5

Least Square Problems

5.1 Introduction

Let the set of data points be (x_i, y_i), $\quad i = 1, 2, ..., m$, and let the curve given by $y = f(x)$ be fitted to this data. If e_i is the error of the approximation at $x = x_i$ due to this fitting then, $e_i = y_i - f(x_i)$. If we write $S = \sum_{i=1}^{m} e_i^2 = \sum_{i=1}^{m} [y_i - f(x_i)]^2$. Then the method of minimizing this error which is the sum of the square of errors is called the method of least squares.

5.1.1 Fitting a Straight Line

Let $Y = a_0 + a_1 x$ be the straight line to be fitted to the given data by the method of least squares. Then the sum of errors is $S = \sum_{i=1}^{m} [y_i - a_0 - a_1 x_i]^2$. S is a function of a_0 and a_1. To minimize S, $\frac{\partial S}{\partial a_0} = 0$ and $\frac{\partial S}{\partial a_1} = 0$. We have,

$$\frac{\partial S}{\partial a_0} = -2\sum_{i=1}^{m} [y_i - a_0 - a_1 x_i], \qquad \frac{\partial S}{\partial a_1} = -2x_i \sum_{i=1}^{m} [y_i - a_0 - a_1 x_i] \tag{5.1}$$

$$\frac{\partial S}{\partial a_0} = 0 \implies -2\sum_{i=1}^{m} [y_i - a_0 - a_1 x_i] = 0$$

$$\implies \sum_{i=1}^{m} y_i = \sum_{i=1}^{m} a_0 + a_1 \sum_{i=1}^{m} x_i$$

$$\implies \sum_{i=1}^{m} y_i = a_1 \sum_{i=1}^{m} x_i + m a_0 \tag{5.2}$$

$$\frac{\partial S}{\partial a_1} = 0 \implies -2x_i \sum_{i=1}^{m} [y_i - a_0 - a_1 x_i] = 0$$

$$\implies \sum_{i=1}^{m} x_i y_i = a_0 \sum_{i=1}^{m} x_i + a_1 \sum_{i=1}^{m} x_i^2 \tag{5.3}$$

The equations 5.2 and 5.3 are called normal equations which can be solved for a_0 and a_1. From the equation 5.2, it can be easily shown that the fitted line passes through the *means* of x_i and y_i,i.e the line satisfies $\overline{y} = a_0 + a_1 \overline{x}$.

5.1.2 Multiple Linear Least Square

Let $z = a_0+a_1x+a_2y$ be a linear equation to be fitted to the given data $(x_1, y_1, z_1), (x_2, y_2, z_2), ..., (x_m, y, z_m)$ by the method of least squares. Then the sum of errors is $S = \sum_{i=1}^{m} [z_i - a_0 - a_1x_i - a_2y_i]^2$. S is a function of a_0, a_1 and a_2. To minimize S:

$$\frac{\partial S}{\partial a_0} = -2\sum_{i=1}^{m} [y_i - a_0 - a_1x_i - a_2y_i] = 0$$

$$\frac{\partial S}{\partial a_1} = -2x_i\sum_{i=1}^{m} [y_i - a_0 - a_1x_i - a_2y_i] = 0$$

$$\frac{\partial S}{\partial a_2} = -2y_i\sum_{i=1}^{m} [y_i - a_0 - a_1x_i - a_2y_i] = 0$$

So, the normal equations are:

$$\begin{aligned}
\sum_{i=1}^{m} z_i &= a_1\sum_{i=1}^{m} x_i + a_2\sum_{i=1}^{m} y_i + ma_0 \\
\sum_{i=1}^{m} z_i\, x_i &= a_1\sum_{i=1}^{m} x_i^2 + a_2\sum_{i=1}^{m} x_iy_i + a_0\sum_{i=1}^{m} x_i \\
\sum_{i=1}^{m} z_i\, y_i &= a_1\sum_{i=1}^{m} x_iy_i + a_2\sum_{i=1}^{m} y_i^2 + a_0\sum_{i=1}^{m} y_i
\end{aligned} \tag{5.4}$$

5.2 Curve Fitting by Polynomials

Let $Y = a_0 + a_1x + a_2x^2 + ... + a_nx^n$ be a polynomial to be fitted to the given data $(x_1, y_1), (x_2, y_2), ..., (x_m, y_m)$ by the method of least squares. Then the sum of errors is $S = \sum_{i=1}^{m} [z_i - a_0 - a_1x_i - a_2y_i]^2$. Then the normal equations are:

$$\begin{aligned}
\sum_{i=1}^{m} y_i &= a_1\sum_{i=1}^{m} x_i + a_2\sum_{i=1}^{m} x_i^2 + ... + ma_0 \\
\sum_{i=1}^{m} x_i\, y_i &= a_0\sum_{i=1}^{m} x_i + a_1\sum_{i=1}^{m} x_i^2 + a_2\sum_{i=1}^{m} x_i^3 + ... + a_n\sum_{i=1}^{m} x_i^{n+1} \\
&\;\;... \\
\sum_{i=1}^{m} x_i^n\, y_i &= a_0\sum_{i=1}^{m} x_i^n + a_1\sum_{i=1}^{m} x_i^{n+1} + a_2\sum_{i=1}^{m} x_i^{n+2} + ... + a_n\sum_{i=1}^{m} x_i^{2n}
\end{aligned} \tag{5.5}$$

This system constitutes of $(n + 1)$ equations in $(n + 1)$ unknowns. For larger value of n the system is *ill conditioned*, so orthogonal polynomials are used to fit such data points.

5.3 Weighted Least Square Approximation

For the errors are weighted by W_i, then the sum of weighed errors is:
$S = \sum_{i=1}^{m} W_i\, e_i^2 = \sum_{i=1}^{m} W_i\, [y_i - f(x_i)]^2$. So that the normal equations of the linear curve fitting $Y = a_0 + a_1 x$ becomes:

$$\begin{aligned} \sum_{i=1}^{m} W_i\, y_i &= a_1 \sum_{i=1}^{m} W_i\, x_i + m a_0 \\ \sum_{i=1}^{m} W_i\, x_i y_i &= a_0 \sum_{i=1}^{m} x W_{i\,i} + a_1 \sum_{i=1}^{m} W_i\, x_i^2 \end{aligned} \tag{5.6}$$

5.4 Linearization of Nonlinear Laws

1. $y = ax + \frac{b}{x}$
   This can be written as $xy = b + ax^2$. Put $xy = Y$, $b = A_0$, $a = A_1$ and $x^2 = X$. Then the given nonlinear equation becomes the linear equation $Y = A_0 + A_1 X$.

2. $y = ae^{bx}$
   This can be written as $xy = b + ax^2$. Put $lny = Y$, $lna = A_0$, $b = A_1$ and $x = X$. Then the given nonlinear equation becomes the linear equation $Y = A_0 + A_1 X$.

5.4.1 Exercise

1. Fit a linear equation to the data points with the given weights.
   $(0, -1)$, $(2, 5)$, $(5, 12)$, $(7, 20)$ and $W = (1, 1, 10, 1)$

2. Fit the a second-degree polynomial to the given data points:
   $(0, 71)$, $(1, 89)$, $(2, 67)$, $(3, 43)$, $(4, 31)$, $(5, 18)$, $(6, 9)$

3. Determine the normal equations for the cubic polynomial fitting.

4. What is the difference between interpolation and curve fitting for a given data points?

5. Convert the following nonlinear equations into suitable linear equations for the curve fitting using linear least square fitting.

   a). $xy^a = b$ b). $y = ab^x$ c). $y = ax^b$

6. Fit a function of the form $y = ax^b$ to the data points: $(61, 350)$, $(26, 400)$, $(7, 500)$, $(2.6, 600)$