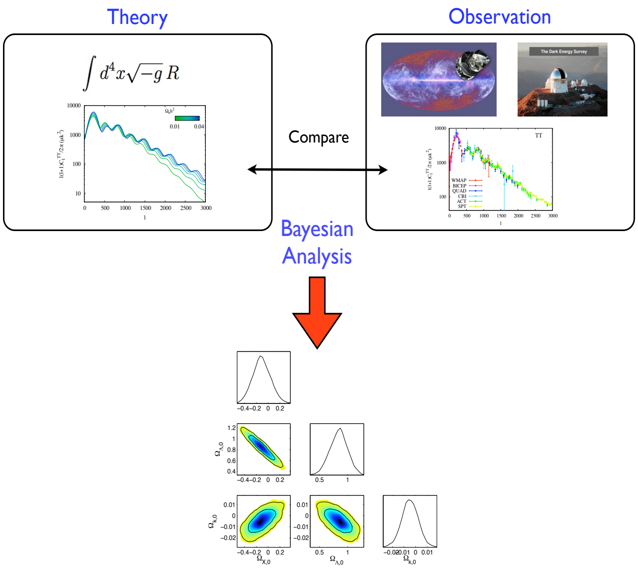
Numerical Methods



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1

Curve Fitting

Data are often given for discrete values along a continuum. However, you may require estimates at points between the discrete values.

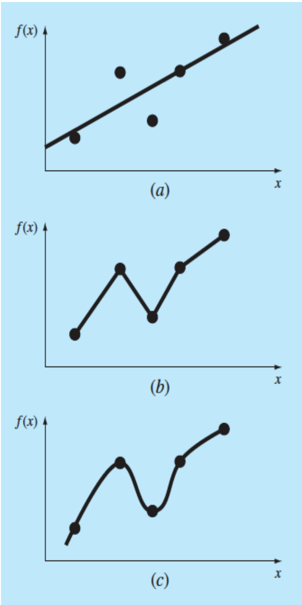
1. Any individual data point may be incorrect, we make no effort to intersect every point. Rather, the curve is designed to follow the pattern of the points taken as a group: least-squares regression.

2. These data are known to be very precise, the basic approach is to fit a curve or a series of curves that pass directly through each of the points: interpolation.

Two types of applications are generally encountered when fitting experimental data: trend analysis and hypothesis testing.

- Trend analysis may be used to predict or forecast values of the dependent variable. This can involve extrapolation beyond the limits of the observed data or interpolation within the range of the data.

- Hypothesis testing: an existing mathematical model is compared with measured data. If the model coefficients are unknown, it may be necessary to determine values that best fit the observed data. Often, alternative models are compared and the 'best' one is selected on the basis of empirical observations.



1.1 Simple Statistics

The arithmetic mean ($\bar{y}$) of a sample is defined as the sum of the individual data points (y_i) divided by the number of points (n), or

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

The most common measure of spread for a sample is the **standard deviation** (s_y) about the mean

$$s_y = \sqrt{\frac{\sum (y_i - \bar{y})^2}{n-1}}$$

or the **variance**:

$$s_y^2 = \frac{\sum (y_i - \bar{y})^2}{n-1}$$

with $n-1$ degrees of freedom.

To compute the standard deviation

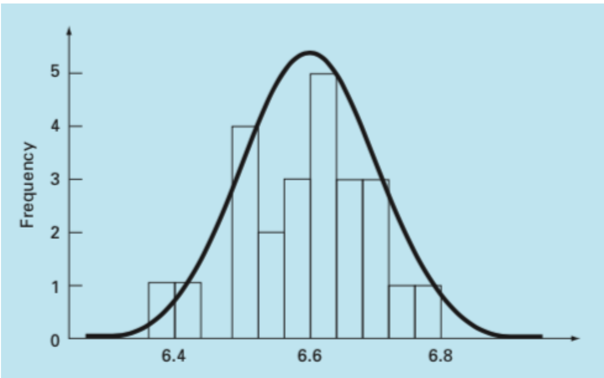
$$s_y^2 = \frac{\sum y_i^2 - (\sum y_i)^2/n}{n-1}$$

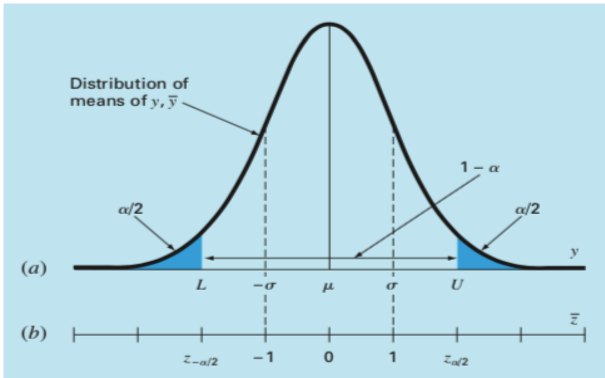
Notice that it does not require precomputation of $\bar{y}$.

1.2 The Normal Distribution

The shape with which these data are spread around the mean. A histogram provides a simple visual representation of the distribution.

If a quantity is normally distributed, the range defined by $y - s_y$ to $y + s_y$ will encompass approximately 68 percent of the total measurements. Similarly, the range defined by $y - 2s_y$ to $y + 2s_y$ will encompass approximately 95 percent.
Because we "infer" properties of the unknown population from a limited sample, the endeavor is called **statistical inference**. Because the results are often reported as estimates of the population parameters, the process is also referred to as **estimation**.





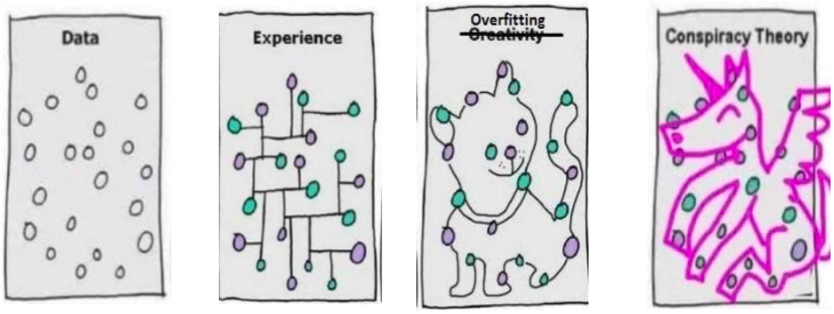
The probability that the true mean of y, μ, falls within the bound from L to U is $1 - \alpha$.
kurtosis, skewness, etc.

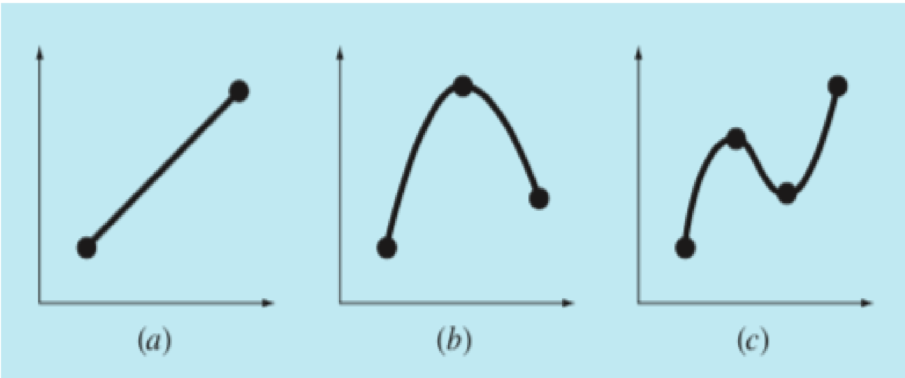
1.3 Interpolation

You will frequently have occasion to estimate intermediate values between precise data points. For $n + 1$ data points, there is one and only one polynomial of order n that passes through all the points.

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

Polynomial interpolation consists of determining the unique nth-order polynomial that fits $n + 1$ data points.





1.3.1 Linear Interpolation

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

$$\frac{f_1(x) - f(x_0)}{x - x_0} = \frac{f(x_1) - f(x_0)}{x_1 - x_0}, \tag{1.1}$$

which can be rearranged to yield

$$f_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0), \tag{1.2}$$

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

1.3.2 Quadratic Interpolation

If three data points are available, this can be accomplished with a second-order polynomial (also called a quadratic polynomial or a parabola)

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1), \tag{1.3}$$

can be expressed as

$$f_2(x) = a_0 + a_1 x + a_2 x^2 \tag{1.4}$$

where

$$\begin{aligned} a_0 &= b_0 - b_1 x_0 + b_2 x_0 x_1, & (1.5) \\ a_1 &= b_1 - b_2 x_0 - b_2 x_1, & (1.6) \\ a_2 &= b_2. & (1.7) \end{aligned}$$

To determine the values of the coefficients

$$b_0 = f(x_0), \tag{1.8}$$

$$b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}, \tag{1.9}$$

$$b_2 = \frac{\frac{f(x_2)-f(x_1)}{x_2-x1} - \frac{f(x_1)-f(x_0)}{x_1-x_0}}{x_2 - x_0}, \tag{1.10}$$

Similar to the finite-divided-difference approximation of the second derivative.

1.3.3 General Form of Newton's Interpolating Polynomials

1.4 Lagrange Polynomial

The problem of determining a polynomial of degree one that passes through the distinct points (x_0, y_0) and (x_1, y_1) is the same as approximating a function f for which $f(x_0) = y_0$ and $f(x_1) = y_1$.

We define the functions

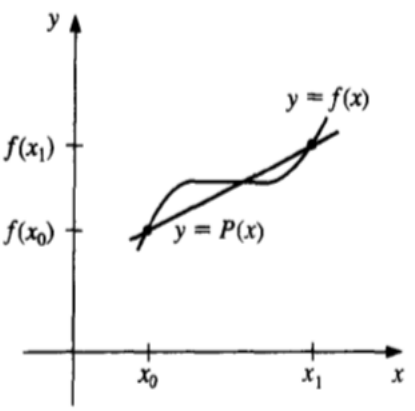
$$L_0(x) = \frac{x - x_1}{x_0 - x_1} \qquad \text{and} \qquad L_1(x) = \frac{x - x_0}{x_1 - x_0}, \tag{1.11}$$

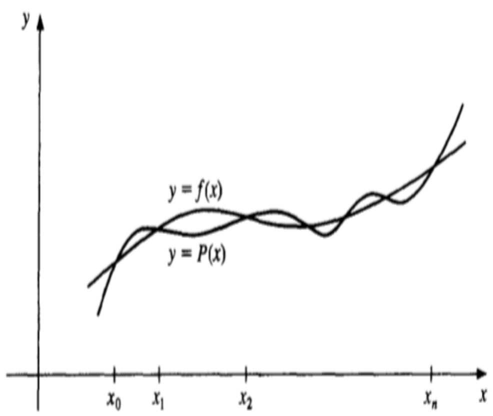
and define

$$P(x) = L_0(x) f(x_0) + L_1(x) f(x_1). \tag{1.12}$$

To generalize the concept of linear interpolation, consider the construction of a polynomial of degree at most n that passes through the $n+1$ points.

x	$f(x)$	First divided differences	Second divided differences	Third divided differences
x_0	$f[x_0]$			
		$f[x_0, x_1] = \dfrac{f[x_1] - f[x_0]}{x_1 - x_0}$		
x_1	$f[x_1]$		$f[x_0, x_1, x_2] = \dfrac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$	
		$f[x_1, x_2] = \dfrac{f[x_2] - f[x_1]}{x_2 - x_1}$		$f[x_0, x_1, x_2, x_3] = \dfrac{f[x_1, x_2, x_3] - f[x_0, x_1, x_2]}{x_3 - x_0}$
x_2	$f[x_2]$		$f[x_1, x_2, x_3] = \dfrac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1}$	
		$f[x_2, x_3] = \dfrac{f[x_3] - f[x_2]}{x_3 - x_2}$		$f[x_1, x_2, x_3, x_4] = \dfrac{f[x_2, x_3, x_4] - f[x_1, x_2, x_3]}{x_4 - x_1}$
x_3	$f[x_3]$		$f[x_2, x_3, x_4] = \dfrac{f[x_3, x_4] - f[x_2, x_3]}{x_4 - x_2}$	
		$f[x_3, x_4] = \dfrac{f[x_4] - f[x_3]}{x_4 - x_3}$		$f[x_2, x_3, x_4, x_5] = \dfrac{f[x_3, x_4, x_5] - f[x_2, x_3, x_4]}{x_5 - x_2}$
x_4	$f[x_4]$		$f[x_3, x_4, x_5] = \dfrac{f[x_4, x_5] - f[x_3, x_4]}{x_5 - x_3}$	
		$f[x_4, x_5] = \dfrac{f[x_5] - f[x_4]}{x_5 - x_4}$		
x_5	$f[x_5]$			





Theorem: If $x_0, x_1, \ldots, x_n$ are $n+1$ distinct numbers and f is a function whose values are given at these numbers, then a unique polynomial $P(x)$ of degree at most n exists with $f(x_k) = P(x_k)$, for each $k = 0, 1, \ldots, n$.

The polynomial is given by

$$P(x) = f(x_0)L_{n,0}(x) + \cdots + f(x_n)L_{n,n}(x) = \sum_{k=0}^{n} f(x_k)L_{n,k}(x), \tag{1.13}$$

where, for each $k = 0, 1, \ldots, n$.

$$
\begin{aligned}
L_{n,k}(x) &= \frac{(x - x_0)(x - x_1)\cdots(x - x_{k-1})(x - x_{k+1})\cdots(x - x_n)}{(x_k - x_0)(x_k - x_1)\cdots(x_k - x_{k-1})(x_k - x_{k+1})\cdots(x_k - x_n)} && (1.14)\\
&= \prod_{i=0, i\neq k}^{n} \frac{x - x_i}{x_k - x_i}. && (1.15)
\end{aligned}
$$

for cases where the order of the polynomial is unknown, the Newton method has advantages because of the insight it provides into the behavior of the different-order formulas. Lagrange version is somewhat easier to program. Because it does not require computation and storage of divided differences, the Lagrange form is often used when the order of the polynomial is known a priori. (here: wiki for hermite)

1.5 Splines

In the previous sections, nth-order polynomials were used to interpolate between $n + 1$ data points. An alternative approach is to apply lower-order polynomials to subsets of data points. Such connecting polynomials are called spline functions.

1.6 Quadratic Splines

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

$$f_i(x) = a_i x^2 + b_i x + c_i,$$

For $n + 1$ data points, there are n intervals and, consequently, $3n$ unknown constants to evaluate. Therefore, $3n$ equations or conditions are required to evaluate the unknowns. These are:

1. The function values of adjacent polynomials must be equal at the interior knots.

$$
\begin{aligned}
a_{i-1}x_{i-1}^2 + b_{i-1}c_{i-1} + c_{i-1} &= f(x_{i-1}) && (1.16)\\
a_i x_{i-1}^2 + b_i x_{i-1} + c_i &= f(x_{i-1}). && (1.17)
\end{aligned}
$$

   for $i = 2$ to n. Because only interior knots are used, each equation provides $n-1$ conditions for a total of $2n - 2$ conditions.

If $f \in C^1[a, b]$ and $x_0, \ldots, x_n \in [a, b]$ are distinct, the unique polynomial of least degree agreeing with f and f' at $x_0, \ldots, x_n$ is the Hermite polynomial of degree at most $2n + 1$ given by

$$H_{2n+1}(x) = \sum_{j=0}^{n} f(x_j) H_{n,j}(x) + \sum_{j=0}^{n} f'(x_j) \hat{H}_{n,j}(x),$$

where

$$H_{n,j}(x) = [1 - 2(x - x_j) L'_{n,j}(x_j)] L^2_{n,j}(x)$$

and

$$\hat{H}_{n,j}(x) = (x - x_j) L^2_{n,j}(x).$$

In this context, $L_{n,j}(x)$ denotes the jth Lagrange coefficient polynomial of degree n defined in Eq. (3.2).

Moreover, if $f \in C^{2n+2}[a, b]$, then

$$f(x) = H_{2n+1}(x) + \frac{(x - x_0)^2 \ldots (x - x_n)^2}{(2n + 2)!} f^{(2n+2)}(\xi),$$

for some ξ with $a < \xi < b$. ∎

2. The first and last functions must pass through the end points.

$$a_1 x_0^2 + b_1 x_0 + c_1 = f(x_0) \tag{1.18}$$

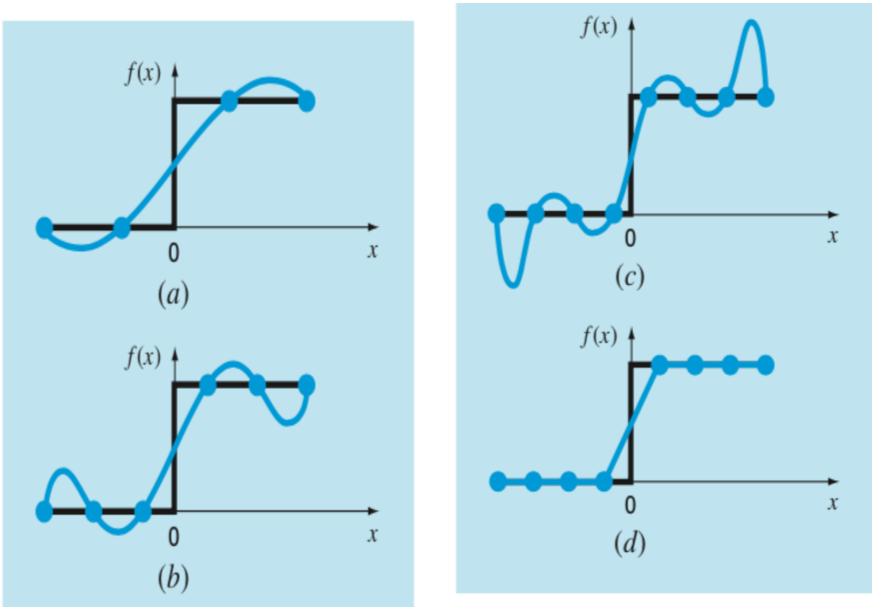
$$a_n x_n^2 + b_n x_n + c_n = f(x_n) \tag{1.19}$$

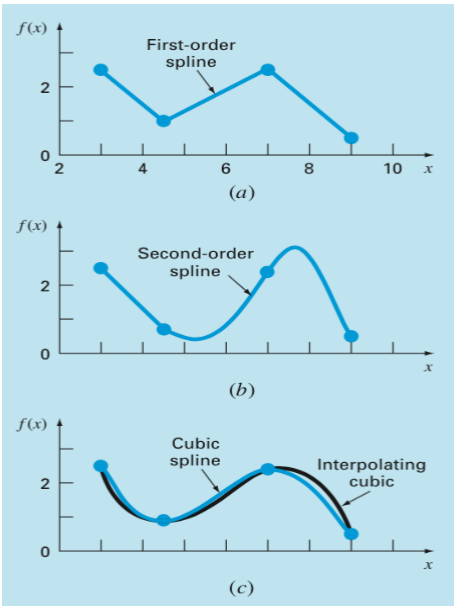
$$\tag{1.20}$$

total of $2n - 2 + 2 = 2n$ conditions.

3. The first derivatives at the interior knots must be equal.

$$2a_{i-1} x_{i-1} + b_{i-1} = 2a_i x_{i-1} + b_i \tag{1.21}$$

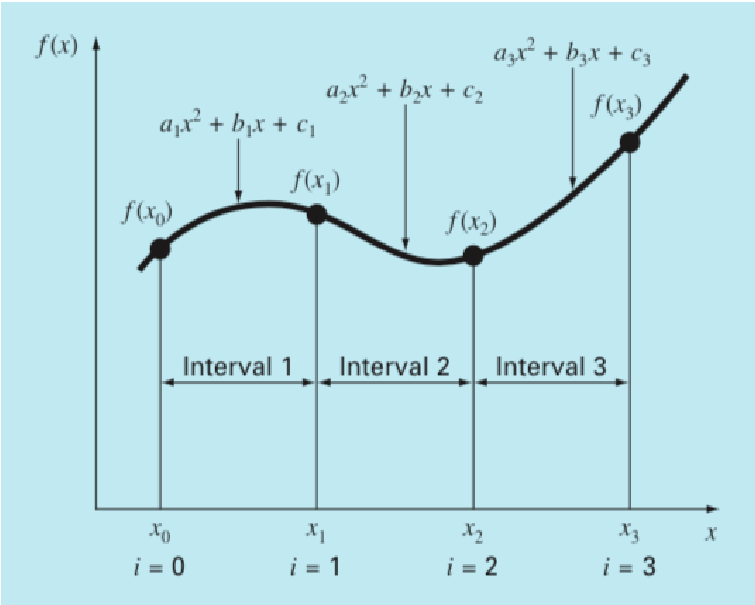




for $i = 2$ to n. This provides another $n - 1$ conditions for a total of $2n + n - 1 = 3n - 1$. Because we have $3n$ unknowns.

4. Assume that the second derivative is zero at the first point.

$$a_1 = 0. \tag{1.22}$$



1.6.1 Bilinear Interpolation

1.7 Least-Squares Regression

Where substantial error is associated with data, polynomial interpolation is inappropriate and may yield unsatisfactory results when used to predict intermediate values.

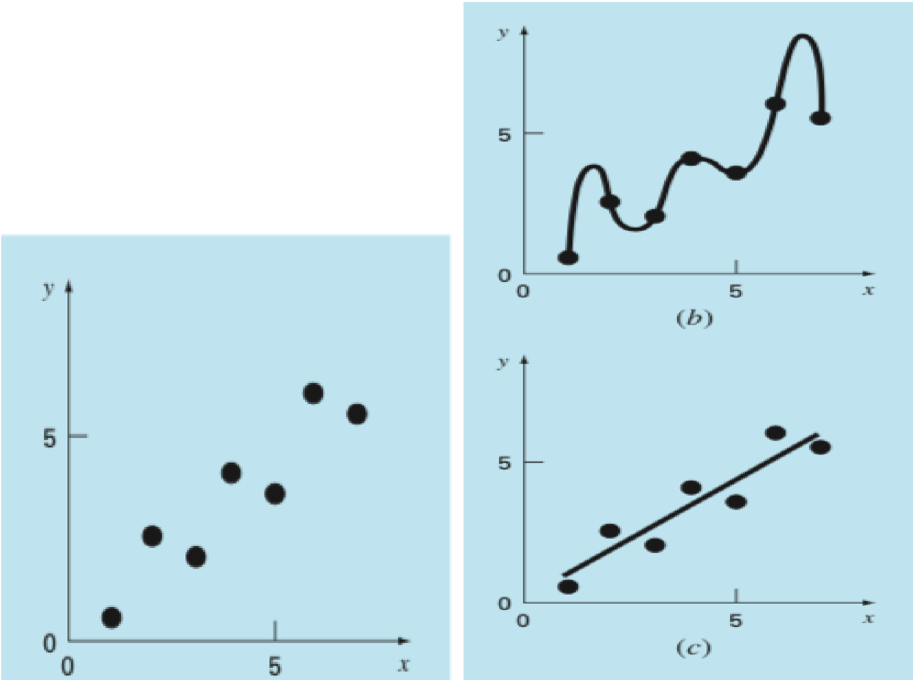
A more appropriate strategy for such cases is to derive an approximating function that fits the shape or general trend of the data without necessarily matching the individual points.

One way to do this is to derive a curve that minimizes the discrepancy between the data points and the curve. A technique for accomplishing this objective, called least- squares regression

1.7.1 Linear Regression

The simplest example of a least-squares approximation is fitting a straight line to a set of paired observations

$$y = a_0 + a_1 x + e$$



The error, or residual, is the discrepancy between the true value of y and the approximate value, predicted by the linear equation.

There are several criteria to minimize of the residual errors.

Minimize the sum of the squares of the residuals between the measured y and the y calculated with the linear model

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

Determining the values of a_0 and a_1 that minimizes this equation.

1.7.2 Least-Squares Fit of a Straight Line

$$\frac{\partial S_r}{\partial a_0} = -2 \sum (y_i - a_0 - a_1 x_i) \tag{1.23}$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum [(y_i - a_0 - a_1 x_i) x_i] \tag{1.24}$$

Setting these derivatives equal to zero will result in a minimum S_r.

$$0 = \sum y_i - \sum a_0 - \sum a_1 x_i \tag{1.25}$$

$$0 = \sum y_i x_i - \sum a_0 x_i - \sum a_1 x_i^2] \tag{1.26}$$

Now, realizing that $\sum a_0 = na_0$

$$na_0 + a_1 \left(\sum x_i\right) = \sum y_i \tag{1.27}$$

$$a_0 \left(\sum x_i\right) + a_1 \left(\sum x_i^2\right) = \sum y_i x_i \tag{1.28}$$

These are called the normal equations, and can be solved simultaneously

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

and

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

This is called the maximum likelihood principle in statistics.

The standard error of the estimate

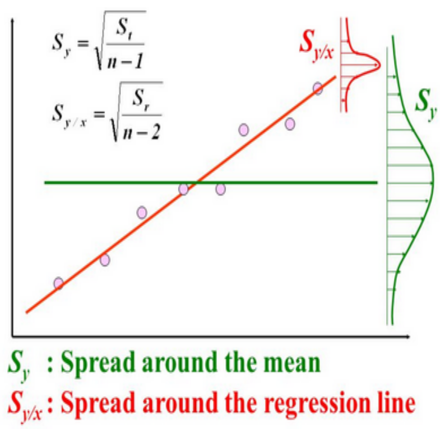
$$s_{y/x} = \sqrt{\frac{S_r}{n-2}}$$

quantifies the spread around the regression line. This concept can be used to quantify the "goodness" of our fit.

The difference between the two quantities, $S_t - S_r$, quantifies the improvement or error reduction due to describing the data in terms of a straight line rather than as an average value. $[S_t = \sum (y_i - \bar{y})^2]$

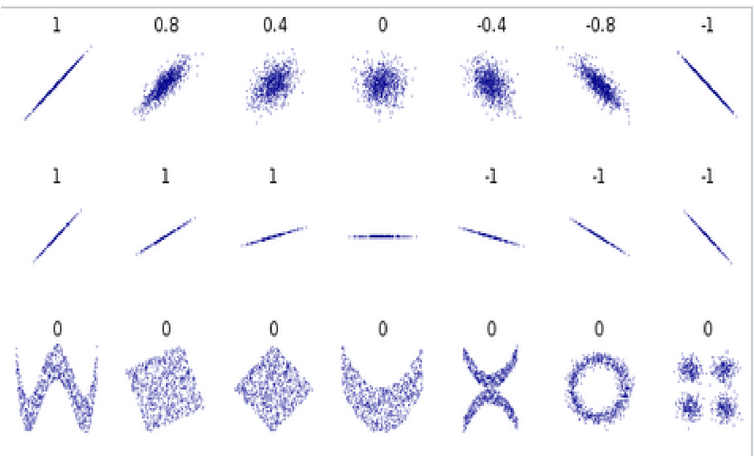
$$r^2 = \frac{S_t - S_r}{S_t}$$

where r^2 is called the coefficient of determination and r is the correlation coefficient For a perfect fit, $S_r = 0$ and $r = 1$, signifying that the line explains 100 percent of the variability of the data. For $r = 0$, $S_r = S_t$ and the fit represents no improvement.



Pearson correlation coefficient

$$r = \frac{n\sum x_i y_i - (\sum x_i)(\sum y_i)}{\sqrt{(n\sum x_i^2 - (\sum x_i)^2)(n\sum y_i^2 - (\sum y_i)^2)}}$$



1.7.3 Linearization of Nonlinear Relationships

In some cases, techniques such as polynomial regression, are appropriate. For others, transformations can be used to express the data in a form that is compatible with linear regression.

One example is the exponential model

$$y = a_1 e^{bx}$$

Another example of a nonlinear model is the simple power equation

$$y = a_2 x^b$$

$$E = \sum_{i=1}^{m} (y_i - b e^{a x_i})^2, \quad \text{in the case of Eq. (8.4),}$$

or

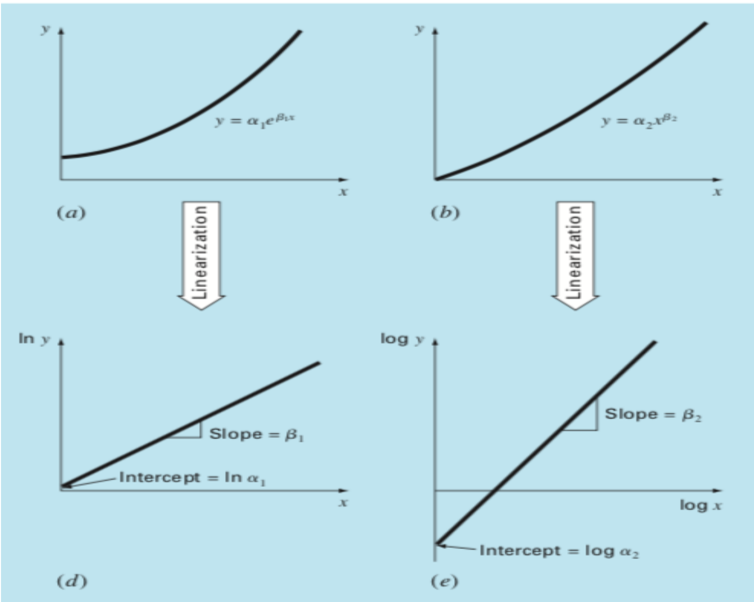
$$E = \sum_{i=1}^{m} (y_i - b x_i^a)^2, \quad \text{in the case of Eq. (8.5).}$$

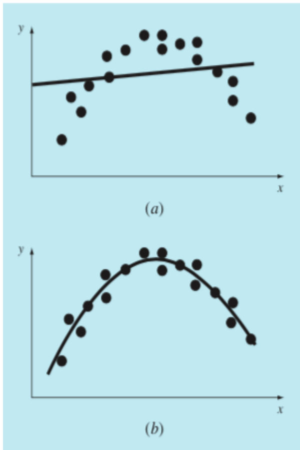
$$\ln y = \ln b + a x, \quad \text{in the case of Eq. (8.4),}$$

and

$$\ln y = \ln b + a \ln x, \quad \text{in the case of Eq. (8.5).}$$

No exact solution to either of these systems in a and b can generally be found.





1.7.4 Polynomial Regression

The least-squares procedure can be readily extended to fit the data to a higher-order polynomial. For example, suppose that we fit a second-order polynomial or quadratic

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

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

$$\frac{\partial S_r}{\partial a_0} = -2\sum(y_i - a_0 - a_1 x_i - a_2 x_i^2) \tag{1.29}$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum[(y_i - a_0 - a_1 x_i - a_2 x_i^2)x_i] \tag{1.30}$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum[(y_i - a_0 - a_1 x_i - a_2 x_i^2)x_i^2] \tag{1.31}$$

$$na_0 + a_1\left(\sum x_i\right) + (\sum x_i^2)a_2 = \sum y_i \tag{1.32}$$

$$a_0\left(\sum x_i\right) + a_1\left(\sum x_i^2\right) + (\sum x_i^3)a_2 = \sum y_i x_i \tag{1.33}$$

$$a_0\left(\sum x_i^2\right) + a_1\left(\sum x_i^3\right) + (\sum x_i^4)a_2 = \sum y_i x_i^2 \tag{1.34}$$

The coefficients of the unknowns can be calculated directly from the observed data. And in general, for a polynomial of order n, we have : (py: the quadratic case in HW.)

$$a_0\sum_{i=1}^{m} x_i^0 + a_1\sum_{i=1}^{m} x_i^1 + a_2\sum_{i=1}^{m} x_i^2 + \cdots + a_n\sum_{i=1}^{m} x_i^n = \sum_{i=1}^{m} y_i x_i^0,$$

$$a_0\sum_{i=1}^{m} x_i^1 + a_1\sum_{i=1}^{m} x_i^2 + a_2\sum_{i=1}^{m} x_i^3 + \cdots + a_n\sum_{i=1}^{m} x_i^{n+1} = \sum_{i=1}^{m} y_i x_i^1,$$

$$\vdots$$

$$a_0\sum_{i=1}^{m} x_i^n + a_1\sum_{i=1}^{m} x_i^{n+1} + a_2\sum_{i=1}^{m} x_i^{n+2} + \cdots + a_n\sum_{i=1}^{m} x_i^{2n} = \sum_{i=1}^{m} y_i x_i^n.$$

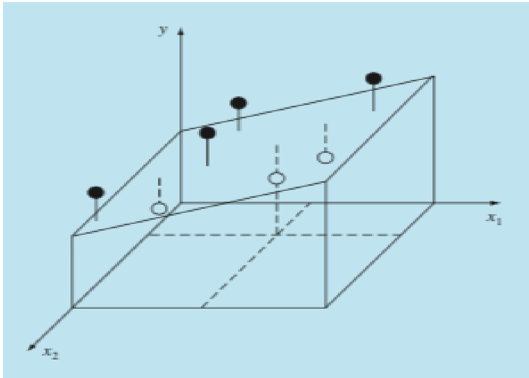
1.7.5 Multiple Linear Regression

Two or more independent variables

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

For this two-dimensional case, the regression "line" becomes a "plane".

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



1.8 Pade

A **rational funcion** r of degree N has the form

$$r(x) \equiv \frac{p(x)}{q(x)}$$

where $p(x)$ and $q(x)$ are polynomial whose degrees sum to N. The rational function whose numerator and denominator have the same or nearly the same degree generally produce approximation results superior to polynomial methods for the same amount of computation effort.

Suppose r is a rational function of degree $N = n + m$ of the form

$$r(x) = \frac{p(x)}{q(x)} = \frac{p_0 + p_1 x + \cdots + p_n x^n}{q_0 + q_1 x + \cdots + q_m x^m}$$

that is used to approximate a function f on a closed interval I containing zero.

The **Pade approximation technique**, which is the extension of Taylor polynomial approximation to rational functions, choses the $N + 1$ parameters so that $f^{(k)}(0) = r^{(k)}(0)$, for each $k = 0, 1, \ldots, N$. When $n = N$ and $m = 0$, the Pade approximation is just the Nth Maclaurin polynomial.
Consider de difference

$$f(x) - r(x) = f(x) - \frac{p(x)}{q(x)} = \frac{f(x)q(x) - p(x)}{q(x)} = \frac{f(x)\sum_{i=0}^{m} q_i x^i - \sum_{i=0}^{n} p_i x^i}{q(x)}$$

and suppose f has the Maclaurin series expansion $f(x) = \sum_{i=0}^{\infty} a_i x^i$. Then

$$f(x) - r(x) = \frac{\sum_{i=0}^{\infty} a_i x^i \sum_{i=0}^{m} q_i x^i - \sum_{i=0}^{n} p_i x^i}{q(x)}$$

The object is to choose the constants $q_i, q_2, \ldots, q_m$ and $p_0, p_1, \ldots, p_n$ so that

$$f^{(k)}(0) - r^{(k)}(0) = 0 \qquad \text{for each } k = 0, 1, \ldots, N.$$

So, the rational function for Pade approximation results from the solution of the $N+1$ linear equations

$$\sum_{i=0}^{k} a_i q_{k-i} = p_k, \qquad k = 0, 1, \ldots N$$

in the $N+1$ unknowns $q_1, q_2, \ldots q_m, p_0, p_1, \ldots p_n$.

(here: do it) The Maclaurin series expansion for e^{-x} if $\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} x^n$. To find the Pade approximation to e^{-x} of degree 5 with $n = 3$ and $m = 2$, we need to choose:

$$\left(1 - x + \frac{x^2}{2} - \frac{x^3}{6} + \cdots\right)(1 + q_1 x + q_2 x^2) - (p_0 + p_1 x + p_2 x^2 + p_3 x^3).$$

Expanding and collecting terms produces

$$\begin{aligned}
x^5 &: \; -\frac{1}{120} + \frac{1}{24}q_1 - \frac{1}{6}q_2 = 0; & x^2 &: \; \frac{1}{2} - q_1 + q_2 = p_2; \\
x^4 &: \; \frac{1}{24} - \frac{1}{6}q_1 + \frac{1}{2}q_2 = 0; & x^1 &: \; -1 + q_1 = p_1; \\
x^3 &: \; -\frac{1}{6} + \frac{1}{2}q_1 - q_2 = p_3; & x^0 &: \; 1 = p_0.
\end{aligned}$$

giving

$$p_0 = 1, \; p_1 = -\frac{3}{5}, \; p_2 = \frac{3}{20}, \; p_3 = -\frac{1}{60}, \; q_1 = \frac{2}{5}, \text{ and } q_2 = \frac{1}{20}.$$

x	e^{-x}	$P_5(x)$	$\lvert e^{-x} - P_5(x)\rvert$	$r(x)$	$\lvert e^{-x} - r(x)\rvert$
0.2	0.81873075	0.81873067	8.64×10^{-8}	0.81873075	7.55×10^{-9}
0.4	0.67032005	0.67031467	5.38×10^{-6}	0.67031963	4.11×10^{-7}
0.6	0.54881164	0.54875200	5.96×10^{-5}	0.54880763	4.00×10^{-6}
0.8	0.44932896	0.44900267	3.26×10^{-4}	0.44930966	1.93×10^{-5}
1.0	0.36787944	0.36666667	1.21×10^{-3}	0.36781609	6.33×10^{-5}

So the Pade approximation is (py: do it)

$$r(x) = \frac{1 - \frac{3}{5}x + \frac{3}{20}x^2 - \frac{1}{60}x^3}{1 + \frac{2}{5}x + \frac{1}{20}x^2}.$$

(hw: Determine all degree 3 Pade approximations for $f(x) = x\ln(x+1)$. Compare the results at $x_i = 0.2i$ for $i = 1, 2, 3, 4, 5$ with the actual values $f(x_i)$)
Although the rational-function approximation gave results superior to the polynomial approximation of the same degree, the approximation has a wide variation in accuracy. This accuracy variations is expected because the Pade approximation is based on a Taylor polynomial representation, and the Taylor representation has a wide variation of accuracy.

Suppose we want to approximate the function f by an $N-$th degree rational function r written in the form

$$r(x) = \frac{\sum_{k=0}^{n} p_k T_k(x)}{\sum_{k=0}^{m} q_k T_k(x)} \qquad \text{where } N = n + m \quad \text{and } q_0 = 1$$

Writing $f(x)$ in a series involving Chebyshev polynomials as

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x)$$

gives

$$f(x) - r(x) = \sum_{k=0}^{\infty} a_k T_k(x) - \frac{\sum_{k=0}^{n} p_k T_k(x)}{\sum_{k=0}^{m} q_k T_k(x)}$$

or

$$f(x) - r(x) = \frac{\sum_{k=0}^{\infty} a_k T_k(x) \sum_{k=0}^{m} q_k T_k(x) - \sum_{k=0}^{n} p_k T_k(x)}{\sum_{k=0}^{m} q_k T_k(x)}.$$

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x),$$

then the orthogonality of the Chebyshev polynomials implies that

$$a_0 = \frac{1}{\pi}\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\,dx \quad \text{and} \quad a_k = \frac{2}{\pi}\int_{-1}^{1} \frac{f(x)T_k(x)}{\sqrt{1-x^2}}\,dx, \quad \text{where } k \geq 1.$$

Figure 1.1: Summary of the .

$$\tilde{P}_5(x) = 1.266066T_0(x) - 1.130318T_1(x) + 0.271495T_2(x) - 0.044337T_3(x)$$
$$+ 0.005474T_4(x) - 0.000543T_5(x).$$

$$\tilde{P}_5(x)[T_0(x) + q_1T_1(x) + q_2T_2(x)] - [p_0T_0(x) + p_1T_1(x) + p_2T_2(x) + p_3T_3(x)].$$

Using the relation (8.18) and collecting terms gives the equations

$$\begin{aligned}
T_0 &: \quad 1.266066 - 0.565159q_1 + 0.1357485q_2 = p_0, \\
T_1 &: \quad -1.130318 + 1.401814q_1 - 0.587328q_2 = p_1, \\
T_2 &: \quad 0.271495 - 0.587328q_1 + 1.268803q_2 = p_2, \\
T_3 &: \quad -0.044337 + 0.138485q_1 - 0.565431q_2 = p_3, \\
T_4 &: \quad 0.005474 - 0.022440q_1 + 0.135748q_2 = 0, \\
T_5 &: \quad -0.000543 + 0.002737q_1 - 0.022169q_2 = 0.
\end{aligned}$$

The solution to this system produces the rational function

$$r_T(x) = \frac{1.055265T_0(x) - 0.613016T_1(x) + 0.077478T_2(x) - 0.004506T_3(x)}{T_0(x) + 0.378331T_1(x) + 0.022216T_2(x)}.$$

Figure 1.2: Summary of the numerical methods covered in this course.

$$r_T(x) = \frac{0.977787 - 0.599499x + 0.154956x^2 - 0.018022x^3}{0.977784 + 0.378331x + 0.044432x^2}.$$

x	e^{-x}	$r(x)$	$\lvert e^{-x} - r(x)\rvert$	$r_T(x)$	$\lvert e^{-x} - r_T(x)\rvert$
0.2	0.81873075	0.81873075	7.55×10^{-9}	0.81872510	5.66×10^{-6}
0.4	0.67032005	0.67031963	4.11×10^{-7}	0.67031310	6.95×10^{-6}
0.6	0.54881164	0.54880763	4.00×10^{-6}	0.54881292	1.28×10^{-6}
0.8	0.44932896	0.44930966	1.93×10^{-5}	0.44933809	9.13×10^{-6}
1.0	0.36787944	0.36781609	6.33×10^{-5}	0.36787155	7.89×10^{-6}

2

Orthogonal Polynomials and Least Squares Approximation

Suppose $f \in C[a, b]$ and that a polynomial $P_n x$ of degree at most n is requires that will minimize the error

$$\int_a^b [f(x) - P_n(x)]^2 dx \tag{2.1}$$

To determine a least squares approximating polynomial; that is, a polynomial to minimize this expression, let

$$P_n(x) = a_x x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0 = \sum_{k=0}^{n} a_k x^k, \tag{2.2}$$

and define,

$$e = e(a_0, a_1, \ldots, a_n) = \int_a^b \left(f(x) - \sum_{k=0}^{n} a_k x^k \right)^2 dx. \tag{2.3}$$

Let Π_n be the set of all polynomials of degree at most n.

The problem is to find real coefficients $a_0, a_1, \ldots, a_n$ that will minimize E. A necessary condition for the numbers $a_0, a_1, \ldots, a_n$ to minimize E is that

$$\frac{\partial E}{\partial a_j} = 0, \quad \text{for each } j = 0, 1, \ldots, n.$$

Hence, to find $P_n(x)$, the $(n + 1)$ linear **normal equations**

$$\sum_{k=0}^{n} a_k \int_a^b x^{j+k}\, dx = \int_a^b x^j f(x)\, dx, \quad \text{for each } j = 0, 1, \ldots, n, \tag{8.6}$$

must be solved for the $(n + 1)$ unknowns a_j. The normal equations always have a unique solution provided $f \in C[a, b]$. (See Exercise 15.)

If $\{\phi_0(x), \phi_1(x), \ldots, \phi_n(x)\}$ is a collection of linearly independent polynomials in $\prod_n$, then any polynomial in $\prod_n$ can be written uniquely as a linear combination of $\phi_0(x)$, $\phi_1(x), \ldots, \phi_n(x)$. ■

An integrable function w is called a **weight function** on the interval I if $w(x) \geq 0$, for all x in I, but $w(x) \not\equiv 0$ on any subinterval of I. ■

Suppose $\{\phi_0, \phi_1, \ldots, \phi_n\}$ is a set of linearly independent functions on $[a, b]$, w is a weight function for $[a, b]$, and, for $f \in C[a, b]$, a linear combination

$$P(x) = \sum_{k=0}^{n} a_k \phi_k(x)$$

is sought to minimize the error

$$E(a_0, \ldots, a_n) = \int_a^b w(x) \left[f(x) - \sum_{k=0}^{n} a_k \phi_k(x) \right]^2 dx.$$

This problem reduces to the situation considered at the beginning of this section in the special case when $w(x) \equiv 1$ and $\phi_k(x) = x^k$, for each $k = 0, 1, \ldots, n$.

The normal equations associated with this problem are derived from the fact that for each $j = 0, 1, \ldots, n$,

$$0 = \frac{\partial E}{\partial a_j} = 2 \int_a^b w(x) \left[f(x) - \sum_{k=0}^{n} a_k \phi_k(x) \right] \phi_j(x)\, dx.$$

The system of normal equations can be written

$$\int_a^b w(x)f(x)\phi_j(x)\,dx = \sum_{k=0}^{n} a_k \int_a^b w(x)\phi_k(x)\phi_j(x)\,dx, \quad \text{for } j = 0, 1, \ldots, n.$$

If the functions $\phi_0, \phi_1, \ldots, \phi_n$ can be chosen so that

$$\int_a^b w(x)\phi_k(x)\phi_j(x)\,dx = \begin{cases} 0, & \text{when } j \neq k, \\ \alpha_j > 0, & \text{when } j = k, \end{cases} \tag{8.7}$$

then the normal equations reduce to

$$\int_a^b w(x)f(x)\phi_j(x)\,dx = a_j \int_a^b w(x)[\phi_j(x)]^2\,dx = a_j\alpha_j,$$

for each $j = 0, 1, \ldots, n$, and are easily solved to give

$$a_j = \frac{1}{\alpha_j}\int_a^b w(x)f(x)\phi_j(x)\,dx.$$

Hence the least squares approximation problem is greatly simplified when the functions $\phi_0, \phi_1, \ldots, \phi_n$ are chosen to satisfy the *orthogonality* condition in Eq. (8.7). The remainder of this section is devoted to studying collections of this type.

Table 10.3 Orthogonal Polynomials Generated by Gram–Schmidt Orthogonalization of $u_n(x) = x^n$, $n = 0, 1, 2, \ldots$

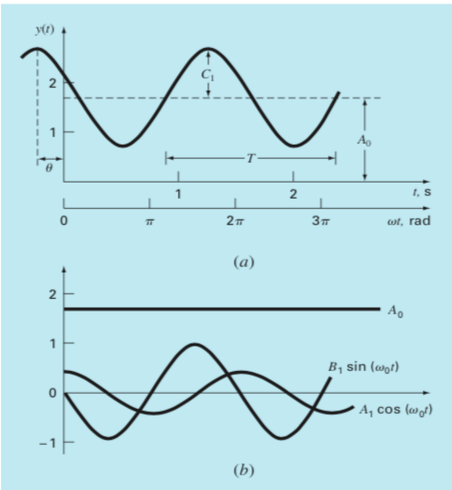
Polynomials	Interval	Weighting function $w(x)$	Standard normalization
Legendre	$-1 \le x \le 1$	1	$\int_{-1}^{1} [P_n(x)]^2\,dx = \frac{2}{2n+1}$
Shifted Legendre	$0 \le x \le 1$	1	$\int_{0}^{1} [P_n^*(x)]^2\,dx = \frac{1}{2n+1}$
Chebyshev I	$-1 \le x \le 1$	$(1-x^2)^{-1/2}$	$\int_{-1}^{1} \frac{[T_n(x)]^2}{(1-x^2)^{1/2}}\,dx = \begin{cases} \pi/2, & n \ne 0 \\ \pi, & n = 0 \end{cases}$
Shifted Chebyshev I	$0 \le x \le 1$	$[x(1-x)]^{-1/2}$	$\int_{0}^{1} \frac{[T_n^*(x)]^2}{[x(1-x)]^{1/2}}\,dx = \begin{cases} \pi/2, & n > 0 \\ \pi, & n = 0 \end{cases}$
Chebyshev II	$-1 \le x \le 1$	$(1-x^2)^{1/2}$	$\int_{-1}^{1} [U_n(x)]^2(1-x^2)^{1/2}\,dx = \frac{\pi}{2}$
Laguerre	$0 \le x < \infty$	e^{-x}	$\int_{0}^{\infty} [L_n(x)]^2 e^{-x}\,dx = 1$
Associated Laguerre	$0 \le x < \infty$	$x^k e^{-x}$	$\int_{0}^{\infty} [L_n^k(x)]^2 x^k e^{-x}\,dx = \frac{(n+k)!}{n!}$
Hermite	$-\infty < x < \infty$	e^{-x^2}	$\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2}\,dx = 2^n \pi^{1/2} n!$

3

Fourier Approximations

Fourier approximation represents a systematic framework for using trigonometric series for this purpose. We will use the cosine

$$f(t) = A_0 + C_1 \cos(w_0 t + \theta)$$



For a function $f \in C[-\pi, \pi]$, we want to find the *continuous least squares* approximation by functions in $\mathcal{T}_n$ in the form

$$S_n(x) = \frac{a_0}{2} + a_n \cos nx + \sum_{k=1}^{n-1} (a_k \cos kx + b_k \sin kx).$$

Since the set of functions $\{\phi_0, \phi_1, \ldots, \phi_{2n-1}\}$ is orthogonal on $[-\pi, \pi]$ with respect to $w(x) \equiv 1$, it follows from Theorem 8.6 that the appropriate selection of coefficients is

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos kx \, dx, \quad \text{for each } k = 0, 1, 2, \ldots, n,$$

and

$$b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin kx \, dx, \quad \text{for each } k = 1, 2, \ldots, n - 1.$$

To determine the trigonometric polynomial from $\mathcal{T}_n$ that approximates

$$f(x) = |x|, \quad \text{for } -\pi < x < \pi,$$

requires finding

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} |x|\,dx = -\frac{1}{\pi}\int_{-\pi}^{0} x\,dx + \frac{1}{\pi}\int_{0}^{\pi} x\,dx = \frac{2}{\pi}\int_{0}^{\pi} x\,dx = \pi,$$

$$a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} |x|\cos kx\,dx = \frac{2}{\pi}\int_{0}^{\pi} x\cos kx\,dx = \frac{2}{\pi k^2}\left[(-1)^k - 1\right],$$

for each $k = 1, 2, \ldots, n$, and

$$b_k = \frac{1}{\pi}\int_{-\pi}^{\pi} |x|\sin kx\,dx = 0, \quad \text{for each } k = 1, 2, \ldots, n-1.$$

$$S_n(x) = \frac{\pi}{2} + \frac{2}{\pi}\sum_{k=1}^{n} \frac{(-1)^k - 1}{k^2}\cos kx.$$

Figure 3.1: Summary of the numericalmethods covered in this course.

3.1 Least-Squares Fit of a Sinusoid

Thus, our goal is to determine coefficient values that minimize

$$S_r = \sum_{i=1}^{N}\{y_i - [A_0 + A_1\cos(w_0 t) + B_1\sin(w_0 t_i)]\}^2$$

or

$$A_0 = \frac{\sum y}{N} \tag{3.1}$$

$$A_1 = \frac{2}{N}\sum y\cos(w_0 t) \tag{3.2}$$

$$B_1 = \frac{2}{N}\sum y\sin(w_0 t) \tag{3.3}$$

$$\begin{bmatrix} N & \sum\cos(\omega_0 t) & \sum\sin(\omega_0 t) \\ \sum\cos(\omega_0 t) & \sum\cos^2(\omega_0 t) & \sum\cos(\omega_0 t)\,\sin(\omega_0 t) \\ \sum\sin(\omega_0 t) & \sum\cos(\omega_0 t)\,\sin(\omega_0 t) & \sum\sin^2(\omega_0 t) \end{bmatrix} \begin{Bmatrix} A_0 \\ A_1 \\ B_0 \end{Bmatrix} = \begin{Bmatrix} \sum y \\ \sum y\cos(\omega_0 t) \\ \sum y\sin(\omega_0 t) \end{Bmatrix}$$

$$A_0 = \frac{\sum y}{N}$$

$$\left.\begin{aligned} A_j &= \frac{2}{N}\sum y\cos(j\omega_0 t) \\ B_j &= \frac{2}{N}\sum y\sin(j\omega_0 t) \end{aligned}\right\} \qquad j = 1, 2, \ldots, m$$

The least squares trigonometric polynomial is, consequently,

$$S_3(z) = \left[\frac{a_0}{2} + a_3\cos 3z + \sum_{k=1}^{2}(a_k\cos kz + b_k\sin kz)\right],$$

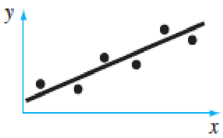
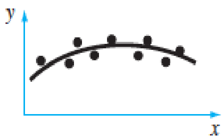
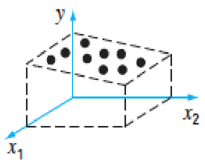
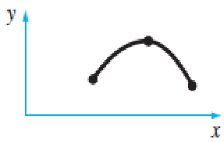
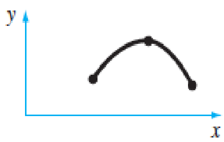
where

$$a_k = \frac{1}{5}\sum_{j=0}^{9} f\left(1 + \frac{z_j}{\pi}\right)\cos kz_j, \quad \text{for } k = 0, 1, 2, 3,$$

and

$$b_k = \frac{1}{5}\sum_{j=0}^{9} f\left(1 + \frac{z_j}{\pi}\right)\sin kz_j, \quad \text{for } k = 1, 2.$$

Method	Error Associated with Data	Match of Individual Data Points	Number of Points Matched Exactly	Programming Effort	Comments
Regression					
Linear regression	Large	Approximate	0	Easy	
Polynomial regression	Large	Approximate	0	Moderate	Round-off error becomes pronounced for higher-order versions
Multiple linear regression	Large	Approximate	0	Moderate	
Nonlinear regression	Large	Approximate	0	Difficult	
Interpolation					
Newton's divided-difference polynomials	Small	Exact	$n + 1$	Easy	Usually preferred for exploratory analyses
Lagrange polynomials	Small	Exact	$n + 1$	Easy	Usually preferred when order is known
Cubic splines	Small	Exact	Piecewise fit of data points	Moderate	First and second derivatives equal at knots

Method	Formulation	Graphical Interpretation	Errors
Linear regression	$y = a_0 + a_1 x$ where $a_1 = \dfrac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - \left(\sum x_i\right)^2}$, $a_0 = \bar{y} - a_1\bar{x}$		$s_{y/x} = \sqrt{\dfrac{S_r}{n-2}}$ $r^2 = \dfrac{S_t - S_r}{S_t}$
Polynomial regression	$y = a_0 + a_1 x + \cdots + a_m x^m$ (Evaluation of a's equivalent to solution of $m + 1$ linear algebraic equations)		$s_{y/x} = \sqrt{\dfrac{S_r}{n-(m+1)}}$ $r^2 = \dfrac{S_t - S_r}{S_t}$
Multiple linear regression	$y = a_0 + a_1 x_1 + \cdots + a_m x_m$ (Evaluation of a's equivalent to solution of $m + 1$ linear algebraic equations)		$s_{y/x} = \sqrt{\dfrac{S_r}{n-(m+1)}}$ $r^2 = \dfrac{S_t - S_r}{S_t}$
Newton's divided-difference interpolating polynomial*	$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$ where $b_0 = f(x_0)$, $b_1 = f[x_1, x_0]$, $b_2 = f[x_2, x_1, x_0]$		$R_2 = (x - x_0)(x - x_1)(x - x_2)\dfrac{f^{(3)}(\xi)}{6}$ or $R_2 = (x - x_0)(x - x_1)(x - x_2)f[x_3, x_2, x_1, x_0]$
Lagrange interpolating polynomial*	$f_2(x) = f(x_0)\left(\dfrac{x - x_1}{x_0 - x_1}\right)\left(\dfrac{x - x_2}{x_0 - x_2}\right) + f(x_1)\left(\dfrac{x - x_0}{x_1 - x_0}\right)\left(\dfrac{x - x_2}{x_1 - x_2}\right) + f(x_2)\left(\dfrac{x - x_0}{x_2 - x_0}\right)\left(\dfrac{x - x_1}{x_2 - x_1}\right)$		$R_2 = (x - x_0)(x - x_1)(x - x_2)\dfrac{f^{(3)}(\xi)}{6}$ or $R_2 = (x - x_0)(x - x_1)(x - x_2)f[x_3, x_2, x_1, x_0]$
Cubic splines	A cubic: $a_i x^3 + b_i x^2 + c_i x + d_i$ is fit to each interval between knots. First and second derivatives are equal at each knot