Optimal Design of Energy Systems

Chapter 4 Equation Fitting

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Chapter 4. Equation fitting

4.1 Mathematical modeling

Equation Development

Key elements

- Performance characteristics of equipment
- Behavior of processes
- Thermodynamic properties of substances

Purposes

- To facilitate the process of system **simulation**
- To develop a mathematical statement for **optimization**

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] => interchanging rows & columns

ex>

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

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4.2 Matrices

- Multiplying two matrices

# of columns of the left matrix = # of rows of the right matrix

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \times \begin{bmatrix} b_{11} & \cdots & b_{1l} \\ \vdots & \ddots & \vdots \\ b_{n1} & \cdots & b_{nl} \end{bmatrix} \Rightarrow m \times l \; matrix$$

4.2 Matrices

- Simultaneous linear equations

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

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4.2 Matrices

- Determinant (scalar)

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

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

cofactor of a_{11}

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

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

Cofactor of a_{ij}

Example 4.1 : Matrices

Evaluate $$\begin{vmatrix} 1 & 2 & -1 & 0 \\ 0 & 1 & 2 & 0 \\ 3 & -1 & 1 & 2 \\ 4 & 2 & 1 & 5 \end{vmatrix}$$

(Solution)

Find row which has many zeros if possible => second row!

$$\det = a_{21}A_{21} + a_{22}A_{22} + a_{23}A_{23} + a_{24}A_{24}$$

$$= (0)A_{21} + (1)(-1)^{2+2}\begin{vmatrix} 1 & -1 & 0 \\ 3 & 1 & 2 \\ 4 & 1 & 5 \end{vmatrix} + (2)(-1)^{2+3}\begin{vmatrix} 1 & 2 & 0 \\ 3 & -1 & 2 \\ 4 & 2 & 5 \end{vmatrix} + (0)A_{24}$$

$$= 0 + 10 + 46 + 0 = 56$$

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4.3 Solution of simultaneous equation

✓ Simultaneous linear equations

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

✓ Matrix form

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

4.3 Solution of simultaneous equation

- Crammer's rule

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

Example 4.2

Using Cramer's rule, get x_2

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

(Solution)

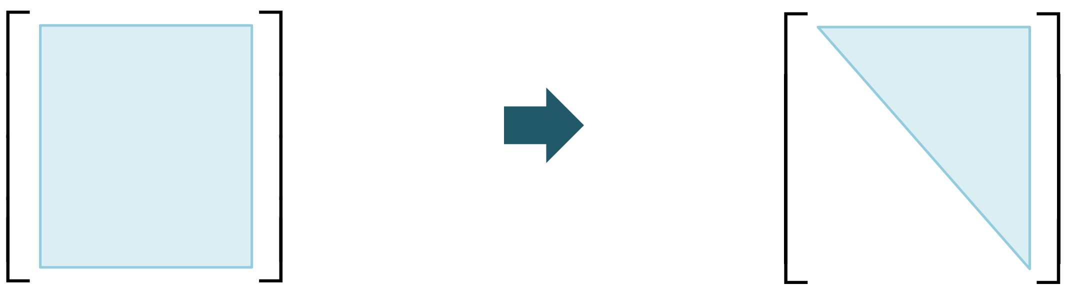
$$x_2 = \frac{\begin{vmatrix} 2 & 3 & -1 \\ 1 & 9 & 2 \\ -1 & 0 & 3 \end{vmatrix}}{\begin{vmatrix} 2 & 1 & -1 \\ 1 & -2 & 2 \\ -1 & 0 & 3 \end{vmatrix}} = \frac{30}{-15} = -2$$

4.3 Solution of simultaneous equation

- Gaussian elimination

Coefficient matrix [A]

Triangular matrix



Back substitution

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4.4 Polynomial representations

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

- degree of the eq = highest exponent of x

- # of data point = degree + 1 → exact expression

  > → best fit

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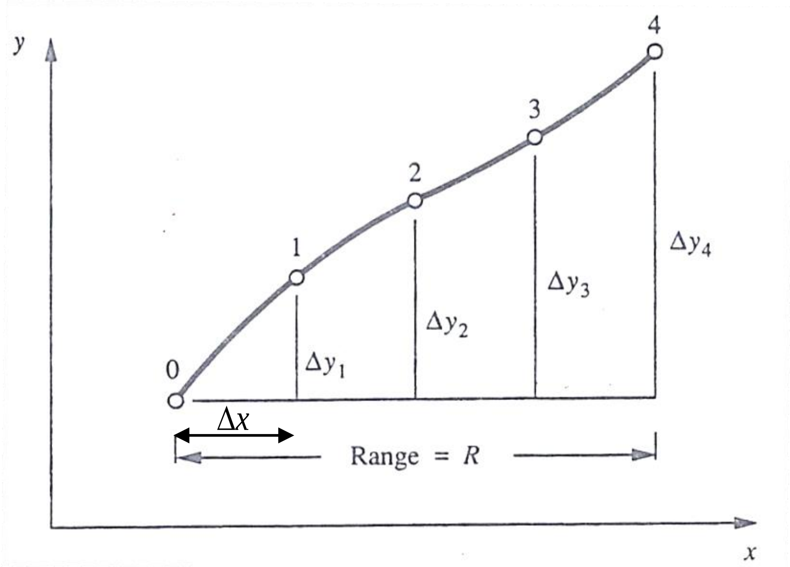
4.6 Simplifications when the independent variable is uniformly spaced

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



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

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)

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

(next page)

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4.6 Simplifications 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)

$$x = x_0, y = y_0$$

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

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

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

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

4.6 Simplifications 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

4.7 Lagrange interpolation

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

$$\Downarrow$$

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

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

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

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

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

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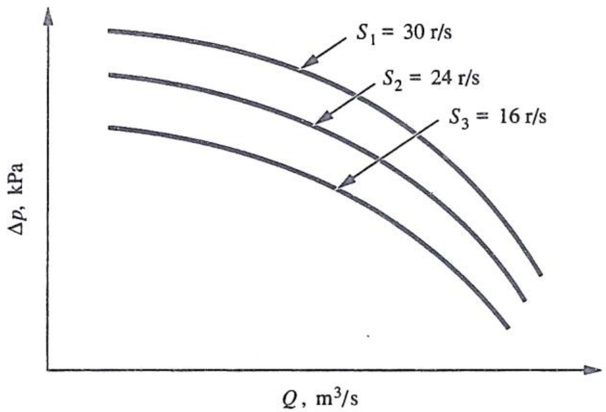
4.8 Function of two variables



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

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

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

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

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

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

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

Example 4.3 : Function of two variables

The range is the difference between the inlet and outlet temperatures of the water. In table below, for example, when the wet-bulb temperature is 20℃ and the range is 10℃, inlet and outlet temperature are 35.9℃ and 25.9℃ each. **Express** the outlet temperature ***t*** in Table below as a function of the wet-bulb temperature (**WBT**) and the range **R**

(Solution)

	Wet-bulb temperature, ℃		
Range, ℃	20	23	26
10	25.9	27.5	29.4
16	27.0	28.4	30.2
22	28.4	29.6	31.3

For 3 WBTs, get parabola that represents (R,t)

i) For WBT = 20℃

(R,t) : (10,25.9), (16,27.0), (22,28.4)

$\Rightarrow t = 24.733 + 0.075006R + 0.004146R^2$

ii) For WBT = 23℃

$\Rightarrow t = 26.667 + 0.041659R + 0.0041469R^2$

iii) For WBT = 26℃

$\Rightarrow t = 28.733 + 0.024999R + 0.0041467R^2$

Example 4.3 : Function of two variables

(Solution)

Set 2nd degree equation (constant terms(C) , WBT) : (24.733,20), (26.667,23), (28.733,26)

$\Rightarrow C = 15.247 + 0.32637WBT + 0.007380WBT^2$

Set 2nd degree equation (coefficient of R , WBT) and (coefficient of R^2 , WBT) as well

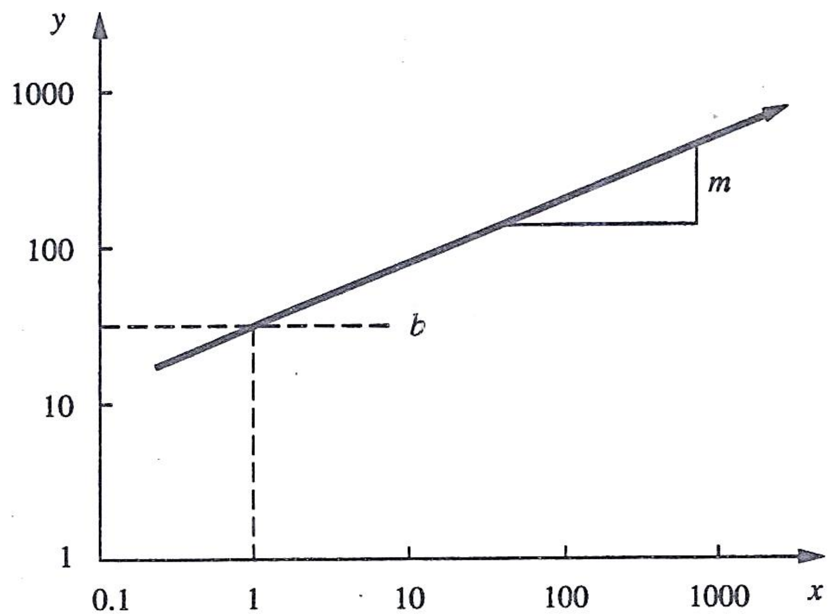
$$t = (15.247 + 0.32637WBT + 0.007380WBT^2) + (0.72375 - 0.050978WBT + 0.000927WBT^2)R + (0.004147 + 0WBT + 0WBT^2)R^2$$

Chapter 4. Equation fitting

4.9 Exponential forms

✓ $y = bx^m$

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



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

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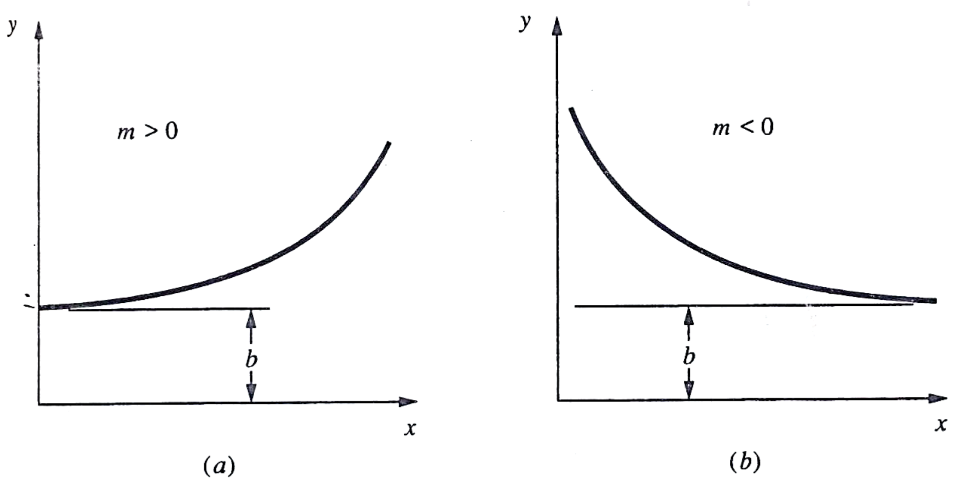
4.9 Exponential forms

✓ $y = b + ax^m$

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

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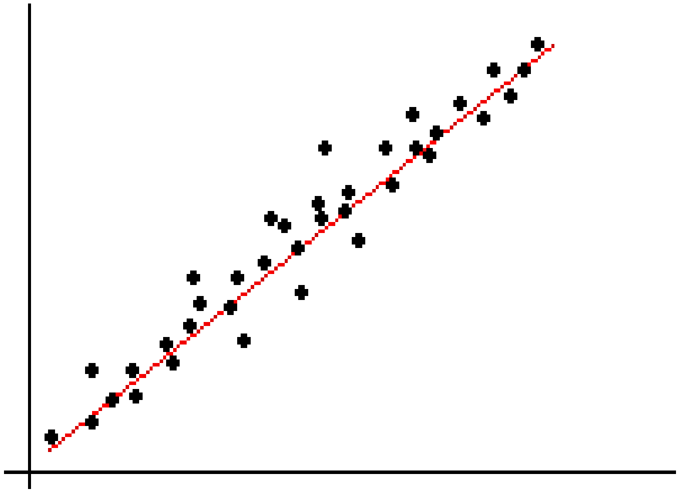
4.10 Best fit : Method of least squares

└ The sum of the squares of the deviation is a minimum

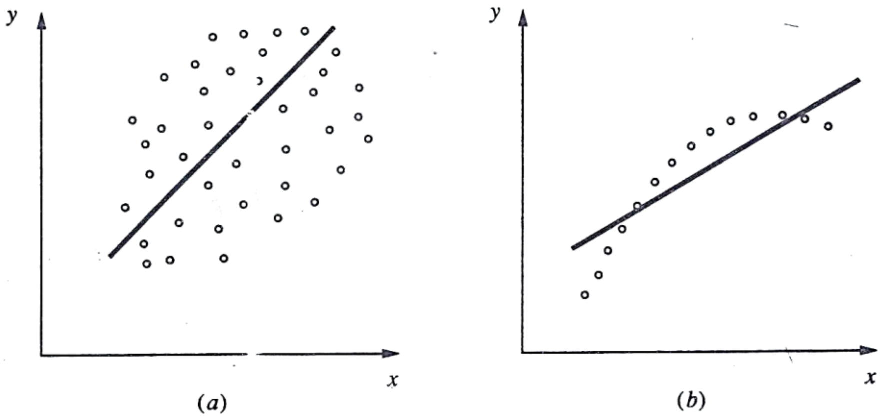


Example of least square method

✓ 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 square for $y = a + bx$

$$z = \sum_{i=1}^{m} (a + bx_i - y_i)^2 \rightarrow \min$$

$$\frac{\partial z}{\partial a} = \sum 2(a + bx_i - y_i) = 0$$

$$\frac{\partial z}{\partial b} = \sum 2(a + bx_i - y_i)x_i = 0$$

$$ma + b\sum x_i = \sum y_i$$

$$a\sum x_i + b\sum x_i{}^2 = \sum x_i y_i$$

Example 4.4 : Best fit : Method of least squares

Determine a_0 and a_1 in the equation $y = a_0 + a_1 x$ to provide a best fit in the sense of least-squares deviation to the data points (1, 4.9), (3, 11.2), (4, 13.7), and (6, 20.1)

(Solution)

$$ma + b\sum x_i = \sum y_i$$

$$a\sum x_i + b\sum x_i^2 = \sum x_i y_i$$

	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
$\sum$	14	49.9	62	213.9

$m = 4$

$4a_0 + 14a_1 = 49.9$

$14a_0 + 62a_1 = 213.9$

➡ $y = 1.908 + 3.019x$

Chapter 4. Equation fitting

4.10 Best fit : Method of Least Squares

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

$$\sum_{i=1}^{m} (a + bx_i + cx_1{}^2 - y_i)^2 \rightarrow min$$

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

4.11 Method of Least Squares Applied to Nonpolynomial Forms

- Method of least squares

  → apply to equation with constant coefficients

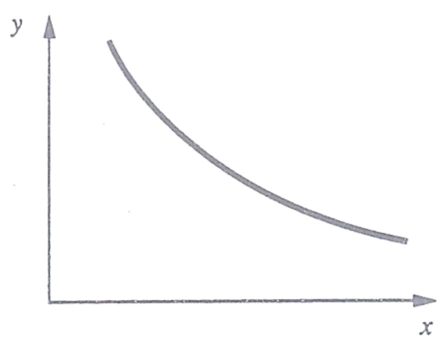
  cf) $y = \sin 2ax + bx^c$

Chapter 4. Equation fitting

4.12 The art of equation fitting

- Choice of the form of the equation

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



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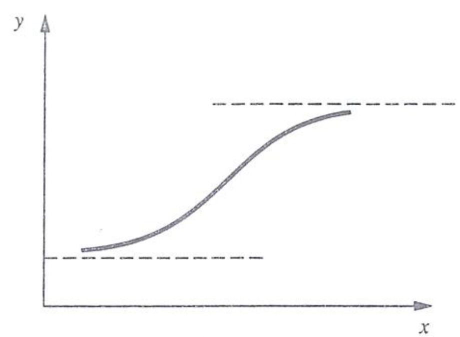

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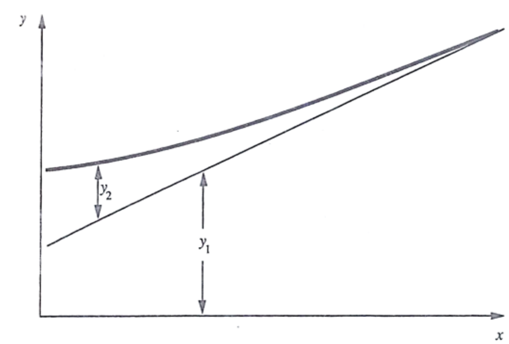

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