Optimal Design of Energy Systems

Chapter 4 Equation Fitting

Min Soo KIM

Department of Mechanical and Aerospace Engineering
Seoul National University

Chapter 4. Equation Fitting

4.1 Mathematical Modeling

- performance characteristics of equipment
- behavior of processes
- thermodynamic properties

- Equation development is required
  - Facilitate the process of system simulation
  - Develop a mathematical statement for optimization

Chapter 4. Equation Fitting

4.2 Matrices

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

Order of matrix $m \times n$

$[A]^T$ Transpose of a matrix [A]

ex>

$$[A] = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \qquad [A]^T = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Chapter 4. Equation Fitting

4.2 Matrices

- Simultaneous linear equations

$$
\begin{aligned}
2x_1 - x_2 + 3x_3 &= 6 \\
x_1 + 3x_2 \quad &= 1 \\
4x_1 - 2x_2 + x_3 &= 0
\end{aligned}
\quad \Rightarrow \quad
\begin{bmatrix} 2 & -1 & 3 \\ 1 & 3 & 0 \\ 4 & -2 & 1 \end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}
=
\begin{bmatrix} 6 \\ 1 \\ 0 \end{bmatrix}
$$

Chapter 4. Equation Fitting

4.2 Matrices

- Determinant

$$D = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = \begin{matrix} +a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ -a_{31}a_{22}a_{13} - a_{21}a_{12}a_{33} - a_{11}a_{23}a_{32} \end{matrix}$$

$$= a_{11}\underline{A_{11}} + a_{21}A_{21} + a_{13}A_{31}$$

↳ cofactor of a_{11}

$$= a_{22}a_{33} - a_{23}a_{32}$$

$$A_{ij} = [(-1)^{i+j}] \begin{vmatrix} submatrix\ \ formed \\ by\ striking\ out \\ \mathrm{i}\ \ th\ row\ and\ \ j\ th \\ column\ of\ [A] \end{vmatrix}$$

Chapter 4. Equation Fitting

4.3 Solution of Simultaneous Equations

✓ Simultaneous linear equations

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

✓ Matrix form

$$[A][X] = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = [B]$$

Chapter 4. Equation Fitting

4.3 Solution of Simultaneous Equations

- Crammer's rule

$$x_i = \frac{\left| [A]\ matrix\ with\ [B]\ matrix\ substituted\ in\ \mathrm{i}th\ column \right|}{|A|}$$

ex>

$$\begin{bmatrix} 2 & 1 & -1 \\ 1 & -2 & 2 \\ -1 & 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 9 \\ 0 \end{bmatrix}$$

$$x_1 = \frac{\begin{vmatrix} 3 & 1 & -1 \\ 9 & -2 & 2 \\ 0 & 0 & 3 \end{vmatrix}}{\begin{vmatrix} 2 & 1 & -1 \\ 1 & -2 & 2 \\ -1 & 0 & 3 \end{vmatrix}} = \frac{-45}{-15} = 3 \quad x_2 = \frac{\begin{vmatrix} 2 & 3 & -1 \\ 1 & 9 & 2 \\ -1 & 0 & 3 \end{vmatrix}}{\begin{vmatrix} 2 & 1 & -1 \\ 1 & -2 & 2 \\ -1 & 0 & 3 \end{vmatrix}} = -2 \quad x_3 = \frac{\begin{vmatrix} 2 & 1 & 3 \\ 1 & -2 & 9 \\ -1 & 0 & 0 \end{vmatrix}}{\begin{vmatrix} 2 & 1 & -1 \\ 1 & -2 & 2 \\ -1 & 0 & 3 \end{vmatrix}} = 1$$

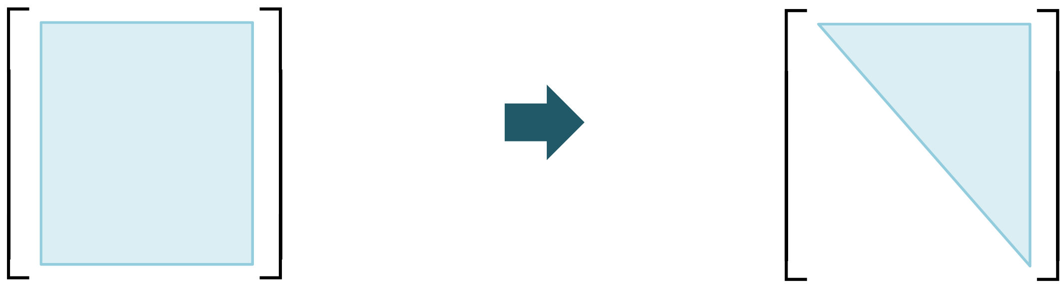
Chapter 4. Equation Fitting

4.3 Solution of Simultaneous Equations

- Gaussian elimination

Coefficient matrix [A]

Triangular matrix



Back substitution

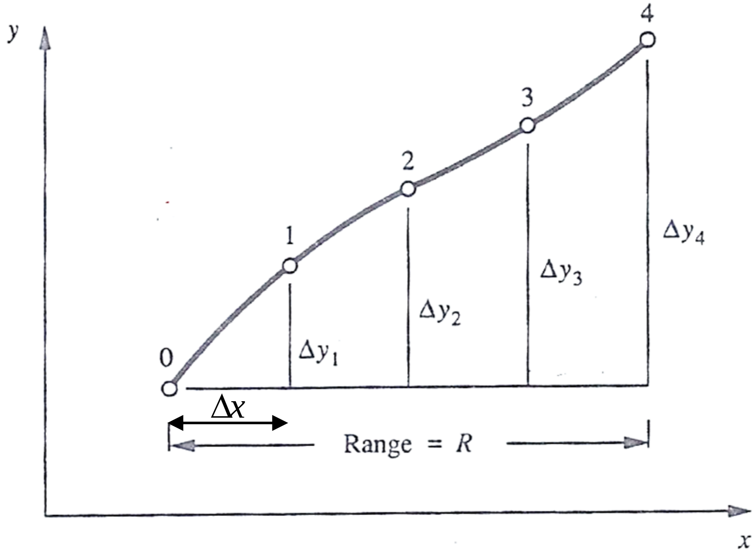
4.4 Polynomial representation

$$y = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

# of data point = n+1	→	exact expression
>	→	best fit

4.6 Simplification when the independent variable is uniformly spaced

$$\Delta x = x_1 - x_0 = \cdots = x_n - x_{n-1}$$



- ✓ Points are equally spaced
- ✓ Derive 4th degree polynomial
- ✓ n=4

$$y = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

4

$$y - y_0 = a_1\left[\frac{n}{R}(x - x_0)\right] + a_2\left[\frac{n}{R}(x - x_0)\right]^2 + a_3\left[\frac{n}{R}(x - x_0)\right]^3 + a_4\left[\frac{n}{R}(x - x_0)\right]^4$$

Eq. (4.16)

(next page)

Chapter 4. Equation Fitting

4.6 Simplification when the independent variable is uniformly spaced

TABLE 4.1
Constants in Eq. (4.16)

Equation	a_4	a_3	a_2	a_1
Fourth degree	$\frac{1}{24}(\Delta y_4 - 4\Delta y_3 + 6\Delta y_2 - 4\Delta y_1)$	$\frac{\Delta y_3}{6} - \frac{\Delta y_2}{2} + \frac{\Delta y_1}{2} - 6a_4$	$\frac{\Delta y_2}{2} - \Delta y_1 - 3a_3 - 7a_4$	$\Delta y_1 - a_2 - a_3 - a_4$
Cubic		$\frac{1}{6}(3\Delta y_1 + \Delta y_3 - 3\Delta y_2)$	$\frac{1}{2}(\Delta y_2 - 2\Delta y_1) - 3a_3$	$\Delta y_1 - a_2 - a_3$
Quadratic			$\frac{1}{2}(\Delta y_2 - 2\Delta y_1)$	$\Delta y_1 - a_2$
Linear				Δy_1

Chapter 4. Equation Fitting

4.6 Simplification when the independent variable is uniformly spaced

- ✓ if substitute (x1,y1)

$$\Delta y_1 = a_1 \frac{4(x_1 - x_0)}{R} + a_2 \left[\frac{4(x_1 - x_0)}{R}\right]^2 + a_3 \left[\frac{4(x_1 - x_0)}{R}\right]^3 + a_4 \left[\frac{4(x_1 - x_0)}{R}\right]^4$$

$$= a_1 + a_2 + a_3 + a_4$$

- ✓ Substitute all the points to Equation (4.16)

$$x = x_0,\ y = y_0$$

$$x = x_1,\ y = \Delta y_1 = a_1 + a_2 + a_3 + a_4$$

$$x = x_2, \qquad \Delta y_2 = 2a_1 + 4a_2 + 8a_3 + 16a_4$$

$$x = x_3, \qquad \Delta y_3 = 3a_1 + 9a_2 + 27a_3 + 64a_4$$

$$x = x_4, \qquad \Delta y_4 = 4a_1 + 16a_2 + 64a_3 + 256a_4$$

Chapter 4. Equation Fitting

4.7 Lagrange Interpolation

$$y = a_0 + a_1 x + a_2 x^2$$

⬇

$$y = c_1(x - x_2)(x - x_3) + c_2(x - x_1)(x - x_3) + c_3(x - x_1)(x - x_2)$$

$$x = x_1, \quad y_1 = c_1(x_1 - x_2)(x_1 - x_3)$$

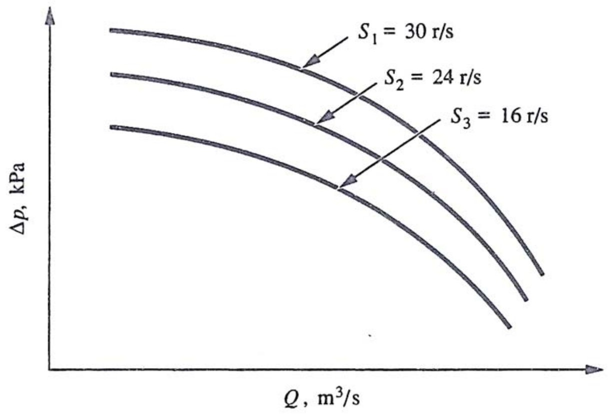
$$x = x_2, \quad y_2 = c_2(x_2 - x_1)(x_2 - x_3)$$

$$x = x_3, \quad y_3 = c_3(x_3 - x_1)(x_3 - x_2)$$

$$y = \sum_{i=1}^{n} y_i \prod_{j=1}^{n} \frac{(x - x_j)\ ommiting\ (x - x_i)}{(x_i - x_j)\ ommiting\ (x_i - x_i)}$$

Chapter 4. Equation Fitting

4.8 Function of two variables



$$S_1 : \Delta P_1 = a_1 + b_1 Q + c_1 Q^2$$

$$S_2 : \Delta P_2 = a_2 + b_2 Q + c_2 Q^2$$

$$S_3 : \Delta P_3 = a_3 + b_3 Q + c_3 Q^2$$

$$\Delta P = a(S) + b(S)Q + c(S)Q^2$$

$$a(S) = A_0 + A_1 S + A_2 S^2$$

$$b(S) = B_0 + B_1 S + B_2 S^2$$

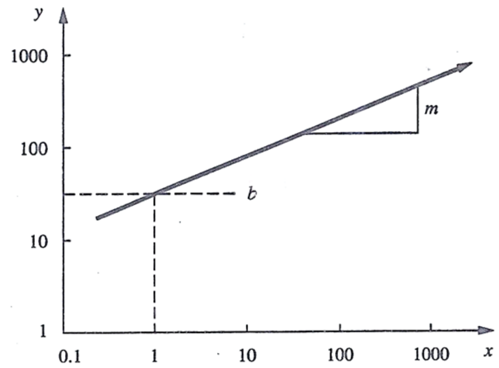
$$c(S) = C_0 + C_1 S + C_2 S^2$$

Chapter 4. Equation Fitting

4.9 Exponential Forms

✓ $y = bx^m$

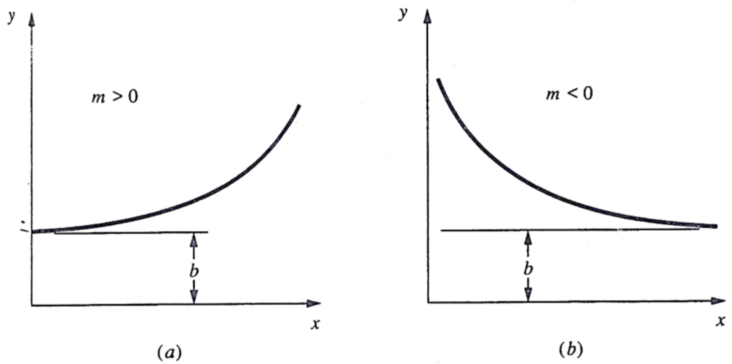
$\ln y = \ln b + m \ln x$



Log-log plot ($y=bx^m$)

✓ $y = b + ax^m$

If y approaches some value b, as $x \to \infty$ or $x \to -\infty$

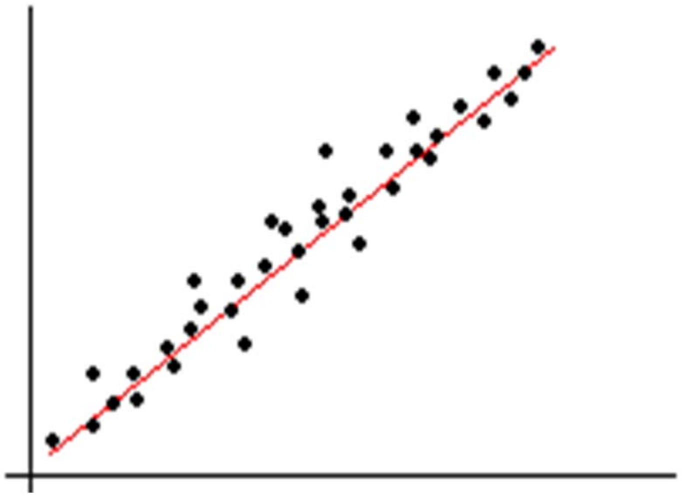


Curve $y=b+ax^m$

- Estimate b
- Calculate m with log-log plot (y-b vs. x)
- Fitting (y vs. x^m)
- Correct value of b

4.10 Best fit : Method of Least Squares

The sum of the squares of the deviation is a minimum

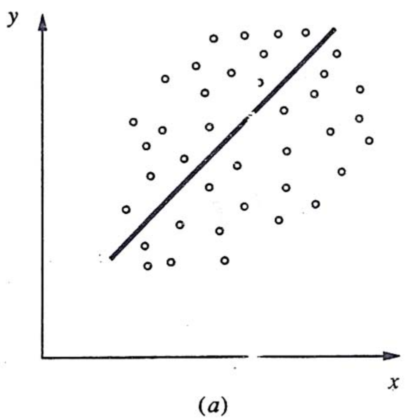


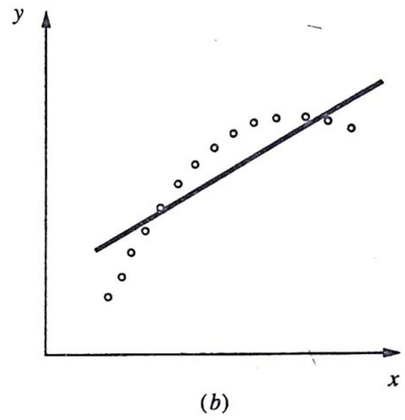
Example of least square method

- ✓ Misuses of least square method

(a) Questionable correlation

(b) Applying too low degree





Misuse of least square method

Chapter 4. Equation Fitting

4.10 Best fit : Method of Least Squares

- Method of least squares for $y = a + bx$

$$
\left.
\begin{aligned}
z &= \sum_{i=1}^{m} (a + bx_i - y_i)^2 \rightarrow \min \\
\frac{\partial z}{\partial a} &= \sum 2(a + bx_i - y_i) = 0 \\
\frac{\partial z}{\partial b} &= \sum 2(a + bx_i - y_i)x_i = 0
\end{aligned}
\right\}
\qquad
\begin{aligned}
ma + b\sum x_i &= \sum y_i \\
a\sum x_i + b\sum x_i^{\,2} &= \sum x_i y_i
\end{aligned}
$$

Chapter 4. Equation Fitting

4.10 Best fit : Method of Least Squares

<Example> provide a best fit (least square)

$$y = a_0 + a_1 x$$

x	y
1	4.9
3	11.2
4	13.7
6	20.1

<Solution>

	x_i	y_i	x_i^2	$x_i y_i$
	1	4.9	1	4.9
	3	11.2	9	33.6
	4	13.7	16	54.8
	6	20.1	36	120.6
Σ	14	49.9	62	213.9

$$4a_0 + 14a_1 = 49.9$$

$$14a_0 + 62a_1 = 213.9$$

$$y = 1.908 + 3.019x$$

Chapter 4. Equation Fitting

4.10 Best fit : Method of Least Squares

- Method of least squares for $y = a + bx + cx^2$

$$
\begin{cases}
a\sum 1 + b\sum x_i + c\sum x_i^{\,2} = \sum y_i \\
a\sum x_i + b\sum x_i^{\,2} + c\sum x_i^{\,3} = \sum y_i x_i \\
a\sum x_i^{\,2} + b\sum x_i^{\,3} + c\sum x_i^{\,4} = \sum y_i x_i^{\,2}
\end{cases}
$$

- For $y = a\sin x + b\ln x$

$$
\begin{cases}
a\sum (\sin x_i)^2 + b\sum (\ln x_i)^{(\sin x_i)} = \sum y_i \sin x_i \\
a\sum (\sin x_i)^{(\ln x_i)} + b\sum (\ln x_i)^2 = \sum y_i \ln x_i
\end{cases}
$$

4.11 Method of Least Squares Applied to Nonpolynomial Forms

- Method of least squares

  → apply to equation with constant coefficients

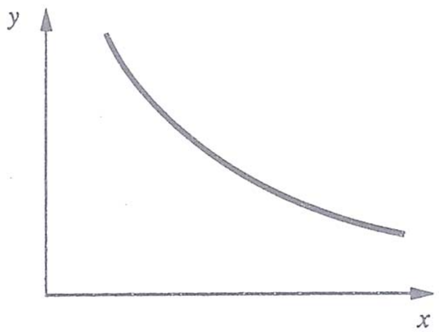
  cf) $y = \sin 2ax + bx^c$

Chapter 4. Equation Fitting

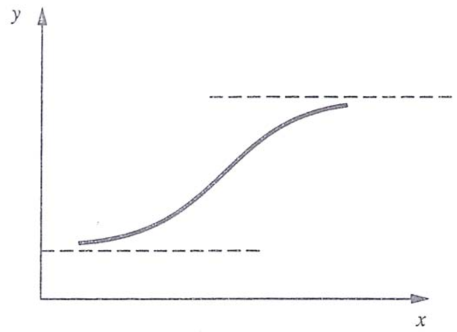
4.12 The are of equation fitting

- Choice of the form of the equation

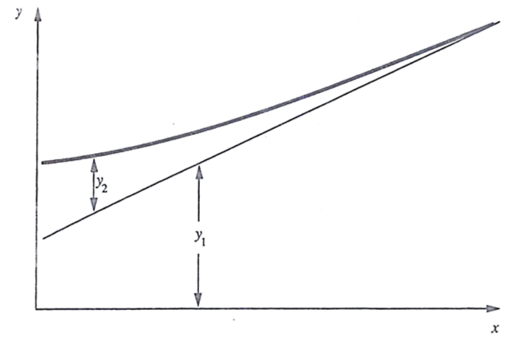
  - Polynomials with negative exponent(1)
  - Exponential eq.(2)
  - Gompertz eq(3) $y = ab^{c^x} \quad where \quad b, c < 1$
  - combination



(1)



(2)



(3)