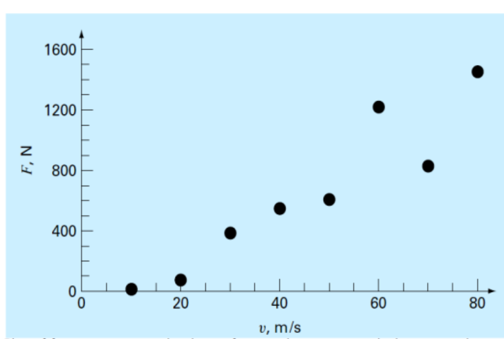
Curve Fitting

Objectives

- Understanding the difference between regression and interpolation.
- Knowing how to fit curve of discrete with least-squares regression.
- Knowing how to compute and understand the meaning of the coefficient of determination.
- Knowing how to perform an interpolation with Newton's polynomial.

In engineering problem, sometime we would like to find the relationships of variables in the form of mathematical models (mathematical equations). It is convenient to predict the change of dependent variables when independent variables vary by using the mathematical models. The mathematical models can be derived not only from laws and theory but also from experimental data which is often given for discrete values. To determine the continuous formulation of those values, we can apply the curve fitting techniques to such data.



Plot of force versus wind velocity for an object suspended in a wind tunnel.

Experimental data for force (N) and velocity (m/s) from a wind tunnel experiment.

***v*, m/s**	10	20	30	40	50	60	70	80
***F*, N**	25	70	380	550	610	1220	830	1450

Fig.1 Example of discrete data.

There are two general approaches for curve fitting:

1. **Regression** – a technique of representing the general trend of the data using a single curve. This curve may not need to intersect all data points. While, the curve shows the pattern of a group of data points.
2. **Interpolation** – a technique of fitting a curve or a series of curve that pass through each of data points. The curve needs to intersect all data points.

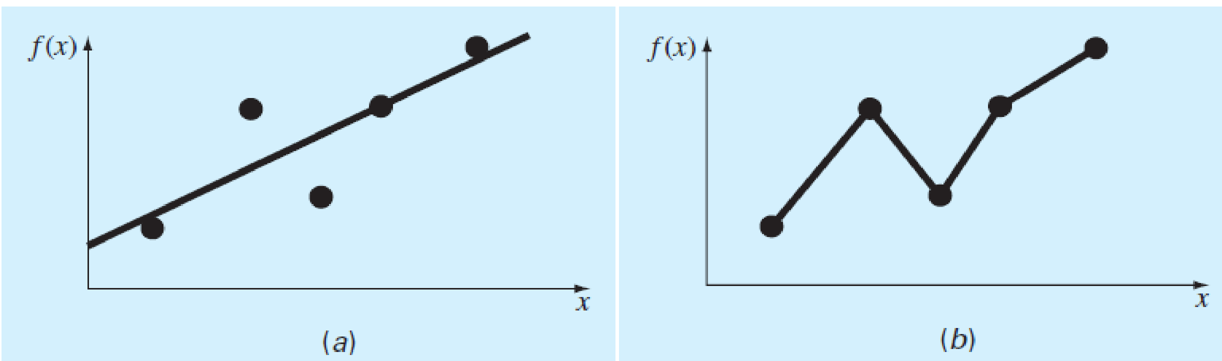
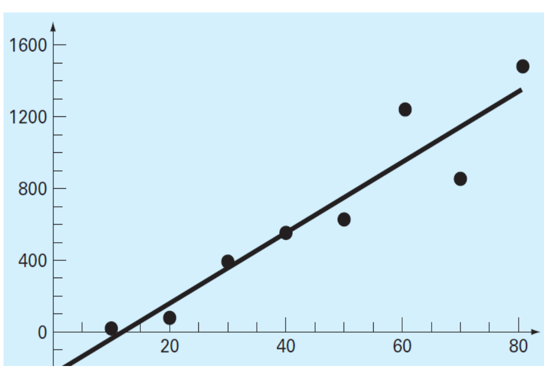


Fig. 2 Comparison between Regression and Interpolation

1. <u>Polynomial Least-Squares Regression</u>

1.1. Linear Least-Squares Regression

The simplest trend curve for curve fitting is a linear line.



$$Y = (a_0 + a_1 X)$$

Fig. 3 The graphical example of linear curve fitting.

However, The difference between the predicted value (by curve fitting) and the data point is existed. The difference is considered as error. A residual error can be derived from

$$e = y - (a_0 + a_1 x) \qquad (1)$$

Where e = the residual error

y = the true value of data point

$a_0 + a_1 x$ = the approximate predicted by the linear equation

The sum of residual errors can be expressed as

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y - (a_0 + a_1 x)) \qquad (2)$$

And the sum squares of the residuals is given by

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y - (a_0 + a_1 x))^2 \qquad (3)$$

The best line which represents the trend of the data must be a line with the minimum sum squares of the residuals.

To complete the linear equation, we need to determine a_0 and a_1 by taking the derivative of S_r with respect to each unknown (a_0 and a_1). Then, we have

$$\frac{\partial S_r}{\partial a_0} = -2\sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i \right) \qquad (4)$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum_{i=1}^{n} \left[\left(y_i - a_0 - a_1 x_i \right) x_i \right] \qquad (5)$$

When the S_r is expected to be minimum as zero, its derivatives equal to zero. Thus,

$$0 = \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} a_0 - \sum_{i=1}^{n} a_1 x_i \tag{6}$$

$$0 = \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} a_0 x_i - \sum_{i=1}^{n} a_1 x_i^2 \tag{7}$$

Where $\sum a_0 = n a_0$. Eq. (6) and (7) can be rearranged as

$$n a_0 + \left(\sum_{i=1}^{n} x_i \right) a_1 = \sum_{i=1}^{n} y_i \tag{8}$$

$$\left(\sum_{i=1}^{n} x_i \right) a_0 + \left(\sum_{i=1}^{n} x_i^2 \right) a_1 = \sum_{i=1}^{n} x_i y_i \tag{9}$$

These equations can be solved for a_0 and a_1 as

$$a_1 = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i \right)^2} \quad , \tag{10}$$

$$a_0 = \bar{y} - a_1 \bar{x} \tag{11}$$

Example 1 Fit a straight line to the values in the following table.

Experimental data for force (N) and velocity (m/s) from a wind tunnel experiment.

***v*, m/s**	10	20	30	40	50	60	70	80
***F*, N**	25	70	380	550	610	1220	830	1450

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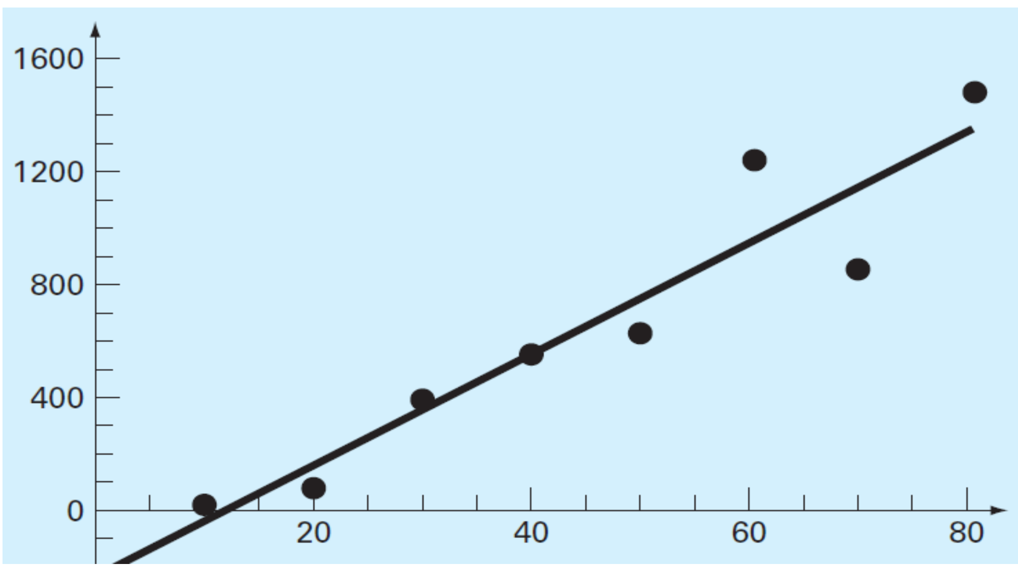
The coefficient of determination, r^2

The r2 is used to measure the goodness of curve fitting. It is given by

$$r^2 = \frac{S_t - S_r}{S_t} \qquad \text{`(12)}$$

Where S_t = Total sum of square which is the square of the difference between an individual data point and the mean of the data.

S_r = the sum squares of the residuals.



Example 2 Determine the coefficient of determination for the curve fitting in Example 1

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1.2. General Polynomial Regression

The least-squares procedure can be extended to fit the data to a higher-order polynomial. For example, using the second-order polynomial or quadratic:

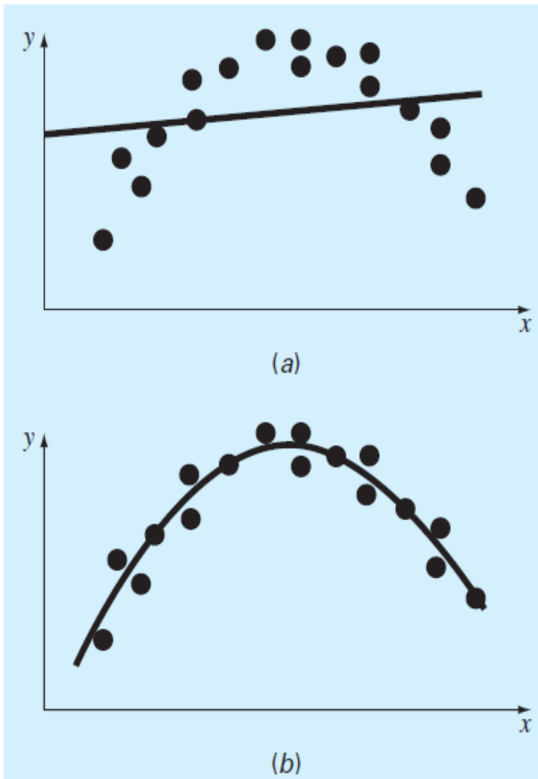

Fig. 4 (a) a linear regression and (b) a second-order polynomial regression.

$$y = a_0 + a_1 x + a_2 x^2 \tag{13}$$

In this case, the sum of squares of residuals is

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - a_2 x_i^2 \right)^2 \tag{14}$$

To generate the least-squares fit, the derivatives of the sum of squares of residuals with respect to each unknown coefficients of the polynomial is expressed as

$$\frac{\partial S_r}{\partial a_0} = -2\sum\left(y_i - a_0 - a_1x_i - a_2x_i^2\right)$$
$$\frac{\partial S_r}{\partial a_1} = -2\sum x_i\left(y_i - a_0 - a_1x_i - a_2x_i^2\right) \tag{15}$$
$$\frac{\partial S_r}{\partial a_2} = -2\sum x_i^2\left(y_i - a_0 - a_1x_i - a_2x_i^2\right)$$

These three equations are set to be zero to minimize the error of prediction. Thus, the equations can be rearranged in the form of the system of equations:

$$na_0 + \left(\sum_{i=1}^{n} x_i\right)a_1 + \left(\sum_{i=1}^{n} x_i^2\right)a_2 = \sum_{i=1}^{n} y_i$$
$$\left(\sum_{i=1}^{n} x_i\right)a_0 + \left(\sum_{i=1}^{n} x_i^2\right)a_1 + \left(\sum_{i=1}^{n} x_i^3\right)a_2 = \sum_{i=1}^{n} x_i y_i \tag{16}$$
$$\left(\sum_{i=1}^{n} x_i^2\right)a_0 + \left(\sum_{i=1}^{n} x_i^3\right)a_1 + \left(\sum_{i=1}^{n} x_i^4\right)a_2 = \sum_{i=1}^{n} x_i^2 y_i$$

Example 3 Fit a second-order polynomial to the following data

x	0	1	2	3	4	5
y	2.1	7.7	13.6	27.2	40.9	61.1

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2. Newton's Interpolation

An interpolation is a technique that can determine the equations for line connecting the adjacent values. It is also used for estimate the unknown valves in between the data points.

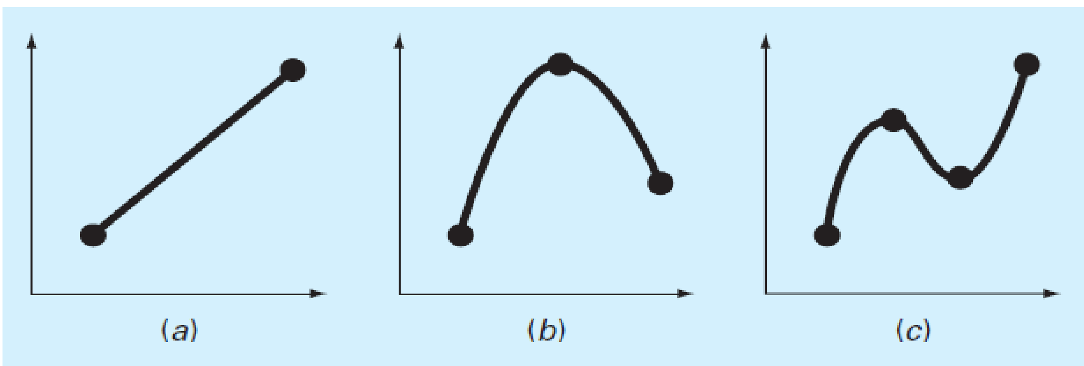

Fig. 5 (a) Linear interpolation, (b) quadratic, and (c) cubic interpolations

2.1. Linear Interpolation

The simplest form of interpolation is to connect two data points with a straight line.

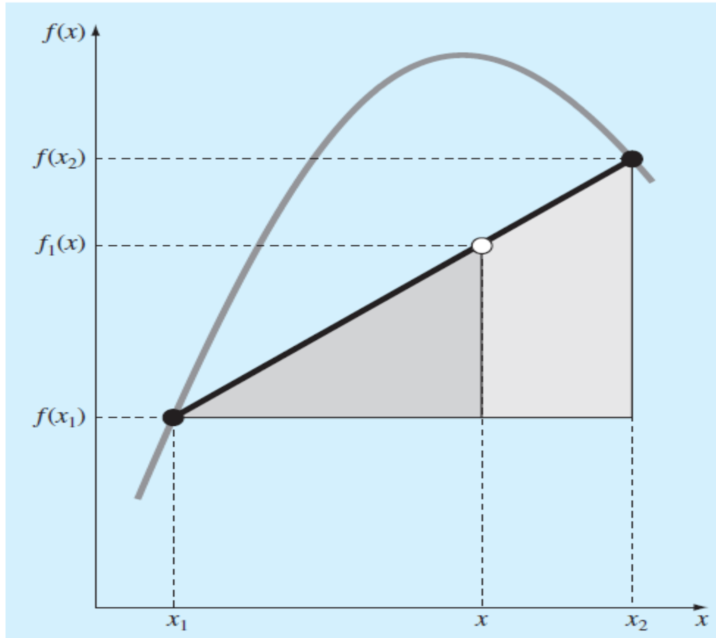

Fig. 6 The concept of linear interpolation

Using similar triangles, the slopes of the line are expressed as

$$slope = \frac{f_1(x) - f(x_1)}{x - x_1} = \frac{f(x_2) - f(x_1)}{x_2 - x_1} \tag{17}$$

$$f_1(x) = f(x_1) + \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x - x_1) \tag{18}$$

$$f_1(x) = C_1 + C_2(x - x_1) \tag{19}$$

Eq. (18) and (19) are the Newton linear-interpolation formula. The notation $f_1(x)$ denotes a first-order interpolating polynomial.

Example 4 Estimate $f(3)$ of the following data using a linear Newton's interpolation.

x	f(x)
1	0
4	1.386
6	1.792
7	1.609

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2.2. G

To fit an (*n-1*)th-order polynomial to the *n* data points, the (*n-1*)th-order polynomial is

$$f_{n-1}(x) = b_1 + b_2(x - x_1) + \cdots + b_n(x - x_1)(x - x_2)\cdots(x - x_{n-1}) \quad (20)$$

Where the coefficients $b_1, b_2, \cdots, b_n$ can be evaluated using the similar scheme as in a linear interpolation. Thus, we have

$$b_1 = f(x_1) \quad (21)$$

$$b_2 = f[x_2, x_1] \quad (22)$$

$$b_3 = f[x_3, x_2, x_1] \quad (23)$$

$$\vdots$$

$$b_3 = f[x_n, x_{n-1}, \ldots, x_2, x_1] \quad (24)$$

Where the bracket function can be evaluated using finite divided differences.

$$f[x_i, x_j] = \frac{f(x_i) - f(x_j)}{x_i - x_j} \tag{25}$$

$$f[x_i, x_j, x_k] = \frac{f[x_i, x_j] - f[x_j, x_k]}{x_i - x_k} \tag{26}$$

$$f[x_n, x_{n-1}, \cdots, x_2, x_1] = \frac{f[x_n, x_{n-1}, \cdots, x_2] - f[x_{n-1}, x_{n-2}, \cdots, x_1]}{x_n - x_1} \tag{27}$$

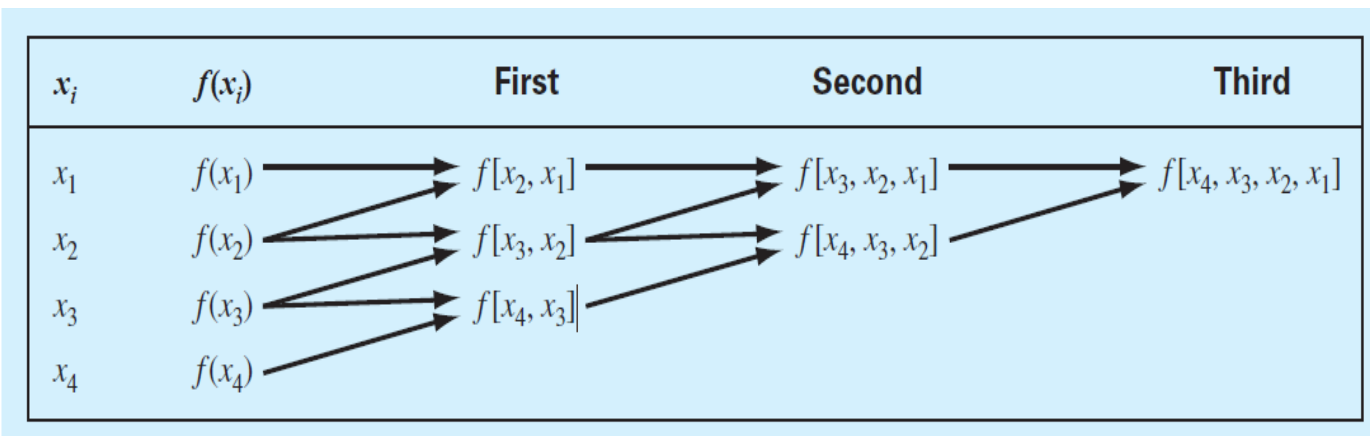

Fig. 6 A divided difference table

For example, the quadratic interpolation, the second-order polynomial is

$$f_2(x) = b_1 + b_2(x - x_1) + b_3(x - x_1)(x - x_2) \tag{28}$$

Where the coefficients are evaluated by

$$b_1 = f(x_1) \tag{29}$$

$$b_2 = f[x_2, x_1] = \frac{f(x_2) - f(x_1)}{x_2 - x_1} \qquad (30)$$

$$b_3 = f[x_3, x_2, x_1] = \frac{\dfrac{f(x_3) - f(x_3)}{x_3 - x_2} - \dfrac{f(x_2) - f(x_1)}{x_2 - x_1}}{x_3 - x_1} \qquad (31)$$

Example 5 Use a second-order Newton polynomial to create the quadratic interpolation formulation of the following data.

x	f(x)
1	0
4	1.386
6	1.792

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Example 6 (a) Fit a straight line to the values in the following table.

(b) And estimate $f(3.6)$ using linear Newton's Interpolation.

x	1	2	3	5	6
f(x)	4.75	4	5.25	19.75	36

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Exercises

1. The acceleration due to gravity at an altitude y above the surface of the earth is given by

y [m]	0	20,000	40,000	60,000	80,000
g [m/s^2]	9.8100	9.7487	9.6879	9.6278	9.5682

Use linear regression to formulate a linear function of the above data

2. Fit a quadratic polynomial to the following data and evaluate the r^2 for the curve fitting.

x	3	4	5	7	8	9	11	12
y	1.6	3.6	4.4	3.4	2.2	2.8	3.8	4.6

3. Use the portion of the given steam table for superheated water at 200 MPa to find

(a) The corresponding entropy, s, for a specific volume, v, of 0.118 with linear interpolation,

(b) The same corresponding entropy using quadratic interpolation.

(c) The volume corresponding to an entropy of 6.45 using linear interpolation.

v [m3/kg]	0.10377	0.11144	0.12547
s [kJ/kg.K]	6.4147	6.5453	6.7664