SE 301: Numerical Methods
Topic 4:
Least Squares Curve Fitting

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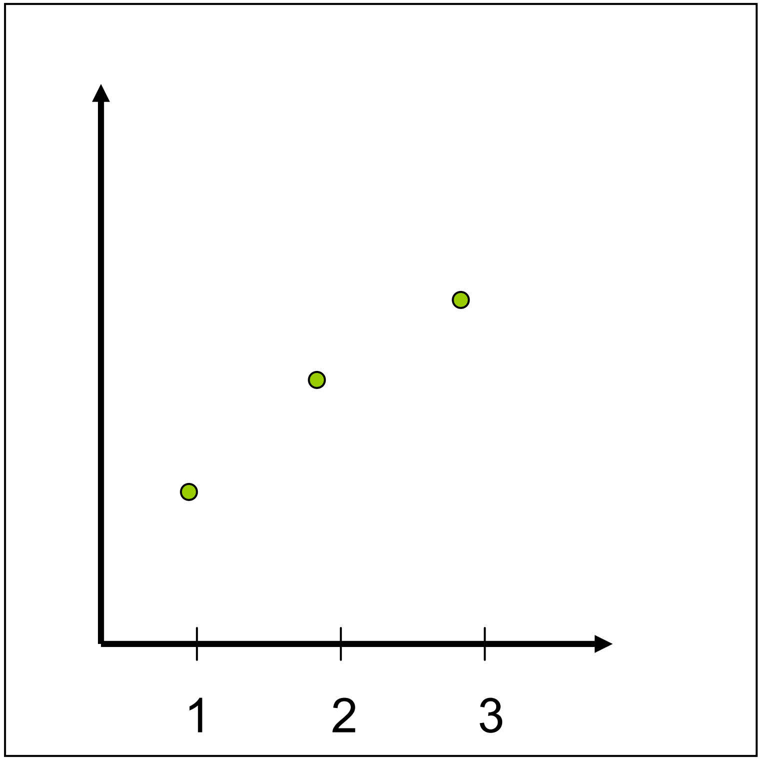
(Term 063)

Motivation

Given a set of experimental data

x	1	2	3
y	5.1	5.9	6.3

- The relationship between x and y may not be clear
- we want to find an expression for f(x)



Curve Fitting

Given a set of tabulated data, find a curve or a function that best represents the data.

Given:

1. The tabulated data
2. The form of the function
3. The curve fitting criteria

Find the unknown coefficients

Selection of the functions

Linear $f(x) = a + bx$

Quadratic $f(x) = a + bx + cx^2$

Polynomial $f(x) = \sum_{k=0}^{n} a_k \; x^k$

General $f(x) = \sum_{k=0}^{m} a_k \; g_k(x)$

$g_k(x)$ are known

Decide on the criterion

1. Least Squares

$$\min_{a,b} \sum_{i=0}^{n} \left| f(x_i) - f_i \right|^2$$

Chapter 17

2. Exact Matching (interplation)

$$f_i = f(x_i)$$

Chapter 18

Least Squares

Given

x_i	x_1	x_2	….	x_n
y_i	y_1	y_2	….	y_n

The form of the function is assumed to be known but the coefficients are unknown

$$y_i = f(x_i) + e_i$$

The difference is assumed to be the result of experimental error

Determine the Unknowns

We want to find a, b to minimize

$$\Phi(a,b)=\sum_{i=1}^{n}\left|f_i-(a+bx_i)\right|^2$$

How do we obtain a and b to minimize $\Phi(a,b)$?

Determine the Unknowns

Necessary condition for the minimum

$$\frac{\partial\ \Phi(a,b)}{\partial\ a}=0$$

$$\frac{\partial\ \Phi(a,b)}{\partial\ b}=0$$

Example 1

x	1	2	3
y	5.1	5.9	6.3

Assume

$$f(x) = a + bx$$

Necessary condition for the minimum

$$\frac{\partial \, \Phi(a,b)}{\partial \, a} = 0$$

$$\frac{\partial \, \Phi(a,b)}{\partial \, b} = 0$$

Remember

$$\frac{d}{dx}\left(\sum_{k=1}^{n} a_i \; x\right) = \sum_{k=1}^{n} a_i$$

$$\frac{\partial}{\partial a}\left(\sum_{k=1}^{n} g_i(x) \; a\right) = \sum_{k=1}^{n} g_i(x)$$

Example 1

$$\frac{\partial\ \Phi(a,b)}{\partial\ a} = 0 = \sum_{k=1}^{N} 2\left(a + b x_k - y_k\right)$$

$$\frac{\partial\ \Phi(a,b)}{\partial\ b} = 0 = \sum_{k=1}^{N} 2\left(a + b x_k - y_k\right) x_k$$

Normal Equations

$$N\,a + \left(\sum_{k=1}^{N} x_k\right) b = \left(\sum_{k=1}^{N} y_k\right)$$

$$\left(\sum_{k=1}^{N} x_k\right) a + \left(\sum_{k=1}^{N} x_k^2\right) b = \left(\sum_{k=1}^{N} x_k\, y_k\right)$$

Example 1

Solving the Normal Equations gives

$$b = \frac{N\left(\sum_{k=1}^{N} x_k\, y_k\right) - \left(\sum_{k=1}^{N} x_k\right)\left(\sum_{k=1}^{N} y_k\right)}{N\left(\sum_{k=1}^{N} x_k^2\right) - \left(\sum_{k=1}^{N} x_k\right)^2}$$

$$a = \frac{1}{N}\left(\left(\sum_{k=1}^{N} y_k\right) - b\left(\sum_{k=1}^{N} x_k\right)\right)$$

Example 1

i	1	2	3	sum
x_i	1	2	3	6
y_i	5.1	5.9	6.3	17.3
x_i^2	1	4	9	14
$x_i\ y_i$	5.1	11.8	18.9	35.8

Example 1

Normal Equations

$$N\,a + \left(\sum_{k=1}^{N} x_k\right) b = \left(\sum_{k=1}^{N} y_k\right)$$

$$\left(\sum_{k=1}^{N} x_k\right) a + \left(\sum_{k=1}^{N} x_k^2\right) b = \left(\sum_{k=1}^{N} x_k\, y_k\right)$$

$$3\,a + \quad 6\,b = 17.3$$

$$6a + 14\,b = 35.8$$

$$Solving \Rightarrow \quad a = 4.5667 \qquad b = 0.60$$

Example 2

x	0.24	0.65	0.95	1.24	1.73	2.01	2.23	2.52
y	0.23	-0.23	-1.1	-0.45	0.27	0.1	-0.29	0.24

It is required to find a function of the form

$$f(x) = a\ \ln(x) + b\ \cos(x) + c\ e^{x}$$

to fit the data.

Example 2

Necessary condition for the minimum

$$\left.\begin{aligned} \frac{\partial\, \Phi(a,b,c)}{\partial\, a} &= 0 \\ \frac{\partial\, \Phi(a,b,c)}{\partial\, b} &= 0 \\ \frac{\partial\, \Phi(a,b,c)}{\partial\, c} &= 0 \end{aligned}\right\} \Rightarrow \textit{Normal Equations}$$

Example 2

$$a\sum_{k=1}^{8}(\ln x_k)^2 + b\sum_{k=1}^{8}(\ln x_k)(\cos x_k) + c\sum_{k=1}^{8}(\ln x_k)(e^{x_k}) = \sum_{k=1}^{8} y_k(\ln x_k)$$

$$a\sum_{k=1}^{8}(\ln x_k)(\cos x_k) + b\sum_{k=1}^{8}(\cos x_k)^2 + c\sum_{k=1}^{8}(\cos x_k)(e^{x_k}) = \sum_{k=1}^{8} y_k(\cos x_k)$$

$$a\sum_{k=1}^{8}(\ln x_k)(e^{x_k}) + b\sum_{k=1}^{8}(\cos x_k)(e^{x_k}) + c\sum_{k=1}^{8}(e^{x_k})^2 = \sum_{k=1}^{8} y_k(e^{x_k})$$

Evaluate the sums and solve the normal equations

How do you judge performance?

Given two or more functions to fit the data,

How do you select the best?

Answer :

Determine the parameters for each function then compute Φ for each one. The function resulting in smaller Φ is the best in the least square sense.

Multiple Regression

Example:

Given the following data

t	0	1	2	3
x	0.1	0.4	0.2	0.2
f(x,t)	3	2	1	2

It is required to determine a function of two variables

$$f(x,t) = a + b\,x + c\,t$$

to explain the data that is best in the least square sense.

Solution of Multiple Regression

Construct Φ , the sum of the square of the error and derive the necessary conditions by equating the partial derivatives with respect to the unknown parameters to zero then solve the equations.

t	0	1	2	3
x	0.1	0.4	0.2	0.2
f(x,t)	3	2	1	2

Solution of Multiple Regression

$$f(x,t) = a + bx + ct$$

$$\Phi(a,b,c) = \sum_{i=1}^{4} \left(a + bx_i + ct_i - f_i\right)^2$$

Necessary conditions

$$\frac{\partial \Phi(a,b,c)}{\partial a} = 2\sum_{i=1}^{4} \left(a + bx_i + ct_i - f_i\right) = 0$$

$$\frac{\partial \Phi(a,b,c)}{\partial b} = 2\sum_{i=1}^{4} \left(a + bx_i + ct_i - f_i\right) x_i = 0$$

$$\frac{\partial \Phi(a,b,c)}{\partial c} = 2\sum_{i=1}^{4} \left(a + bx_i + ct_i - f_i\right) t_i = 0$$

SE301: Numerical Methods
Lecture 13:

Nonlinear least squares problems + More

- Examples of nonlinear least squares
- Solution of inconsistent equations
- Continuous least square problems

Outlines

- Examples of nonlinear least squares
- Solution of inconsistent equations
- Continuous least square problems

Nonlinear Problem

Given

x	1	2	3
y	2.4	5.	9

find a fuction of the form ae^{bx} that best fit the data.

$$\Phi = \sum_{i=1}^{3} \left(ae^{bx_i} - y_i \right)^2$$

Normal Equations are obtained using

$$\frac{\partial \Phi}{\partial a} = 0 = \sum_{i=1}^{3} \left(ae^{bx_i} - y_i \right) e^{bx_i}$$

$$\frac{\partial \Phi}{\partial b} = 0 = \sum_{i=1}^{3} \left(ae^{bx_i} - y_i \right) a\, b\, e^{bx_i}$$

Alternative Solution
(Linearization Method)

Given

x	1	2	3
y	2.4	5.	9

find a fuction of the form ae^{bx} that best fit the data.

$$\text{Define } z = \ln(y) = \ln(a) + bx$$

$$Let\ \ \alpha = \ln(a)\ \ and\ \ z_i = \ln(y_i)$$

$$\text{Instead of using } \quad \Phi = \sum_{i=1}^{3} \left(ae^{bx_i} - y_i \right)^2$$

$$\text{We will use} \quad \Phi = \sum_{i=1}^{3} \left(\alpha + bx_i - z_i \right)^2 \quad \text{(easier to solve)}$$

Inconsistent System of Equations

Problem :

Solve the following system of equations

$$\begin{bmatrix} 1 & 2 \\ 2 & 2 \\ 3 & 4.1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 4 \\ 6 \\ 10 \end{bmatrix}$$

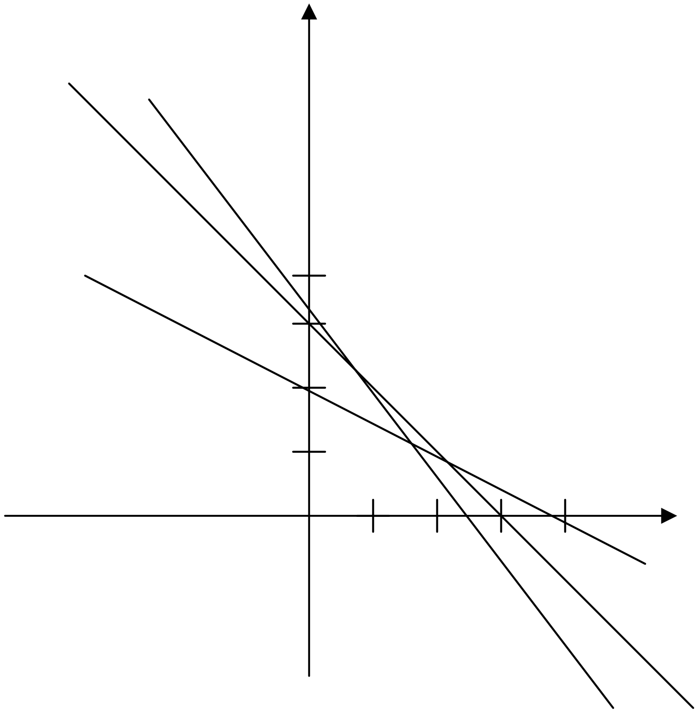
This is inconsistent system of Equations

No solution

Inconsistent System of Equations

Reasons

Inconsistent equations may occur because of errors in formulating the problem, errors in collecting the data or computational errors.



Solution if all lines intersect at one point

Inconsistent System of Equations
Formulation as a least squares problem

We can view the equations as

$$\begin{bmatrix} 1 & 2 \\ 2 & 2 \\ 3 & 4.1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 4 \\ 6 \\ 10 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{bmatrix}$$

Find x_1 and x_2 to minimize the least squares error

Solution

$$\Phi = (x_1 + 2x_2 - 4)^2 + (2x_1 + 2x_2 - 6)^2 + (3x_1 + 4.1x_2 - 10)^2$$

Find x_1 and x_2 to minimize Φ

$$\frac{\partial \Phi}{\partial x_1} = 0 = 2(x_1 + 2x_2 - 4) + 4(2x_1 + 2x_2 - 6) + 6(3x_1 + 4.1x_2 - 10)$$

$$0 = (2 + 8 + 18)x_1 + (4 + 8 + 24.6)x_2 + (-8 - 24 - 60)$$

$$28x_1 + 36.6x_2 = 92$$

$$\frac{\partial \Phi}{\partial x_2} = 0 = 4(x_1 + 2x_2 - 4) + 4(2x_1 + 2x_2 - 6) + 8.2(3x_1 + 4.1x_2 - 10)$$

$$0 = (4 + 8 + 24.6)x_1 + (8 + 8 + 33.62)x_2 + (-16 - 24 - 82)$$

$$36.6x_1 + 49.62x_2 = 122$$

Solution

Normal equations:

$$28x_1 + 36.6x_2 = 92$$

$$36.6x_1 + 49.62x_2 = 122$$

Solution:

$$\Rightarrow x_1 = 2.0048, x_2 = 0.9799$$

Examples
(Linearization Method)

Given

x	1	2	3
y	0.23	.2	.14

find a fuction of the form $1/(\mathrm{ax}+\mathrm{b})$ that best fit the data.

$$f(x) = \frac{1}{\mathrm{ax}+\mathrm{b}}$$

$$\text{Define } z = \frac{1}{y} = \mathrm{ax}+\mathrm{b}$$

$$Let\ z_i = \frac{1}{y_i}$$

$$\text{Instead of using } \Phi = \sum_{i=1}^{3}\left(\frac{1}{\mathrm{ax}+\mathrm{b}} - y_i\right)^2$$

$$\text{We will use } \Phi = \sum_{i=1}^{3}\left(ax_i + b - z_i\right)^2$$

HW

- Check WebCT for HW problems and due date