Least-Square Curve Fitting Procedure

Let the set of data points be $(x_i, y_i), i = 1, 2, \ldots, m$, and let the curve given by $Y = f(x)$ be fitted to this data. At $x = x_i$, the experimental (or observed) value of the ordinate is y_i and the corresponding value on the fitting curve is $f(x_i)$. If e_i is the error of approximation at $x = x_i$, then we have

$$e_i = y_i - f(x_i). \tag{4.1}$$

If we write

$$\begin{aligned} S &= [y_1 - f(x_1)]^2 + [y_2 - f(x_2)]^2 + \cdots + [y_m - f(x_m)]^2 \\ &= e_1^2 + e_2^2 + \cdots + e_m^2. \end{aligned} \tag{4.2}$$

Fitting a Straight Line

Let $Y = a_0 + a_1 x$ be the straight line to be fitted to the given data. Then, corresponding to Eq. (4.2) we have

$$S = [y_1 - (a_0 + a_1 x_1)]^2 + [y_2 - (a_0 + a_1 x_2)]^2 + \cdots + [y_m - (a_0 + a_1 x_m)]^2. \quad (4.3)$$

For S to be minimum, we have

$$\frac{\partial S}{\partial a_0} = 0 = -2[y_1 - (a_0 + a_1 x_1)] - 2[y_2 - (a_0 + a_1 x_2)] - \cdots - 2[y_m - (a_0 + a_1 x_m)]$$

(4.4a)

and

$$\frac{\partial S}{\partial a_1} = 0 = -2x_1[y_1 - (a_0 + a_1 x_1)] - 2x_2[y_2 - (a_0 + a_1 x_2)]$$

$$- \cdots - 2x_m[y_m - (a_0 + a_1 x_m)]. \tag{4.4b}$$

The above equations simplify to

$$ma_0 + a_1(x_1 + x_2 + \cdots + x_m) = y_1 + y_2 + \cdots + y_m \tag{4.5a}$$

and

$$a_0(x_1 + x_2 + \cdots + x_m) + a_1(x_1^2 + x_2^2 + \cdots + x_m^2) = x_1 y_1 + x_2 y_2 + \cdots + x_m y_m \tag{4.5b}$$

or, more compactly to

$$ma_0 + a_1 \sum_{i=1}^{m} x_i = \sum_{i=1}^{m} y_i \tag{4.6a}$$

and

$$a_0 + \sum_{i=1}^{m} x_i + a_1 \sum_{i=1}^{m} x_i^2 = \sum_{i=1}^{m} x_i y_i. \tag{4.6b}$$

Since the x_i and y_i are known quantities, Eqs. (4.5) or (4.6), called the *normal equations*, can be solved for the two unknown a_0 and a_1.

Differentiating Eqs. (4.4a) and (4.4b) with respect to a_0 to a_1 respectively, we find that $\partial^2 S/\partial a_0^2$ and $\partial^2 S/\partial a_1^2$ will both be positive at the points a_0 and a_1. Hence these values provide a *minimum* of S.

Examples

Example 4.1 The table below gives the temperatures T (in °C) and lengths l (in mm) of a heated rod. If $l = a_0 + a_1 T$, find the best values for a_0 and a_1.

T (in °C)	l (in mm)
20	800.3
30	800.4
40	800.6
50	800.7
60	800.9
70	801.0

Solution

To use formulae (4.6), we require ΣT, ΣI, ΣT^2 and ΣTI, and these are computed as in the following table:

T (in °C)	I (in mm)	T^2	TI
20	800.3	400	16006
30	800.4	900	24012
40	800.6	1600	32024
50	800.7	2500	40035
60	800.9	3600	48054
70	801.0	4900	56070
270	4803.9	13900	216201

Using formulae (4.6) we then obtain

$$6a_0 + 270a_1 = 4803.9 \quad \text{and} \quad 270a_0 + 13900a_1 = 216201,$$

from which we get $a_0 = 800$ and $a_1 = 0.0146$.

Linear Curve Fitting Method

Certain experimental values of x & y are given below. If $y = a_0 + a_1 x$, then find the approximate values of a_0 and a_1.

x	0	2	5	7
y	-1	5	12	20

Answer:

$$4a_0 + 14a_1 = 36$$
$$14a_0 + 78a_1 = 210$$
$$a_0 = -1.1381 \text{ and } a_1 = 2.8966$$

Non-Linear Curve Fitting Method

- Taking a straight line as an approximation for a curve is not sufficient for some curves.
- The following non-linear curve fitting methods can be used in such cases:
  - Polynomial of *n*th Degree
  - Power Function
  - Exponential Function

Polynomial of *n*th Degree

Polynomial of the nth degree Let the polynomial of the nth degree, viz.,

$$Y = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n \tag{4.8}$$

be fitted to the data points (x_i, y_i), $i = 1, 2, \ldots, m$. We then have

$$S = [y_1 - (a_0 + a_1 x_1 + \cdots + a_n x_1^n)]^2 + [y_2 - (a_0 + a_1 x_2 + \cdots + a_n x_2^n)]^2$$

$$+ \cdots + [y_m - (a_0 + a_1 x_m + \cdots + a_n x_m^n)]^2. \tag{4.9}$$

Equating, as before, the first partial derivatives to zero and simplifying, we get the following normal equations

$$\left.\begin{aligned}
ma_0 + a_1\sum_{i=1}^{m} x_i + a_2\sum_{i=1}^{m} x_i^2 + \cdots + a_n\sum_{i=1}^{m} x_i^n &= \sum_{i=1}^{m} y_i \\
a_0\sum_{i=1}^{m} x_i + a_1\sum_{i=1}^{m} x_i^2 + \cdots + a_n\sum_{i=1}^{m} x_i^{n+1} &= \sum_{i=1}^{m} x_i y_i \\
&\vdots \\
a_0\sum_{i=1}^{m} x_i^n + a_1\sum_{i=1}^{m} x_i^{n+1} + \cdots + a_n\sum_{i=1}^{m} x_i^{2n} &= \sum_{i=1}^{m} x_i^n y_i.
\end{aligned}\right\} \tag{4.10}$$

These are $(n+1)$ equations in $(n+1)$ unknowns and hence can be solved for $a_0, a_1, \ldots, a_n$. Equation (4.8) then gives the required polynomial of the nth degree.

Polynomial of *n*th Degree : Example

Fit a polynomial of second degree to the data points given in the following table.

x	0	1	2
y	1	6	17

Polynomial of *n*th Degree: Example

Solution

To find the 2nd degree polynomial, we need to find $\sum x_i$, $\sum y_i$, $\sum x_i^2$, $\sum x_i^3$, $\sum x_i^4$, $\sum x_i y_i$ and $\sum x_i^2 y_i$.

We know that

$$ma_0 + a_1\sum x_i + a_2\sum x_i^2 = \sum y_i$$
$$a_0 \sum x_i + a_1\sum x_i^2 + a_n\sum x_i^3 = \sum x_i y_i$$
$$a_0 \sum x_i^2 + a_1\sum x_i^3 + a_n\sum x_i^4 = \sum x_i^2 y_i$$

x	y	x2	x3	x4	xy	x2y
0	1	0	0	0	0	0
1	6	1	1	1	6	6
2	17	4	8	16	34	68
3	24	5	9	17	40	74

Therefore, substituting all known values from the table,

$$3a_0 + 3a_1 + 5a_2 = 24$$

$$3a_0 + 5a_1 + 9a_2 = 40$$

$$5a_0 + 9a_1 + 17a_2 = 74,$$

Answer: $a_0 = 1, a_1 = 2, a_2 = 3$

The polynomial is: $1 + 2x + 3x^2$

Power Function

- In power function method we approximate the actual curve by substituting y_i by a power function of x.
- Then, the approximation Y becomes a power function of x.
- Let, $Y = f(x) = ax^c$ (i.e., a power function of x)
- Taking logarithms of both sides, we get $\log y = \log a + c \log x$
- This equation is in the form $Y = a_0 + a_1 x$, where $Y = \log y$, $a_0 = \log a$, $a_1 = c$ and $x = \log x$.
- Now we can use the least square method to solve this equation.

Exponential Function

- In exponential function method we approximate the actual curve by substituting y_i by an exponential function of x.
- Then, the approximation Y becomes a exponential function of x.
- Let, $Y = f(x) = a_0 e^{a_1 x}$ (i.e., a exponential function of x)
- Taking logarithms of both sides, we get $\log y = \log a_0 + a_1 x$
- This equation is in the form $Y = a_0 + a_1 x$, where $Y = \log y$, $a_0 = \log a_0$.
- Now we can use the least square method to solve this equation.

Exponential Function : Example

Determine the constants a and b by the method of least square such that $y = ae^{bx}$ fits the following data

x	0	1	2
y	1	6	17

Solution:

Given, $y = ae^{bx}$

Taking logarithm on both side,

$$\ln y = \ln a + bx$$

Setting, $\ln y = Y$, $\ln a = a_0$ and $b = a_1$ we get, $y = a_0 + a_1 x$

Exponential Function : Example

Using the least square method,

$5\ a_0 + 30\ a_1 = 17.025$

$30\ a_0 + 220\ a_1 = 122.150$

So, $a_0 = 0.405$, $a_1 = 0.5$

Hence,

$a = e^{a_0} = e^{0.405} = 1.499$

$b = a_1 = 0.5$

X = x	y	Y = ln y	X2	XY
2	4.077	1.405	4	2.811
4	11.084	2.406	16	9.622
6	30.128	3.405	36	20.433
8	81.897	4.405	64	35.244
10	222.620	5.405	100	54.055
30	349.806	17.0272	220	122.164

Weighted Least Square Approximation

In the previous section, we have minimized the sum of squares of the errors. A more general approach is to minimize the weighted sum of the squares of the errors taken over all data points. If this sum is denoted by S, then instead of Eq. (4.2), we have

$$
\begin{aligned}
S &= W_1[y_1 - f(x_1)]^2 + W_2[y_2 - f(x_2)]^2 + \cdots + W_m[y_m - f(x_m)]^2 \\
&= W_1 e_1^2 + W_2 e_2^2 + \cdots + W_m e_m^2. \qquad (4.24)
\end{aligned}
$$

In (4.24), the W_i are prescribed positive numbers and are called *weights*. A weight is prescribed according to the relative accuracy of a data point. If all the data points are accurate, we set $W_i = 1$ for all i. We consider again the linear and nonlinear cases below.

Linear Weighted Least Square Approximation

Let $Y = a_0 + a_1 x$ be the straight line to be fitted to the given data points, viz. $(x_1, y_1), \ldots, (x_m, y_m)$. Then

$$S(a_0, a_1) = \sum_{i=1}^{m} W_i \left[y_i - (a_0 + a_1 x_i)\right]^2. \tag{4.25}$$

For maxima or minima, we have

$$\frac{\partial S}{\partial a_0} = \frac{\partial S}{\partial a_1} = 0, \tag{4.26}$$

which give

$$\frac{\partial S}{\partial a_0} = -2 \sum_{i=1}^{m} W_i \left[y_i - (a_0 + a_1 x_i)\right] = 0 \tag{4.27}$$

and

$$\frac{\partial S}{\partial a_1} = -2\sum_{i=1}^{m} W_i\,[y_i - (a_0 + a_1 x_i)]\,x_i = 0. \tag{4.28}$$

Simplification yields the system of equations for a_0 and a_1:

$$a_0 \sum_{i=1}^{m} W_i + a_1 \sum_{i=1}^{m} W_i x_i = \sum_{i=1}^{m} W_i y_i \tag{4.29}$$

and

$$a_0 \sum_{i=1}^{m} W_i x_i + a_1 \sum_{i=1}^{m} W_i x_i^2 = \sum_{i=1}^{m} W_i x_i y_i, \tag{4.30}$$

which are the *normal equations* in this case and are solved to obtain a_0 and a_1. We consider Example 4.2 again to illustrate the use of weights.

Examples

Example 4.6 Suppose that in the data of Example 4.2, the point (5, 12) is known to be more reliable than the others. Then we prescribe a weight (say, 10) corresponding to this point only and all other weights are taken as unity. The following table is then obtained.

x	y	W	Wx	Wx^2	Wy	Wxy
0	−1	1	0	0	−1	0
2	5	1	2	4	5	10
5	12	10	50	250	120	600
7	20	1	7	49	20	140
14	36	13	59	303	144	750

The normal Eqs. (4.29) and (4.30) then give

$$13a_0 + 59a_1 = 144 \tag{i}$$

$$59a_0 + 303a_1 = 750. \tag{ii}$$

Solution to eqs. (i) and (ii) gives

$$a_0 = -1.349345 \quad \text{and} \quad a_1 = 2.73799.$$

The 'linear least squares approximation' is therefore given by

$$y = -1.349345 + 2.73799x.$$

We obtain

$$y(5.0) \approx 12.34061 = 12.34061,$$

which is a better approximation than that obtained in Example 4.2.

Nonlinear Weighted Least Square Approximation

We now consider the least squares approximation of a set of m data points (x_i, y_i), $i = 1, 2, \ldots, m$, by a polynomial of degree $n < m$. Let

$$y = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n \tag{4.31}$$

be fitted to the given data points. We then have

$$S(a_0, a_1, \ldots, a_n) = \sum_{i=1}^{m} W_i \left[y_i - (a_0 + a_1 x_i + \cdots + a_n x_i^n)\right]^2. \tag{4.32}$$

If a minimum occurs at $(a_0, a_1, \ldots, a_n)$, then we have

$$\frac{\partial S}{\partial a_0} = \frac{\partial S}{\partial a_1} = \frac{\partial S}{\partial a_2} = \cdots = \frac{\partial S}{\partial a_n} = 0. \tag{4.33}$$

These conditions yield the normal equations

$$\left.\begin{aligned} a_0\sum_{i=1}^{m} W_i + a_1\sum_{i=1}^{m} W_i x_i + \cdots + a_n\sum_{i=1}^{m} W_i x_i^n &= \sum_{i=1}^{m} W_i y_i \\ a_0\sum_{i=1}^{m} W_i x_i + a_1\sum_{i=1}^{m} W_i x_i^2 + \cdots + a_n\sum_{i=1}^{m} W_i x_i^{n+1} &= \sum_{i=1}^{m} W_i x_i y_i \\ &\vdots \\ a_0\sum_{i=1}^{m} W_i x_i^n + a_1\sum_{i=1}^{m} W_i x_i^{n+1} + \cdots + a_n\sum_{i=1}^{m} W_i x_i^{2n} &= \sum_{i=1}^{m} W_i x_i^n y_i. \end{aligned}\right\} \qquad (4.34)$$

Equations (4.34) are $(n+1)$ equations in $(n+1)$ unknowns $a_0, a_1, \ldots, a_n$. If the x_i are distinct with $n < m$, then the equations possess a 'unique' solution.