TMC: Curve Fitting & Interpolation

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CURVE FITTING

Describes techniques to fit curves (*curve fitting*) to discrete data to obtain intermediate estimates.

There are two general approaches two curve fitting:

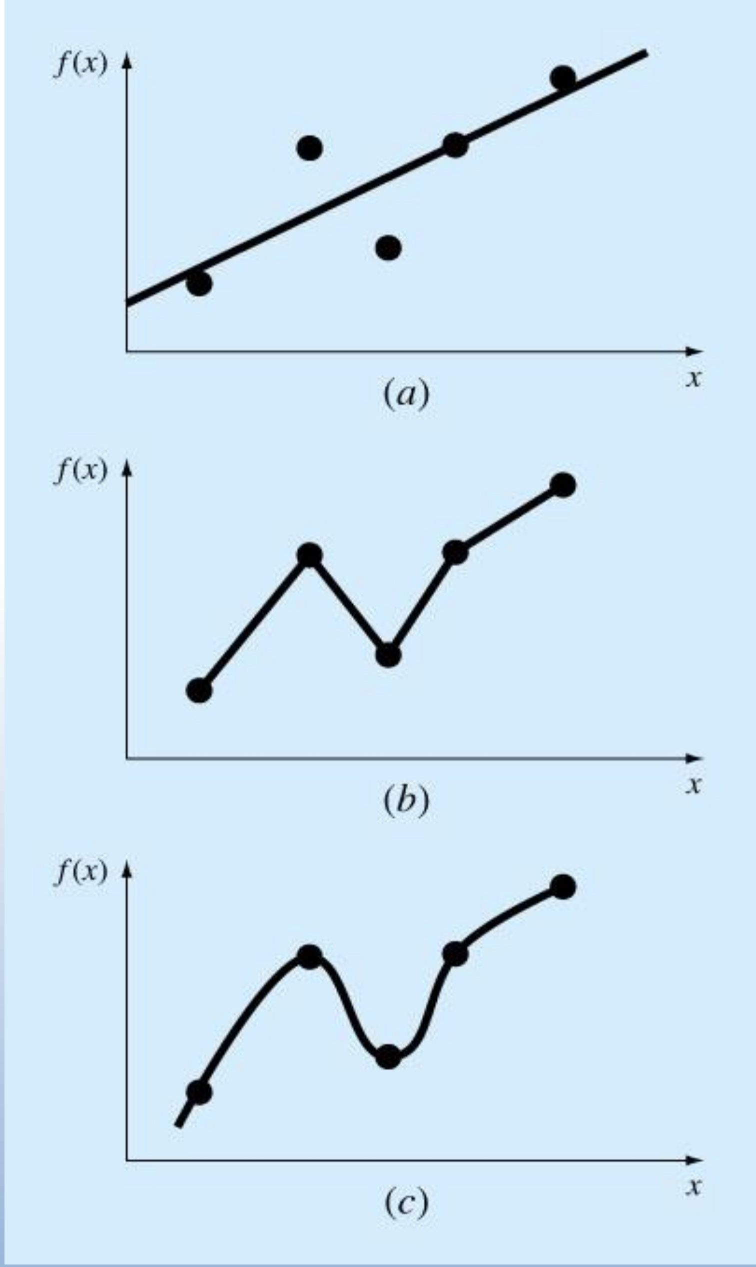
- *Data exhibit a significant degree of scatter*. The strategy is to derive a single curve that represents the general trend of the data.

- *Data is very precise.* The strategy is to pass a curve or a series of curves through each of the points.

In engineering, two types of applications are encountered:

-*Trend analysis*. Predicting values of dependent variable, may include extrapolation beyond data points or interpolation between data points.

-*Hypothesis testing*. Comparing existing mathematical model with measured data.



Three attempts to fit a "best" curve through five data points.
(a) Least-squares regression,
(b) linear interpolation,
(c) curvilinear interpolation.

Mathematical Background

Simple Statistics

If several measurements are made of a particular quantity, additional insight can be gained by summarizing the data in one or more well chosen statistics that convey as much information as possible about specific characteristics of the data set.

These descriptive statistics are most often selected to represent

The location of the center of the distribution of the data,

The degree of spread of the data.

Arithmetic mean. The sum of the individual data points (y_i) divided by the number of points (n).

$$\bar{y} = \frac{\sum y_i}{n}$$

$$i = 1, \ldots, n$$

Standard deviation. The most common measure of a spread for a sample.

$$s_y = \sqrt{\frac{S_t}{n-1}}$$

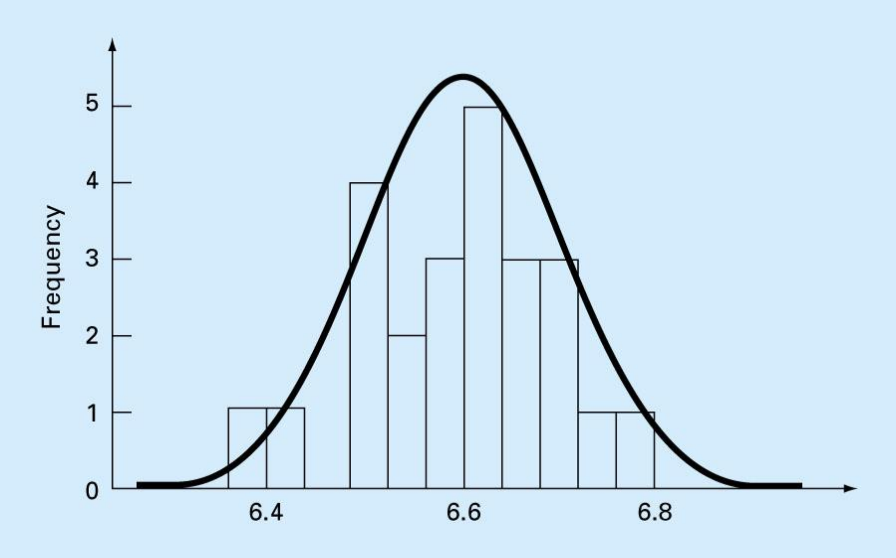
$$S_t = \sum (y_i - \bar{y})^2$$

Variance. Representation of spread by the square of the standard deviation.

$$s_y^2 = \frac{\sum (y_i - \bar{y})^2}{n-1} \quad \text{Degrees of freedom}$$

Coefficient of variation. Has the utility to quantify the spread of data.

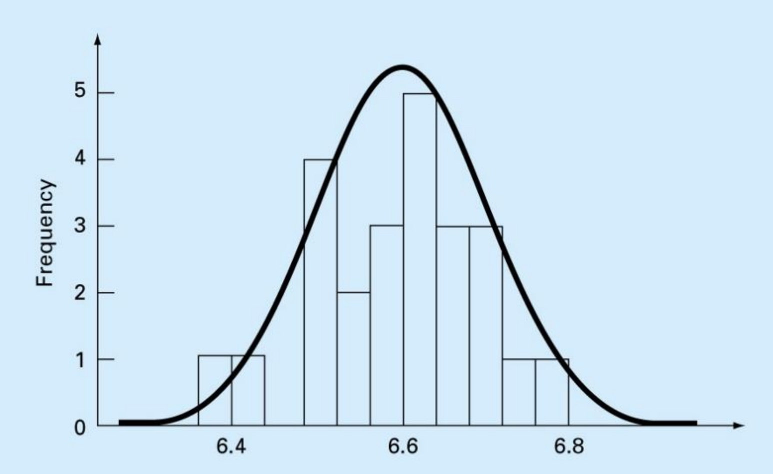
$$c.v. = \frac{s_y}{\bar{y}} 100\%$$



A histogram used to depict the distribution of data. As the number of data points increases, the histogram could approach the smooth, bell-shaped curve called the normal distribution.

Example

Compute the mean, variance, standard deviation, and coefficient of variation for the data in the following table



				Interval	
i	y_i	$(y_i - \bar{y})^2$	Frequency	Lower Bound	Upper Bound
1	6.395	0.042025	1	6.36	6.40
2	6.435	0.027225	1	6.40	6.44
3	6.485	0.013225			
4	6.495	0.011025			
5	6.505	0.009025	4	6.48	6.52
6	6.515	0.007225			
7	6.555	0.002025	2	6.52	6.56
8	6.555	0.002025			
9	6.565	0.001225			
10	6.575	0.000625	3	6.56	6.60
11	6.595	0.000025			
12	6.605	0.000025			
13	6.615	0.000225			
14	6.625	0.000625	5	6.60	6.64
15	6.625	0.000625			
16	6.635	0.001225			
17	6.655	0.003025			
18	6.655	0.003025	3	6.64	6.68
19	6.665	0.004225			
20	6.685	0.007225			
21	6.715	0.013225	3	6.68	6.72
22	6.715	0.013225			
23	6.755	0.024025	1	6.72	6.76
24	6.775	0.030625	1	6.76	6.80
Σ	158.4	0.217000			

Example

The data is added in the table, and the results are used to compute the *mean*:

$$\bar{y} = \frac{158.4}{24} = 6.6$$

As in the table, the sum of the squares of the residuals is 0.217000, which can be used to compute the *standard deviation*:

$$s_y = \sqrt{\frac{0.217}{24-1}} = 0.097133$$

the *variance*:

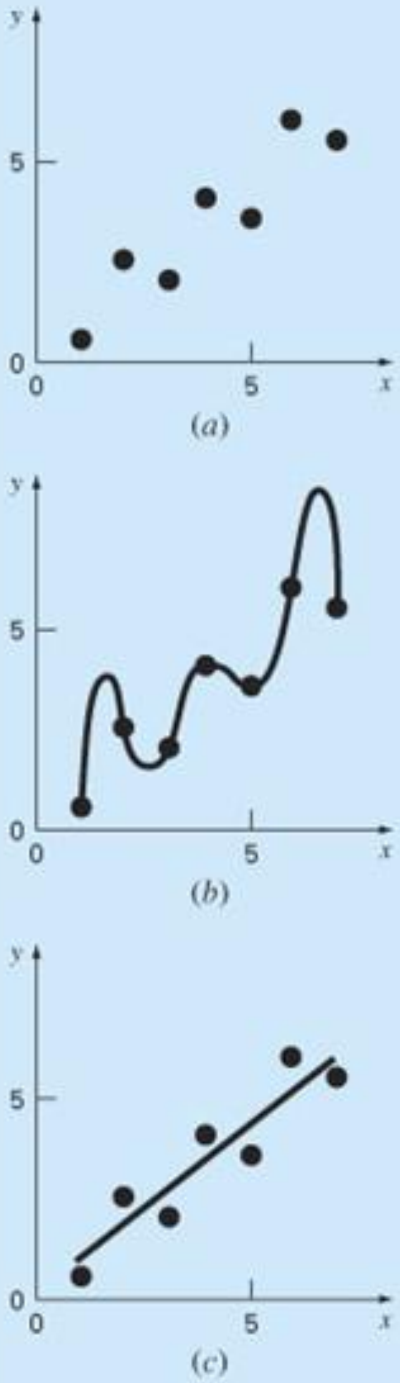
$$s_y{}^2 = 0.009435$$

and the *coefficient of variation*:

$$c.v. = \frac{0.097133}{6.6} 100\% = 1.47\%$$

PART A

LEAST SQUARES REGRESSION



Linear Regression

Fitting a straight line to a set of paired observations: *$(x_1, y_1), (x_2, y_2),\ldots,(x_n, y_n)$.*

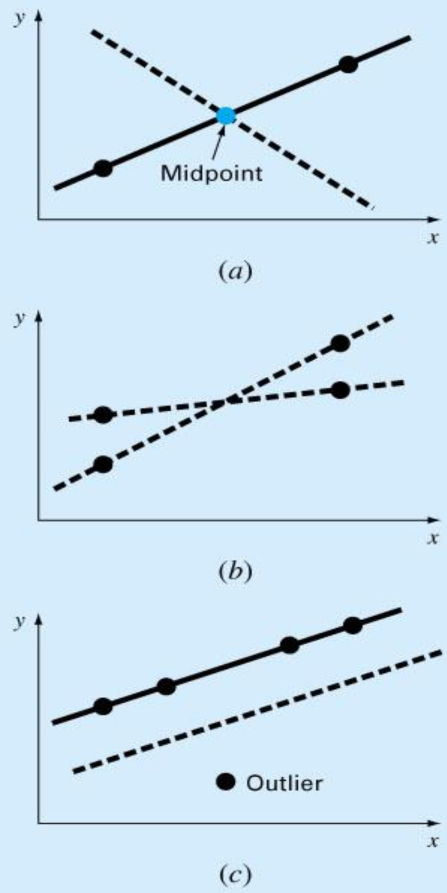
$y=a_0+a_1x+e$

a_1- slope

a_0- intercept

e- error, or residual, between the model and the observations

Criteria for a "Best" Fit



Minimize the sum of the residual errors for all available data:

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - a_o - a_1 x_i)$$

n = total number of points

However, this is an inadequate criterion, so is the sum of the absolute values

$$\sum_{i=1}^{n} |e_i| = \sum_{i=1}^{n} |y_i - a_0 - a_1 x_i|$$

Best strategy is to minimize the sum of the squares of the residuals between the measured y and the y calculated with the linear model:

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_{i,\text{measured}} - y_{i,\text{model}})^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$$

Yields a unique line for a given set of data.

List-Squares Fit of a Straight Line

$$\frac{\partial S_r}{\partial a_o} = -2\sum (y_i - a_o - a_1 x_i) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum \left[(y_i - a_o - a_1 x_i) x_i\right] = 0$$

$$0 = \sum y_i - \sum a_0 - \sum a_1 x_i \qquad \sum a_0 + \sum a_1 x_i = \sum y_i$$

$$0 = \sum y_i x_i - \sum a_0 x_i - \sum a_1 x_i^2 \qquad \sum a_0 x_i + \sum a_1 x_i^2 = \sum y_i x_i$$

$$\left.\begin{aligned} &\sum a_0 = n a_0 \\ &n a_0 + \left(\sum x_i\right) a_1 = \sum y_i \end{aligned}\right\}$$

Normal equations, can be solved simultaneously

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - \left(\sum x_i\right)^2}$$

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

Mean values

Example

Fit a straight line to the x and y values in the first two columns of the following table

x_i	y_i	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1x_i)^2$
1	0.5	8.5765	0.1687
2	2.5	0.8622	0.5625
3	2.0	2.0408	0.3473
4	4.0	0.3265	0.3265
5	3.5	0.0051	0.5896
6	6.0	6.6122	0.7972
7	5.5	4.2908	0.1993
Σ	24.0	22.7143	2.9911

$$n = 7 \qquad \sum x_i y_i = 119.5 \qquad \sum x_i^2 = 140$$

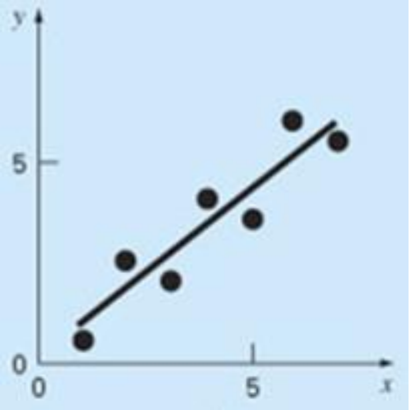
$$\sum x_i = 28 \qquad \bar{x} = \frac{28}{7} = 4$$

$$\sum y_i = 24 \qquad \bar{y} = \frac{24}{7} = 3.428571$$

$$a_1 = \frac{7(119.5) - 28(24)}{7(140) - (28)^2} = 0.8392857$$

$$a_0 = 3.428571 - 0.8392857(4) = 0.07142857$$

y=0.07142857+0.8392857x



Quantification of Error of Linear Regression

If

Total sum of the squares around the mean for the dependent variable, y, is S_t

Sum of the squares of residuals around the regression line is S_r

Then

S_t-S_r quantifies the improvement or error reduction due to describing data in terms of a straight line rather than as an average value.

$$r^2 = \frac{S_t - S_r}{S_t}$$

r^2-coefficient of determination

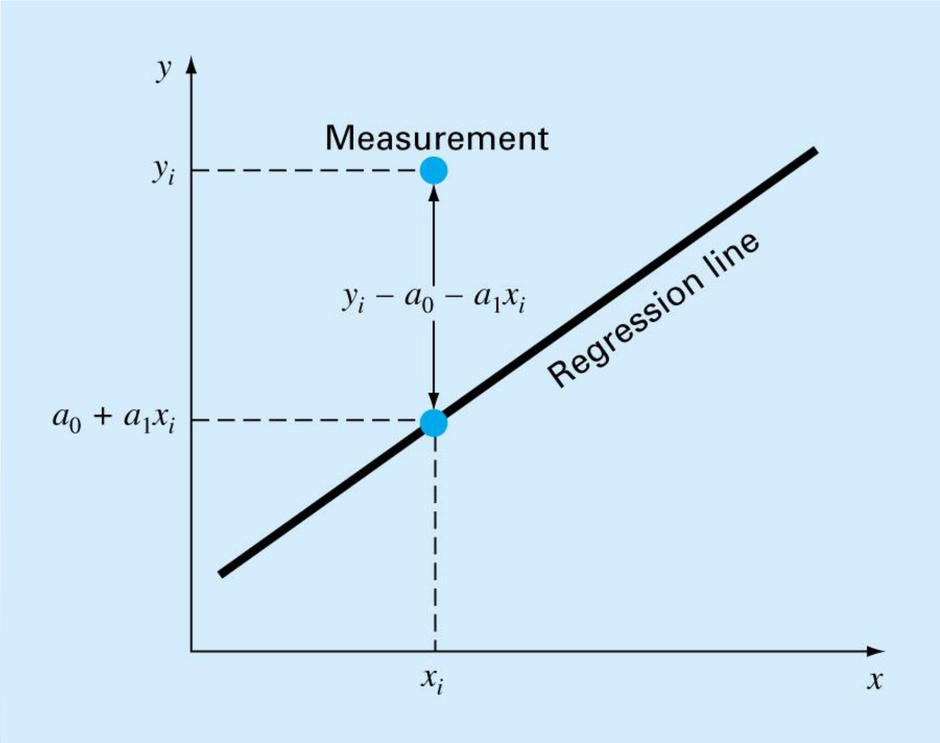
Sqrt(r^2) – correlation coefficient

For a perfect fit, S_r=0 and r=r2=1, signifying that the line explains 100 percent of the variability of the data.

For r=r2=0, S_r=S_t, the fit represents no improvement.

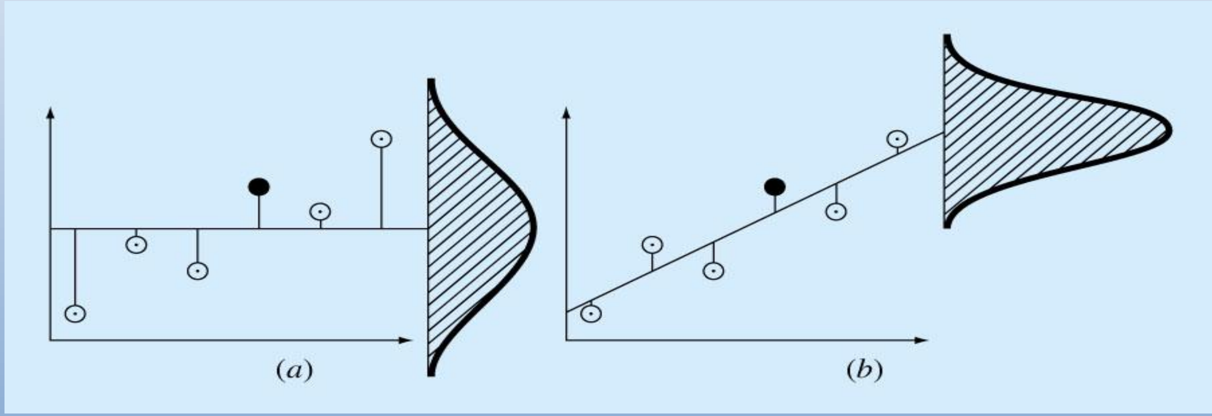
Quantification of Error of Linear Regression

The residual in linear regression represents the vertical distance between a data point and the straight line.



standard error of the estimate

$$s_{y/x} = \sqrt{\frac{S_r}{n-2}}$$



Example

Compute the total standard deviation, the standard error of the estimate and the correlation coefficient for the data in the following table

x_i	y_i	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1 x_i)^2$
1	0.5	8.5765	0.1687
2	2.5	0.8622	0.5625
3	2.0	2.0408	0.3473
4	4.0	0.3265	0.3265
5	3.5	0.0051	0.5896
6	6.0	6.6122	0.7972
7	5.5	4.2908	0.1993
Σ	24.0	22.7143	2.9911

Example

Solution:

The standard deviation is

$$s_y = \sqrt{\frac{22.7143}{7-1}} = 1.9457$$

and the standard error of the estimate is

$$s_{y/x} = \sqrt{\frac{2.9911}{7-2}} = 0.7735$$

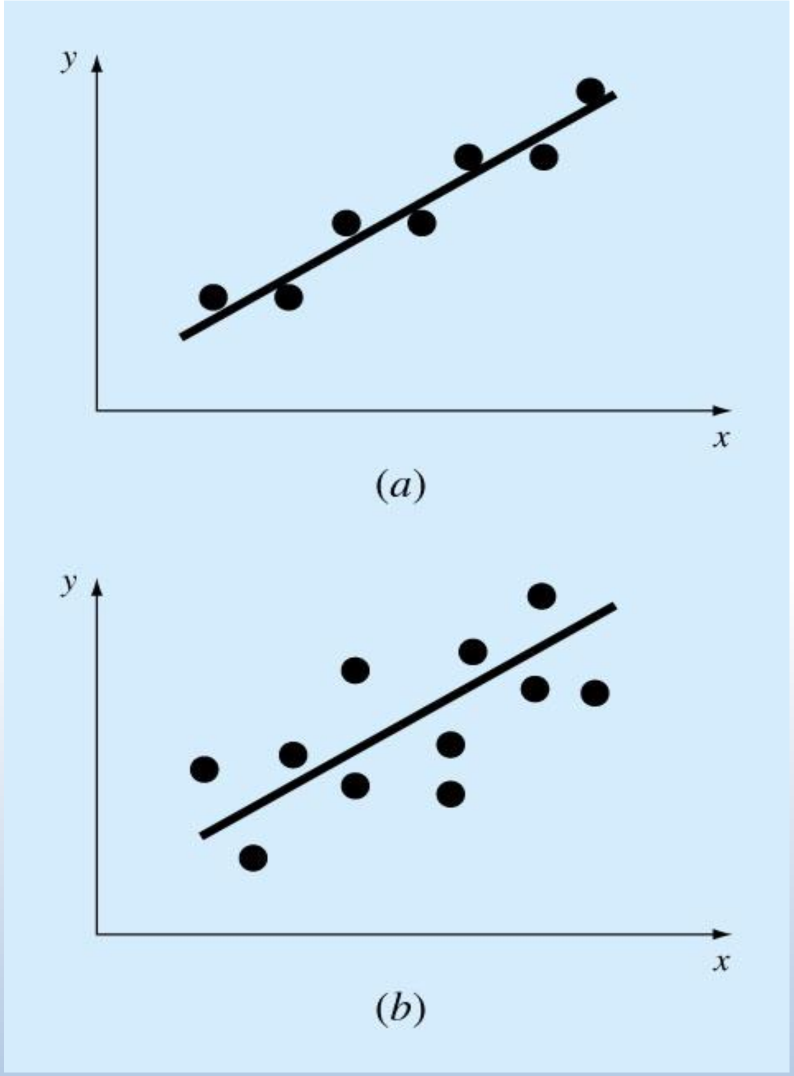
Thus, because $s_{y/x} < s_y$, the linear regression model has merit. The extent of the improvement is quantified by

$$r^2 = \frac{22.7143 - 2.9911}{22.7143} = 0.868$$

Or

$$r = \sqrt{0.868} = 0.932$$

These results indicate that 86.8 percent of the original uncertainty has been explained by the linear model.



Examples of linear regression with
(a) small residual errors
(b) large residual errors.

Polynomial Regression

Some engineering data is poorly represented by a straight line. For these cases a curve is better suited to fit the data.

The least squares method can readily be extended to fit the data to higher order polynomials.

Second-order polynomial

Suppose that we fit a second-order polynomial or quadratic

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

For this case the sum of the squares of the residuals is

$$S_r = \sum_{i=1}^{n} (y - a_0 - a_1 x_i - a_2 {x_i}^2)^2$$

we take the derivative for each of the unknown coefficients of the polynomial, as in

$$\frac{\partial S_r}{\partial a_o} = -2 \sum (y_i - a_o - a_1 x_i - a_2 x_i^2)$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum \left[(y_i - a_o - a_1 x_i - a_2 x_i^2) x_i \right]$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum \left[(y_i - a_o - a_1 x_i - a_2 x_i^2) x_i^2 \right]$$

Second-order polynomial

These equations can be set equal to zero and rearranged to develop the following set of normal equations:

$$\sum a_0 + \sum a_1 x_i + \sum a_2 x_i^2 = \sum y_i$$

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

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

For this case, the standard error is formulated as

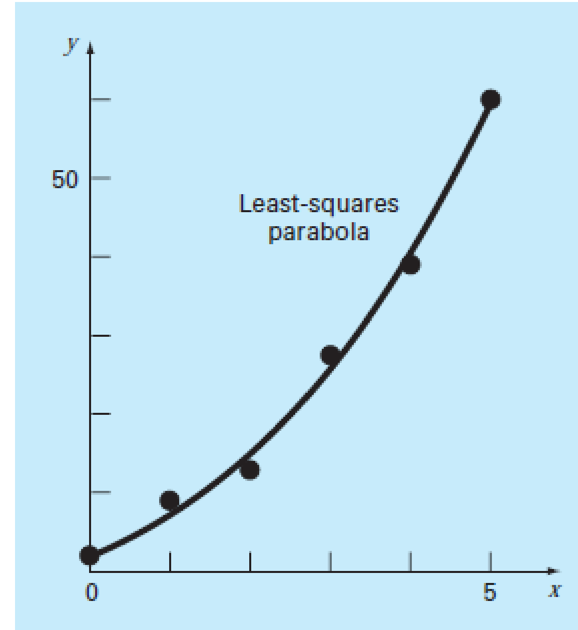
$$s_{y/x} = \sqrt{\frac{S_r}{n-(m+1)}}$$

Example

Fit a second-order polynomial to the data in the first two columns of the following table

x_i	y_i	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1x_i - a_2x_i^2)^2$
0	2.1	544.44	0.14332
1	7.7	314.47	1.00286
2	13.6	140.03	1.08158
3	27.2	3.12	0.80491
4	40.9	239.22	0.61951
5	61.1	1272.11	0.09439
Σ	152.6	2513.39	3.74657

Example



Solution:

From the given data,

$$m = 2 \qquad \sum x_i = 15 \qquad \sum x_i^4 = 979$$
$$n = 6 \qquad \sum y_i = 152.6 \qquad \sum x_i y_i = 585.6$$
$$\bar{x} = 2.5 \qquad \sum x_i^2 = 55 \qquad \sum x_i^2 y_i = 2488.8$$
$$\bar{y} = 25.433 \qquad \sum x_i^3 = 225$$

Therefore, the simultaneous linear equations are

$$\begin{bmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 152.6 \\ 585.6 \\ 2488.8 \end{Bmatrix}$$

Solving these equations through a technique such as Gauss elimination gives $a_0 = 2.47857$, $a_1 = 2.35929$, and $a_2 = 1.86071$. Therefore, the least-squares quadratic equation for this case is

$$y = 2.47857 + 2.35929x + 1.86071x^2$$

The standard error of the estimate based on the regression polynomial is

$$s_{y/x} = \sqrt{\frac{3.74657}{6-3}} = 1.12$$

The coefficient of determination is

$$r^2 = \frac{2513.39 - 3.74657}{2513.39} = 0.99851$$

and the correlation coefficient is $r = 0.99925$.

Multiple Linear Regression

A useful extension of linear regression is the case where y is a linear function of two or more independent variables. For example, y might be a linear function of x_1 and x_2, as in

$$y = a_0 + a_1 x_1 + a_2 x_2 + e$$

The sum of the squares of the residuals is

$$S_r = \sum_{i=1}^{n} (y - a_0 - a_1 x_{i1} - a_2 x_{2i})^2$$

and differentiating with respect to each of the unknown coefficients

$$\frac{\partial S_r}{\partial a_o} = -2 \sum (y_i - a_o - a_1 x_{1i} - a_2 x_{2i})$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum \left[(y_i - a_o - a_1 x_{1i} - a_2 x_{2i}) x_{1i} \right]$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum \left[(y_i - a_o - a_1 x_{1i} - a_2 x_{2i}) x_{2i} \right]$$

Multiple Linear Regression

The coefficients yielding the minimum sum of the squares of the residuals are obtained by

setting the partial derivatives equal to zero and expressing the result in matrix form as

$$\begin{bmatrix} n & \sum x_{1i} & \sum x_{2i} \\ \sum x_{1i} & \sum {x_{1i}}^2 & \sum x_{1ix2i} \\ \sum x_{2i} & \sum x_{1ix2i} & \sum {x_{2i}}^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_{1i} y_i \\ \sum x_{2i} y_i \end{bmatrix}$$

The standard error is formulated as

$$s_{y/x} = \sqrt{\frac{S_r}{n-(m+1)}}$$

Example

The following data was calculated from the equation $y = 5 + 4x1 - 3x2$

x_1	x_2	y
0	0	5
2	1	10
2.5	2	9
1	3	0
4	6	3
7	2	27

Example

Solution: Computations required to develop the normal equations for the problem

	y	x_1	x_2	x_1^2	x_2^2	x_1x_2	x_1y	x_2y
	5	0	0	0	0	0	0	0
	10	2	1	4	1	2	20	10
	9	2.5	2	6.25	4	5	22.5	18
	0	1	3	1	9	3	0	0
	3	4	6	16	36	24	12	18
	27	7	2	49	4	14	189	54
Σ	54	16.5	14	76.25	54	48	243.5	100

The result is

$$\begin{bmatrix} 6 & 16.5 & 14 \\ 16.5 & 76.25 & 48 \\ 14 & 48 & 54 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 54 \\ 243.5 \\ 100 \end{bmatrix}$$

which can be solved using a method such as Gauss elimination for $a_0=5$, $a_1=4$, $a_2=-3$

Algorithm for implementation of polynomial and multiple linear regression

Step 1: Input order of polynomial to be fit, m.

Step 2: Input number of data points, n.

Step 3: If $n < m + 1$, print out an error message that regression is impossible and terminate the process.

If $n \geq m + 1$, continue.

Step 4: Compute the elements of the normal equation in the form of an augmented matrix.

Step 5: Solve the augmented matrix for the coefficients $a_0, a_1, a_2, \ldots, a_m$, using an elimination method.

Step 6: Print out the coefficients.

General Linear Least Squares

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \cdots + a_m z_m + e$$

$z_0,\ z_1,\ \ldots,\ z_m$ are $m+1$ basis functions

$$\{Y\} = [Z]\{A\} + \{E\}$$

$[Z]$ – matrix of the calculated values of the basis functions at the measured values of the independent variable

$\{Y\}$ – observed valued of the dependent variable

$\{A\}$ – unknown coefficients

$\{E\}$ – residuals

$$S_r = \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{m} a_j z_{ji} \right)^2$$

Minimized by taking its partial derivative w.r.t. each of the coefficients and setting the resulting equation equal to zero

Nonlinear Regression

As with linear least squares, nonlinear regression is based on determining the values of the parameters that *minimize the sum of the squares of the residuals*. However, for the nonlinear case, *the solution must proceed in an iterative fashion*.

Ex: $f(x) = a_0(1 - e^{-a_1 x})$

The *Gauss-Newton method* is one algorithm for minimizing the sum of the squares of the residuals between data and nonlinear equations. The key concept underlying the technique is that a *Taylor series expansion* is used to express the original nonlinear equation in an approximate, linear form. Then*, least-squares theory* can be used to obtain new estimates of the parameters that move in the direction of minimizing the residual.

Nonlinear Regression

First, the relationship between the nonlinear equation and the data can be expressed generally as

$$y_i = f(x_i; a_0, a_1, \dots, am) + ei$$

where

y_i = a measured value of the dependent variable,

$f\ (x_i;\ a_0, a_1, \dots, a_m)$ = the equation that is a function of the independent variable xi and a nonlinear function of the parameters $a_0, a_1, \dots, a_m$, and

e_i = a random error

For convenience, this model can be expressed in abbreviated form by omitting the parameters,

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

The nonlinear model can be expanded in a Taylor series around the parameter values and curtailed after the first derivative.

Nonlinear Regression

For example, for a two-parameter case,

$$f(x_i)_{j+1} = f(x_i)_j + \frac{\partial f(xi)_j}{\partial a_0}\Delta a_0 + \frac{\partial f(xi)_j}{\partial a_1}\Delta a_1$$

where

j = the initial guess,

j + 1 = the prediction,

$\Delta a_0 = a_{0,j+1} - a_{0,j}$,

$\Delta a_1 = a_{1,\,j+1} - a_{1,\,j}$.

Thus, we have linearized the original model with respect to the parameters

$$y_i - f(x_i)_j = \frac{\partial f(xi)_j}{\partial a_0}\Delta a_0 + \frac{\partial f(xi)_j}{\partial a_1}\Delta a_1 + e_i$$

Nonlinear Regression

Or in matrix form

$$\{D\} = [Z_j]\{\Delta A\} + \{E\}$$

where

- [Zj] is the matrix of partial derivatives of the function evaluated at the initial guess j,

$$[Zj] = \begin{bmatrix} \dfrac{\partial f_1}{\partial a_0} & \dfrac{\partial f_1}{\partial a_1} \\ \dfrac{\partial f_2}{\partial a_0} & \dfrac{\partial f_2}{\partial a_1} \\ \vdots & \vdots \\ \dfrac{\partial fn}{\partial a_0} & \dfrac{\partial fn}{\partial a_1} \end{bmatrix}$$

where

n = the number of data points and

$\partial f_i/\partial a_k$ = the partial derivative of the function with respect to the kth parameter evaluated at the ith data point.

Nonlinear Regression

- The vector {D} contains the differences between the measurements and the function values,

$$\{D\} = \begin{Bmatrix} y_1 - f(x_1) \\ y_1 - f(x_1) \\ \vdots \\ y_1 - f(x_1) \end{Bmatrix}$$

- The vector {ΔA} contains the changes in the parameter values,

$$\{\Delta A\} = \begin{Bmatrix} \Delta a_0 \\ \Delta a_1 \\ \vdots \\ \Delta a_m \end{Bmatrix}$$

We have $[Z_j]^T\{D\} = [Z_j]^T[Z_j]\{\Delta A\}$

Thus, solving the above equation for {ΔA},

$$\{A\}_{j+1} = \{A\}_j + \{\Delta A\}$$

This procedure is repeated until the solution converges—that is, until $|\varepsilon_a|_k < \varepsilon_s$

$$|\varepsilon_a|_k = \left| \frac{a_{k,j+1} - a_{k,j}}{a_{k,j+1}} \right| 100\%$$

Example

Fit the function $f(x; a_0, a_1) = a_0(1 - e^{-a1x})$ to the data:

x	0.25	0.75	1.25	1.75	2.25
y	0.28	0.57	0.68	0.74	0.79

Use initial guesses of a_0=1.0 and a_1=1.0 for the parameters. Note that for these guesses, the initial sum of the squares of the residuals is 0.0248.

The partial derivatives of the function with respect to the parameters are

$$\frac{\partial f}{\partial a_0} = 1 - e^{-a_1 x}$$

and

$$\frac{\partial f}{\partial a_1} = a_0 x e^{-a_1 x}$$

$$[Z_0] = \begin{bmatrix} 0.2212 & 0.1947 \\ 0.5276 & 0.3543 \\ 0.7135 & 0.3581 \\ 0.8262 & 0.3041 \\ 0.8946 & 0.2371 \end{bmatrix}$$

This matrix multiplied by its transpose results in

$$[Z_0]^T[Z_0] = \begin{bmatrix} 2.3193 & 0.9489 \\ 0.9489 & 0.4404 \end{bmatrix}$$

which in turn can be inverted to yield

$$[[Z_0]^T[Z_0]]^{-1} = \begin{bmatrix} 3.6397 & -7.8421 \\ -7.8421 & 19.1678 \end{bmatrix}$$

The vector {D} consists of the differences between the measurements and the model predictions,

$$\{D\} = \begin{Bmatrix} 0.28 - 0.2212 \\ 0.57 - 0.5276 \\ 0.68 - 0.7135 \\ 0.74 - 0.8262 \\ 0.79 - 0.8946 \end{Bmatrix} = \begin{Bmatrix} 0.0588 \\ 0.0424 \\ -0.0335 \\ -0.0862 \\ -0.1046 \end{Bmatrix}$$

It is multiplied by $[Z_0]^T$ to give

$$[Z_0]^T\{D\} = \begin{bmatrix} -0.1533 \\ -0.0365 \end{bmatrix}$$

The vector $\{\Delta A\}$ is then calculated by solving Eq. (17.35) for

$$\Delta A = \begin{Bmatrix} -0.2714 \\ 0.5019 \end{Bmatrix}$$

which can be added to the initial parameter guesses to yield

$$\begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix} + \begin{Bmatrix} -0.2714 \\ 0.5019 \end{Bmatrix} = \begin{Bmatrix} 0.7286 \\ 1.5019 \end{Bmatrix}$$

The computation would then be repeated until these values fell below the prescribed stopping criterion. The final result is a_0 = 0.79186 and a_1 = 1.6751. These coefficients give a sum of the squares of the residuals of 0.000662

PART B

INTERPOLATION

Interpolation

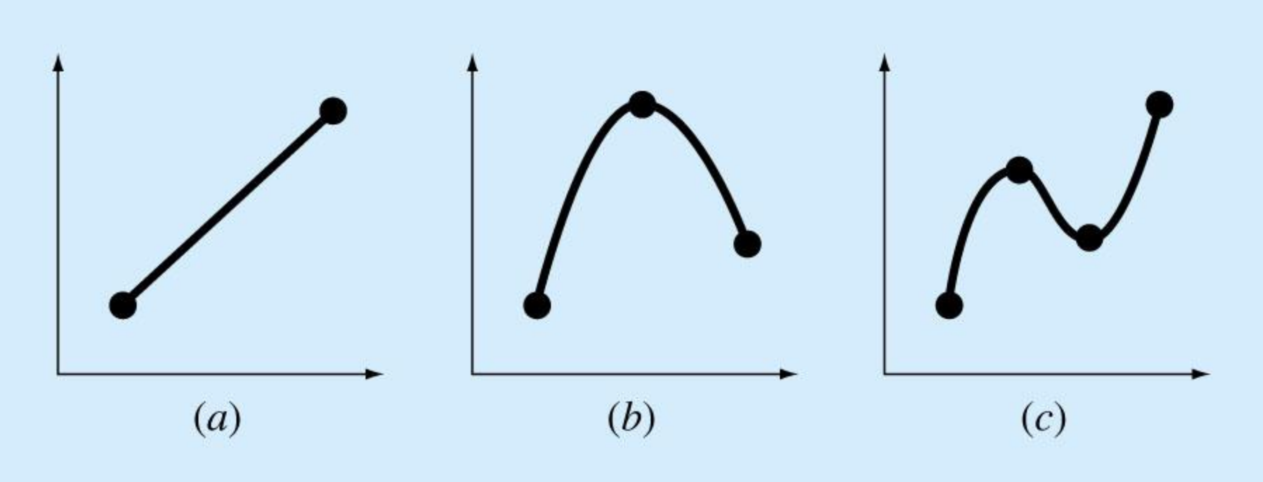
Estimation of intermediate values between precise data points. The most common method is:

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

Although there is one and only one *n*th-order polynomial that fits *n+1* points, there are a variety of mathematical formats in which this polynomial can be expressed:

The Newton polynomial

The Lagrange polynomial



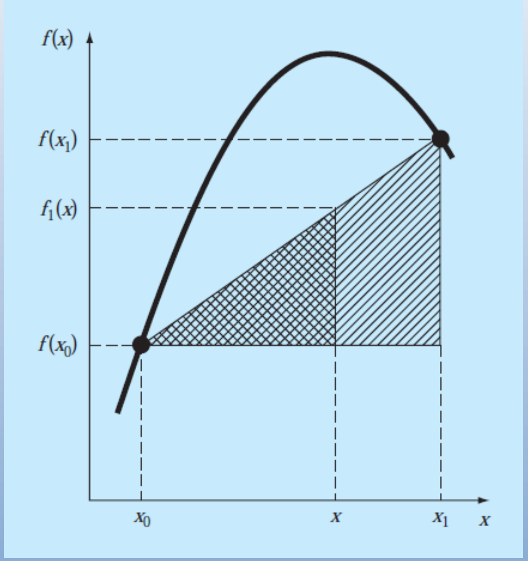
Linear Interpolation

Linear Interpolation is the simplest form of interpolation, connecting two data points with a straight line.

$$\frac{f_1(x) - f(x_0)}{x - x_0} = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$f_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0)$$

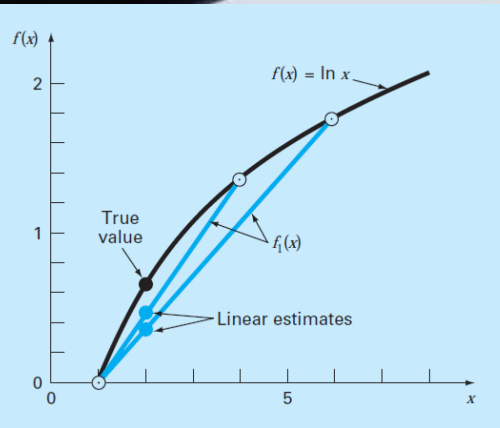
$f_1(x)$ designates that this is a first-order interpolating polynomial.



The shaded areas indicate the similar triangles used to derive the linear-interpolation formula

Example

Estimate the natural logarithm of 2 using linear interpolation. First, perform the computation by interpolating between In1=0 and In6=1.791759. Then, repeat the procedure, but use a smaller interval from In 1 to In4 (1.386294). Note that the true value of In 2 is 0.6931472.



We use a linear interpolation for In(2) from x0=1 and x1=9 to give

$$f_1(2) = 0 + \frac{1.791759 - 0}{6 - 1}(2 - 1) = 0.3583519$$

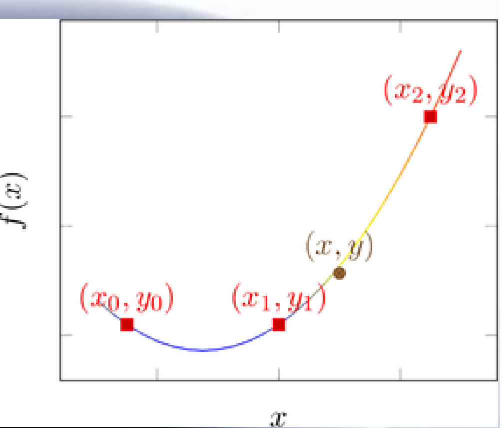
which represents an error of ε_t = 48.3%.

Using the smaller interval from x0 = 1 to x1 = 4 yields

$$f_1(2) = 0 + \frac{1.386294 - 0}{4 - 1}(2 - 1) = 0.4620981$$

Thus, using the shorter interval reduces the percent relative error to ε_t = 33.3%.

Quadratic Interpolation



If three data points are available, the estimate is improved by introducing some curvature into the line connecting the points.

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

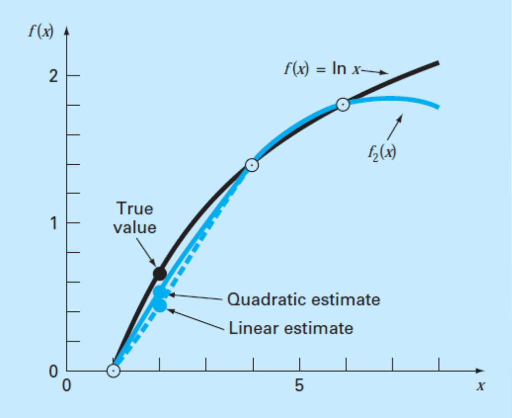
A simple procedure can be used to determine the values of the coefficients.

$$x = x_0 \qquad b_0 = f(x_0)$$

$$x = x_1 \qquad b_1 = \frac{f(x_1) - f(x_0)}{x - x_0}$$

$$x = x_2 \qquad b_2 = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$

Example



Fit a second-order polynomial to the three points used in the above example:

x0 = 1 f(x0) = 0

x1 = 4 f(x1) = 1.386294

x2 = 6 f(x2) = 1.791759

Use the polynomial to evaluate ln 2.

$$b0 = 0$$

$$b1 = \frac{1.386294 - 0}{4 - 1} = 0.4620981$$

$$b2 = \frac{\frac{1.791759 - 1.386294}{6 - 4} - 0.4620981}{6 - 1} = -0.0518731$$

So,

$$f2(x) = 0 + 0.4620981(x - 1) - 0.0518731(x - 1)(x - 4)$$

which can be evaluated at x=2 for

$$f2(2) = 0.5658444$$

which represents a relative error of εt = 18.4%.

General Form of Newton's Interpolating Polynomials

$$f_n(x) = f(x_0) + (x - x_0) f[x_1, x_0] + (x - x_0)(x - x_1) f[x_2, x_1, x_0] \\ + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1}) f[x_n, x_{n-1}, \cdots, x_0]$$

$$\begin{aligned} b_0 &= f(x_0) \\ b_1 &= f[x_1, x_0] \\ b_2 &= f[x_2, x_1, x_0] \\ &\vdots \\ b_n &= f[x_n, x_{n-1}, \cdots, x_1, x_0] \end{aligned}$$

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

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

$$\vdots$$

$$f[x_n, x_{n-1}, \ldots, x_1, x_0] = \frac{f[x_n, x_{n-1}, \ldots, x_1] - f[x_{n-1}, x_{n-2}, \ldots, x_0]}{x_n - x_0}$$

General Form of Newton's Interpolating Polynomials

i	x_i	$f(x_i)$	First	Second	Third
0	x_0	$f(x_0)$	$f[x_1, x_0]$	$f[x_2, x_1, x_0]$	$f[x_3, x_2, x_1, x_0]$
1	x_1	$f(x_1)$	$f[x_2, x_1]$	$f[x_3, x_2, x_1]$	
2	x_2	$f(x_2)$	$f[x_3, x_2]$		
3	x_3	$f(x_3)$			

Newton's divided-difference interpolating polynomial

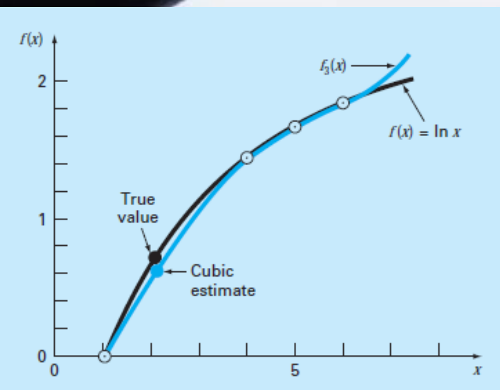
$$f_n(x) = f(x_0) + (x - x_0)f[x_1, x_0] + (x - x_0)(x - x_1)f[x_2, x_1, x_0] + \cdots$$
$$+ (x - x_0)(x - x_1)\cdots(x - x_{n-1})f[x_n, x_{n-1}, \ldots, x_0]$$

Errors of Newton's Interpolating Polynomials

$$R_n \cong f[x_{n+1}, x_n, x_{n-1}, \ldots, x_0](x - x_0)(x - x_1)\cdots(x - x_n)$$

Example

In the previous example, data points at x0=1, x1=4, and x2=6 were used to estimate ln2 with a parabola. Now, adding a fourth point [x3=5; f(x3)=1.609438], estimate ln2 with a third-order Newton's interpolating polynomial.



The third-order polynomial with n=3 is

$$f_3(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1) + b_3(x - x_0)(x - x_1)(x - x_2)$$

The first divided differences for the problem are [Eq. (18.12)]

$$f[x_1, x_0] = \frac{1.386294 - 0}{4 - 1} = 0.4620981$$

$$f[x_2, x_1] = \frac{1.791759 - 1.386294}{6 - 4} = 0.2027326$$

$$f[x_3, x_2] = \frac{1.609438 - 1.791759}{5 - 6} = 0.1823216$$

The second divided differences are

$$f[x_2, x_1, x_0] = \frac{0.2027326 - 0.4620981}{6 - 1} = -0.05187311$$

$$f[x_3, x_2, x_1] = \frac{0.1823216 - 0.2027326}{5 - 4} = -0.02041100$$

The third divided difference is [Eq. (18.14) with $n = 3$]

$$f[x_3, x_2, x_1, x_0] = \frac{-0.02041100 - (-0.05187311)}{5 - 1} = 0.007865529$$

The results for $f[x_1, x_0]$, $f[x_2, x_1, x_0]$, and $f[x_3, x_2, x_1, x_0]$ represent the coefficients b_1, b_2, and b_3, respectively

$$f_3(x) = 0 + 0.4620981(x - 1) - 0.05187311(x - 1)(x - 4) + 0.007865529(x - 1)(x - 4)(x - 6)$$

which can be used to evaluate f3(2) = 0.6287686, which represents a relative error of εt = 9.3%.

Lagrange Interpolating Polynomials

The Lagrange interpolating polynomial is simply a reformulation of the Newton's polynomial that avoids the computation of divided differences:

$$f_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i)$$

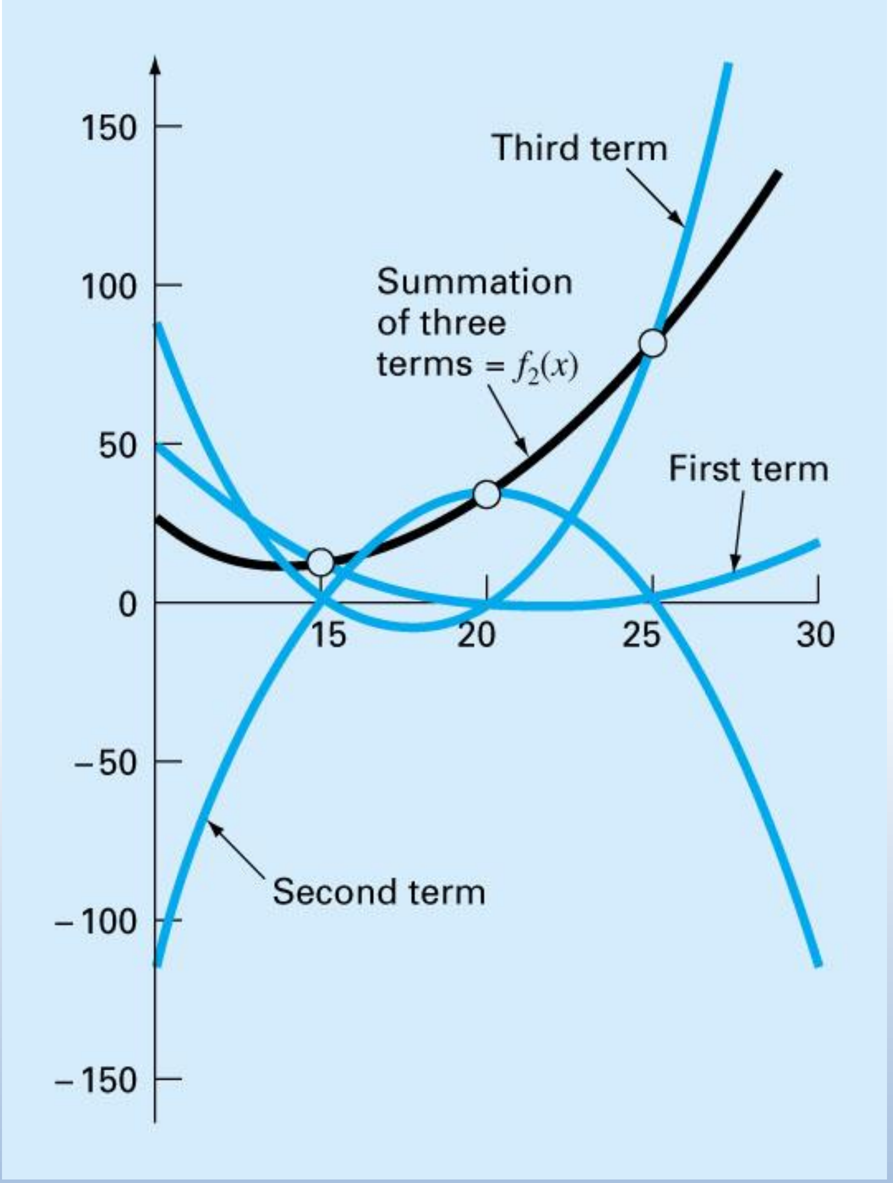
$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$$f_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

$$f_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

•As with Newton’s method, the Lagrange version has an estimated error of:

$$R_n = f[x, x_n, x_{n-1}, \ldots, x_0] \prod_{i=0}^{n} (x - x_i)$$


150
100
50
0
−50
−100
−150
15
20
25
30
Third term
Summation
of three
terms = $f_2(x)$
First term
Second term

Example

Use a Lagrange interpolating polynomial of the first and second order to evaluate ln 2 on the basis of the data such as

x0 = 1 f(x0) = 0

x1 = 4 f(x1) = 1.386294

x2 = 6 f(x2) = 1.791760

The first-order polynomial can be used to obtain the estimate at x = 2,

$$f_1(2) = \frac{2-4}{1-4}0 + \frac{2-1}{4-1}1.386294 = 0.4620981$$

In a similar fashion, the second-order polynomial is developed as

$$\begin{aligned} f_2(2) &= \frac{(2-4)(2-6)}{(1-4)(1-6)}0 + \frac{(2-1)(2-6)}{(4-1)(4-6)}1.386294 \\ &+ \frac{(2-1)(2-4)}{(6-1)(6-4)}1.791760 = 0.5658444 \end{aligned}$$

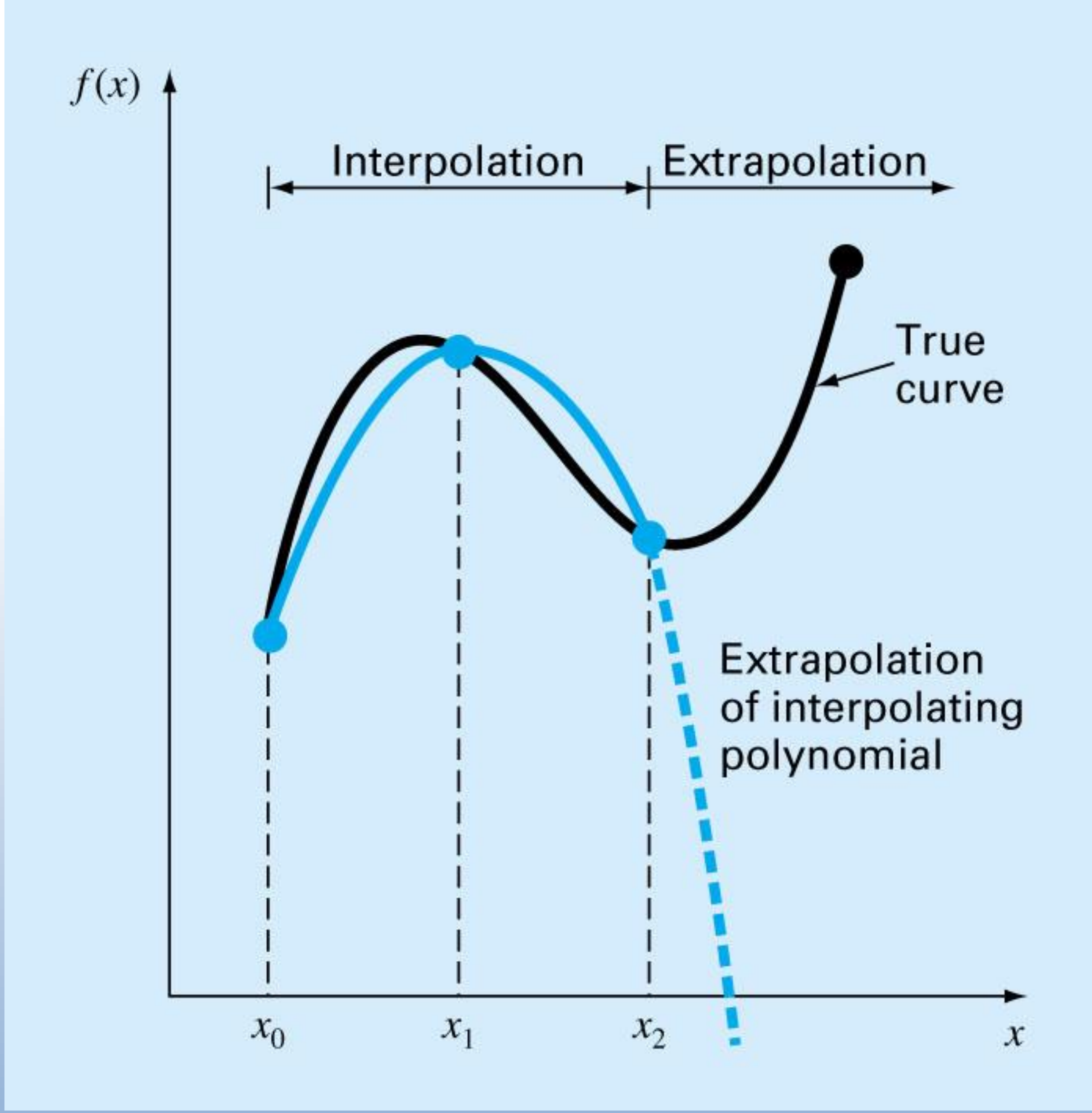
Coefficients of an Interpolating Polynomial

Although both the Newton and Lagrange polynomials are well-suited for determining intermediate values between points, *they do not provide a polynomial in conventional form*:

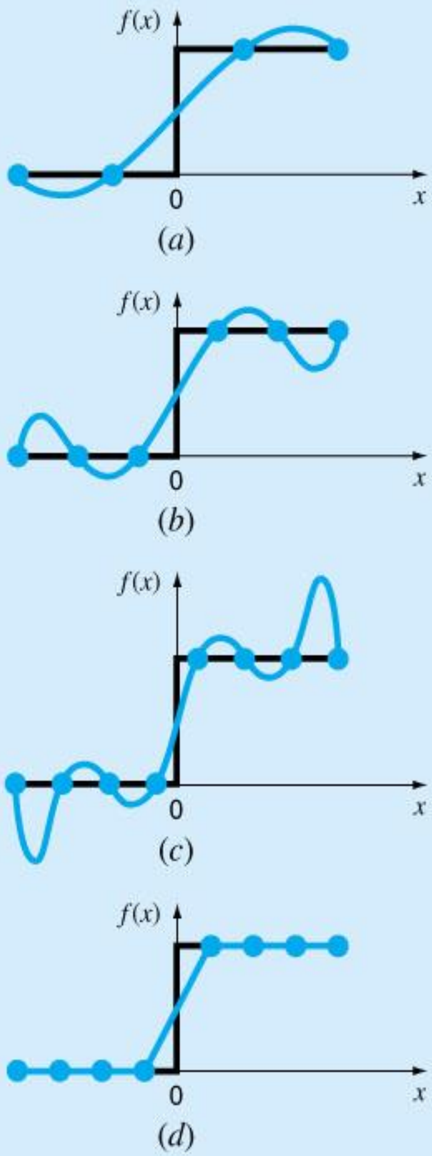
$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_x x^n$$

Since *n+1* data points are required to determine *n+1* coefficients, simultaneous linear systems of equations can be used to calculate “*a*”s.

If you are interested in determining an intermediate point, employ Newton or Lagrange interpolation.



f(x)
Interpolation
Extrapolation
True
curve
Extrapolation
of interpolating
polynomial
x_0
x_1
x_2
x



Spline Interpolation

There are cases where polynomials can lead to erroneous results because of round off error and overshoot.

Alternative approach is to *apply lower-order polynomials to subsets of data points.* Such connecting polynomials are called spline functions.

A visual representation of a situation where the splines are superior to higher-order interpolating polynomials. The function to be fit undergoes an abrupt increase at x= 0.
Parts (a) through (c) indicate that the abrupt change induces oscillations in interpolating polynomials.
In contrast, because it is limited to third-order curves with smooth transitions, a linear spline (d) provides a much more acceptable approximation.

Linear Spline

The simplest *connection between two points is a straight line*. The first-order splines for a group of ordered data points can be defined as a set of linear functions,

$f(x) = f(x_0) + m_0(x - x_0) \qquad x_0 \leq x \leq x_1$

$f(x) = f(x_1) + m_1(x - x_1) \qquad x_1 \leq x \leq x_2$

.

.

.

$f(x) = f(x_{n-1}) + m_{n-1}(x - x_{n-1}) \qquad x_{n-1} \leq x \leq x_n$

where m_i is the slope of the straight line connecting the points:

$$m_i = \frac{f(x_{i+1}) - f(xi)}{x_{i+1} - xi}$$

Example

Fit the data in the following table with first-order splines. Evaluate the function at x = 5.

x	$f(x)$
3.0	2.5
4.5	1.0
7.0	2.5
9.0	0.5

The data can be used to determine the slopes between points. For example, for the interval x = 4.5 to x = 7 the slope can be computed

$$m = \frac{2.5 - 1}{7 - 4.5} = 0.6$$

The value at x = 5 is 1.3.

Quadratic Spline

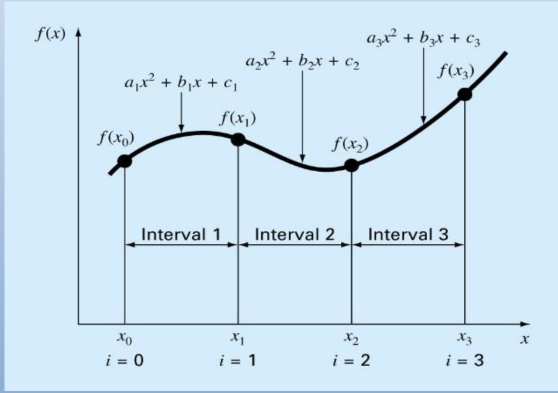
The objective in quadratic splines is to derive a second-order polynomial for each interval between data points. The polynomial for each interval can be represented generally as

$$f_i(x) = aix^2 + bix + c_i$$

1. *The function values of adjacent polynomials must be equal at the interior knots*. This condition can be represented as

$a_{i-1}x^2_{i-1} + b_{i-1}x_{i-1} + c_{i-1} = f(xi_{-1})$
$a_i x^2_{i-1} + bixi_{-1} + c_i = f(xi_{-1})$
for i = 2 to n. Because only interior knots are used, each equation provide n − 1 conditions for a total of 2n − 2 conditions.

2. *The first and last functions must pass through the end points*. This adds two additional equations:
$a_1x^2_0 + b_1x_0 + c_1 = f(x_0)$
$a_nx^2_n + bnxn + cn = f(x_n)$
for a total of 2n − 2 + 2 = 2n conditions.



Quadratic Spline

3. *The first derivatives at the interior knots must be equal*. The first derivative of f(x) is

$$f_i'(x) = 2a_i x + b_i$$

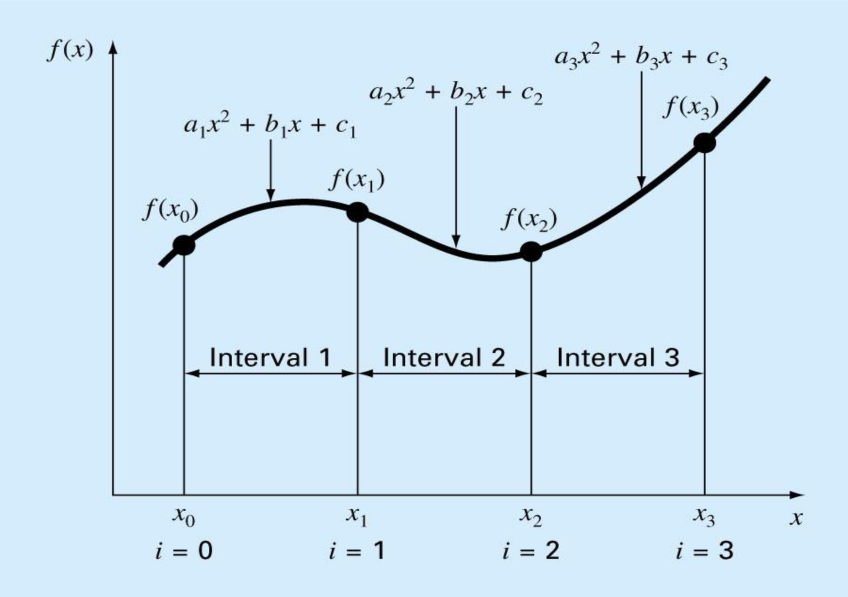
Therefore, the condition can be represented generally as

$$2a_{i-1}x_{i-1} + b_{i-1} = 2a_i x_{i-1} + b_i$$

for i = 2 to n. This provides another n − 1 conditions for a total of 2n + n − 1 = 3n − 1.

4. *Assume that the second derivative is zero at the first point*. Because the second derivative of $f_i(x)$ is $2a_i$, this condition can be expressed mathematically as

$$a_1 = 0$$



Example

Fit quadratic splines to the same data used in the following table. Use the results to estimate the value at x = 5.

x	$f(x)$
3.0	2.5
4.5	1.0
7.0	2.5
9.0	0.5

For the present problem, we have four data points and n=3 intervals. Therefore, 3(3)=9 unknowns must be determined. Constraint #1 yields 2(3) − 2 = 4 conditions:

$$20.25a_1 + 4.5b_1 + c_1 = 1.0$$
$$20.25a_2 + 4.5b_2 + c_2 = 1.0$$
$$49a_2 + 7b_2 + c_2 = 2.5$$
$$49a_3 + 7b_3 + c_3 = 2.5$$

Passing the first and last functions through the initial and final values adds 2 more (Constraint #2):

$$9a_1 + 3b_1 + c_1 = 2.5$$
$$81a_3 + 9b_3 + c_3 = 0.5$$

Example

Continuity of derivatives creates an additional 3 − l = 2 (Constraint #3):

$$9a1 + b1 = 9a2 + b2$$
$$14a2 + b2 = 14a3 + b3$$

Finally, Constraint #4 specifies that a1 = 0. Because this equation specifies a1 exactly, the problem reduces to solving eight simultaneous equations. These conditions can be expressed in matrix form as

$$\begin{bmatrix} 4.5 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 20.25 & 4.5 & 1 & 0 & 0 & 0 \\ 0 & 0 & 49 & 7 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 49 & 7 & 1 \\ 3 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 81 & 9 & 1 \\ 1 & 0 & -9 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 14 & 1 & 0 & -14 & -1 & 0 \end{bmatrix} \begin{Bmatrix} b1 \\ c1 \\ a2 \\ b2 \\ c2 \\ a3 \\ b3 \\ c3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 1 \\ 2.5 \\ 2.5 \\ 2.5 \\ 0.5 \\ 0 \\ 0 \end{Bmatrix}$$

These equations can be solved using techniques from Part Three, with the results:

$$a1 = 0 \quad b1 = -1 \quad c1 = 5.5$$
$$a2 = 0.64 \quad b2 = -6.76 \quad c2 = 18.46$$
$$a3 = -1.6 \quad b3 = 24.6 \quad c3 = -91.$$

which can be substituted into the original quadratic equations to develop the following relationships for each interval:

$$f1(x) = -x + 5.5 \quad 3.0 \leq x \leq 4.5$$
$$f2(x) = 0.64x2 - 6.76x + 18.46 \quad 4.5 \leq x \leq 7.0$$
$$f3(x) = -1.6x2 + 24.6x - 91.3 \quad 7.0 \leq x \leq 9.0$$

When we use f2, the prediction for x = 5 is, therefore,

$$f2(5) = 0.64(5)2 - 6.76(5) + 18.46 = 0.66$$

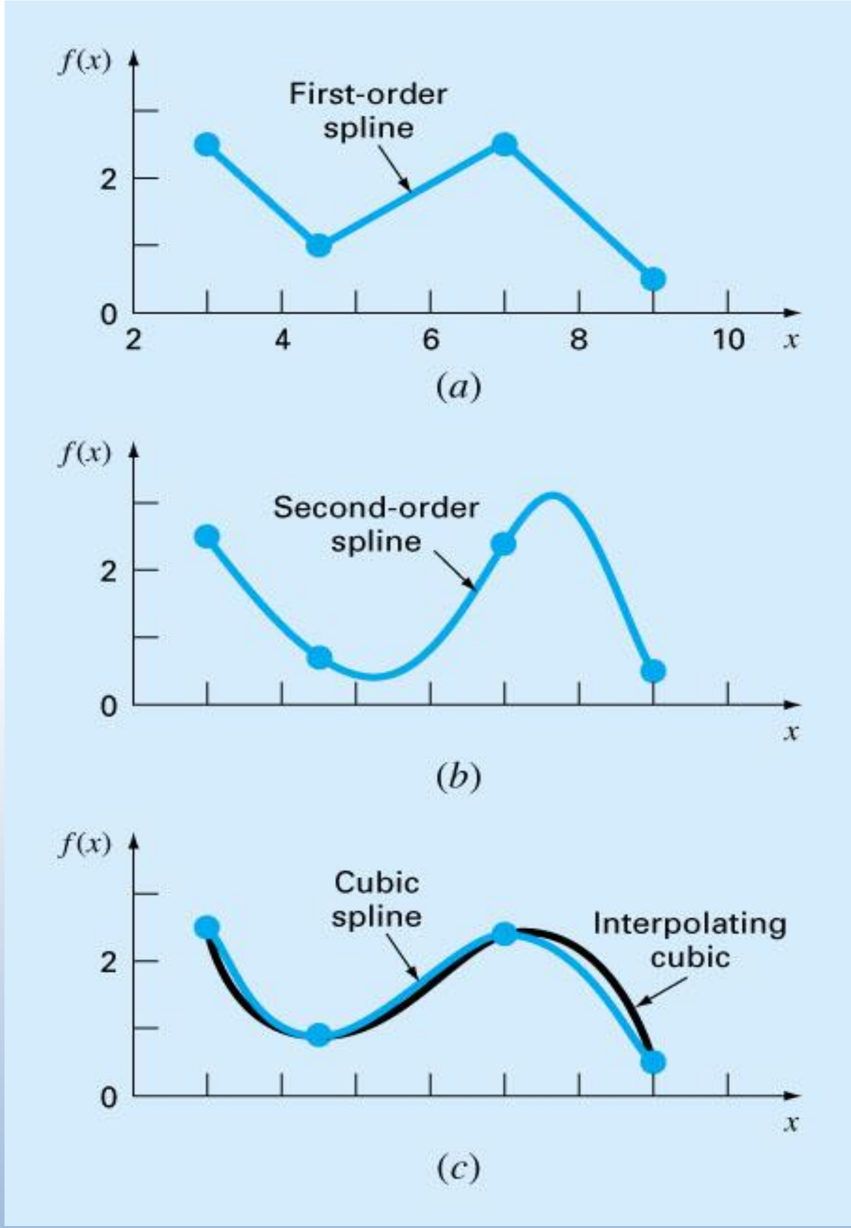
Cubic Splines

The objective in cubic splines is to derive a third-order polynomial for each interval between knots, as in

$$f_i(x) = a_i x^3 + bix^2 + cix + di$$

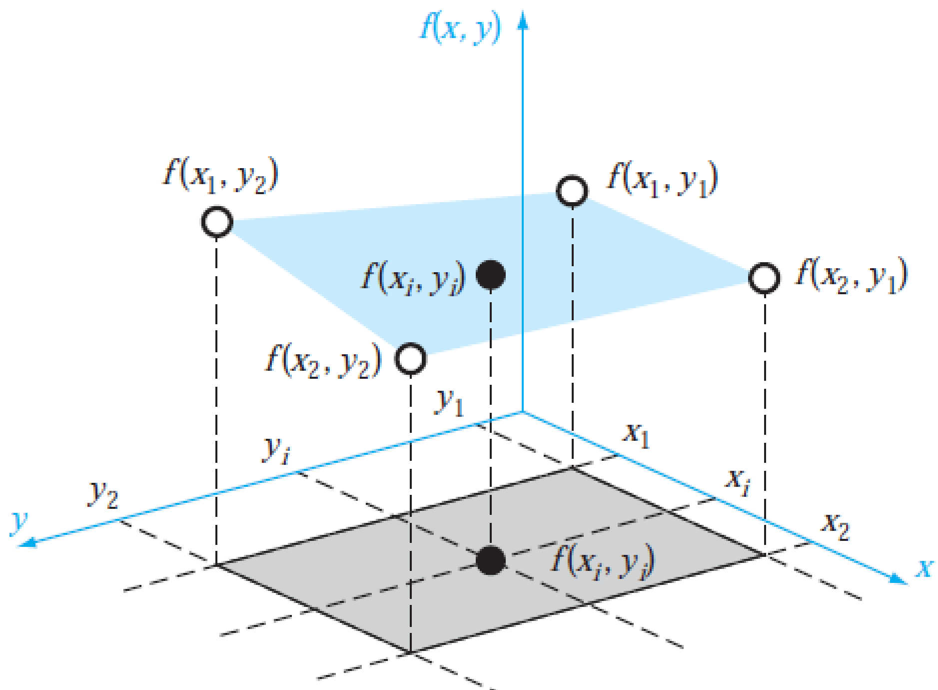
Thus, for n + 1 data points (i = 0, 1, 2, . . . , n), there are n intervals and, consequently, *4n unknown constants* to evaluate. Just as for quadratic splines, 4n conditions are required to evaluate the unknowns. These are:

1. The function values must be equal at the interior knots (2n − 2 conditions).
2. The first and last functions must pass through the end points (2 conditions).
3. The first derivatives at the interior knots must be equal (n − 1 conditions).
4. The second derivatives at the interior knots must be equal (n − 1 conditions).
5. The second derivatives at the end knots are zero (2 conditions).


f(x)
First-order
spline
2
0
2
4
6
8
10
x
(a)
f(x)
Second-order
spline
2
0
x
(b)
f(x)
Cubic
spline
Interpolating
cubic
2
0
x
(c)

MULTIDIMENSIONAL INTERPOLATION

The interpolation methods for one-dimensional problems can be extended to multidimensional interpolation. In the present section, we will describe the simplest case of two dimensional interpolation in Cartesian coordinates.



Bilinear Interpolation

First, we can hold the y value fixed and apply one-dimensional linear interpolation in the x direction. Using the Lagrange form, the result at (xi, y1) is

$$f(xi, y1) = \frac{xi - x2}{x1 - x2} f(x1, y1) + \frac{xi - x1}{x2 - x1} f(x2, y1)$$

And at (xi,y2) is

$$f(xi, y2) = \frac{xi - x2}{x1 - x2} f(x1, y2) + \frac{xi - x1}{x2 - x1} f(x2, y2)$$

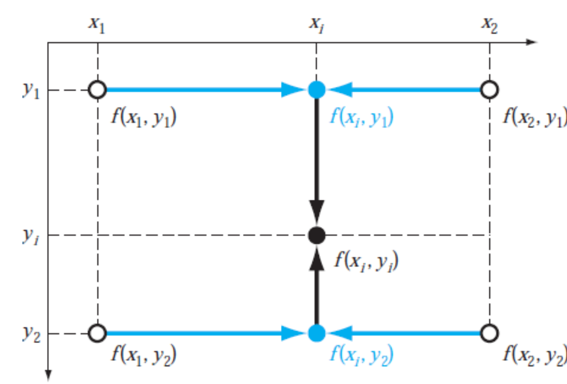
These points can then be used to linearly interpolate along the y dimension to yield the final result,

$$f(xi, yi) = \frac{yi - y2}{y1 - y2} f(xi, y1) + \frac{yi - y1}{y2 - y1} f(xi, y2)$$

A single equation can be developed

$$f(xi, yi) = \frac{xi - x2}{x1 - x2} \frac{yi - y2}{y1 - y2} f(x1, y1) + \frac{xi - x1}{x2 - x1} \frac{yi - y2}{y1 - y2} f(x21, y1)$$

$$+ \frac{xi-x2}{x1-x2} \frac{yi-y1}{y2-y1} f(x1, y2) + \frac{xi-x1}{x2-x1} \frac{yi-y1}{y2-y1} f(x1, y1)$$



Any Questions?

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