 \\ 1 & 2.5 \\ 1 & 4.1 \end{pmatrix} \text{ and } \mathbf{M^T} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -4.5 & -3.2 & -1.4 & 0.8 & 2.5 & 4.1 \end{pmatrix}$$

and so

$$\mathbf{M^TM} = \begin{pmatrix} 6 & -1.7 \\ -1.7 & 56.15 \end{pmatrix}$$

and
$$\mathbf{M^T y} = \begin{pmatrix} 23.9 \\ 28.98 \end{pmatrix}.$$

This then gives us
$$\begin{pmatrix} 6 & -1.7 \\ -1.7 & 56.15 \end{pmatrix} \begin{pmatrix} c \\ m \end{pmatrix} = \begin{pmatrix} 23.9 \\ 28.98 \end{pmatrix}.$$

Rewriting this as a system of linear equations and solving yields,

$$c = 4.16529 \qquad \text{and} \qquad m = 0.642226.$$

This gives us the equation $y = 0.642226x + 4.16529$ as the equation of the line that is the best fit to above set of data.