

Chapter 5

Polynomial Approximation and interpolation

Definition(Polynomial): A polynomial $P_n(x)$ of degree $\leq n$ is a function of the form

$$P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0,$$

where n is non-negative integer and a_n, a_{n-1}, \dots, a_0 are real constants.

Polynomials are easy to differentiate, integrate and have simple structure. Their importance is that they can **uniformly approximate** the continuous functions.

Importance: We can **approximate a continuous function by polynomials** on a closed and bounded interval.

We can get easy form of a complicated function in the form of a polynomial by this approximation. So, it will be easy to deal with the polynomials rather than the complicated functions.

How to approximate: The **Taylor's polynomials** is used to approximate the functions.

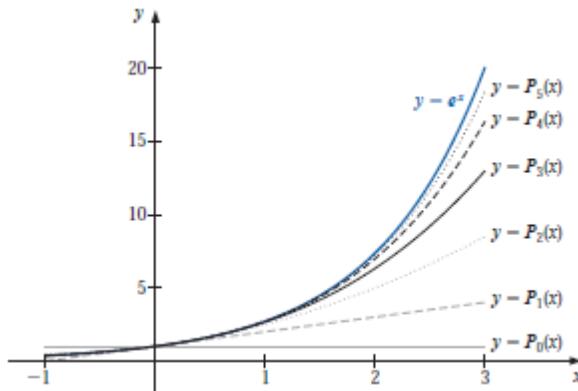
Example: Let $f(x) = e^x$

n th -degree Taylor's polynomials for $f(x)$ about zero is $P_n(x) = \sum_{k=0}^n \frac{f^{(k)}(0)}{k!} x^k$,

so, $P_n(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!}$, if we truncate up to desired degree of approximate polynomials, then we can write:

$$\begin{aligned} P_0(x) &= 1, & P_1(x) &= 1 + x, & P_2(x) &= 1 + x + \frac{x^2}{2}, & P_3(x) &= 1 + x + \frac{x^2}{2} + \frac{x^3}{6}, \\ P_4(x) &= 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24}, & \text{and} & & P_5(x) &= 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \frac{x^5}{120}. \end{aligned}$$

From the following graph of the polynomial approximation we can see that for the higher-degree polynomials, the error becomes less and it approaches to the function $f(x) = e^x$.



Limitations of Taylor's polynomial approximation:

Note: (i) By Taylor's polynomials approximation, we can get better approximation only for higher order differentiable functions.

(ii) This approximation does not give better for all functions: for example $f(x) = \frac{1}{x}$,

Taylor's polynomial about $x = 1$ is given by

$$P_n(x) = \sum_{k=0}^n \frac{f^{(k)}(1)}{k!} (x-1)^k = \sum_{k=0}^n (-1)^k (x-1)^k.$$

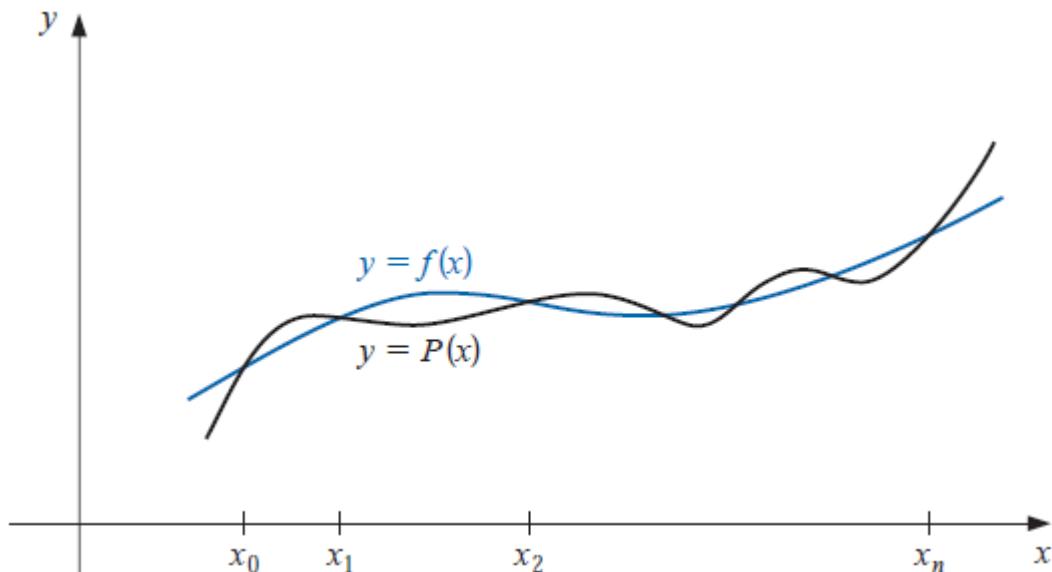
To approximate $f(3) = 1/3$ by $P_n(3)$ for increasing values of n , we obtain the values in Table 3.1—rather a dramatic failure! When we approximate $f(3) = 1/3$ by $P_n(3)$ for larger values of n , the approximations become increasingly inaccurate.

Table 3.1

n	0	1	2	3	4	5	6	7
$P_n(3)$	1	-1	3	-5	11	-21	43	-85

Now, there is another method i.e. [polynomial interpolation](#) to find the approximate form of any function f . In this method, we can approximate a function without even knowing a function but a few data about f .

Interpolation: Given $(n + 1)$ points data points $(x_i, y_i), i = 0, 1, 2, \dots, n$, at which function passes, then approximate in form of a polynomial function $P(x)$ of degree atmost n such that $f(x_i) = P(x_i), i = 0, 1, 2, \dots, n$. Such a polynomial is said to be interpolate the data.



Theorem 1 (Existence and Uniqueness). Given a real-valued function $f(x)$ and $n + 1$ distinct points x_0, x_1, \dots, x_n , there exists a unique polynomial $P_n(x)$ of degree $\leq n$ which interpolates the unknown $f(x)$ at points x_0, x_1, \dots, x_n .

Methods to interpolate:

1. Lagrange Interpolation
2. Newton's interpolation

Lagrange Interpolating Polynomials

Linear Interpolation: Approximate a function that passes through two points $(x_0, y_0), (x_1, y_1)$ i.e. $y_0 = f(x_0)$, $y_1 = f(x_1)$ by polynomial of atmost one degree i.e. linear polynomial $P_1(x)$.

Interpolating polynomial should satisfy $f(x_0) = P_1(x_0), f(x_1) = P_1(x_1)$.

Using this polynomial for approximation within the interval given by the endpoints is called polynomial interpolation.

Define the functions

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} \quad \text{and} \quad L_1(x) = \frac{x - x_0}{x_1 - x_0}.$$

The linear Lagrange interpolating polynomial through (x_0, y_0) and (x_1, y_1) is
 $P_1(x) = L_0(x)f(x_0) + L_1(x)f(x_1) = \frac{x - x_1}{x_0 - x_1}f(x_0) + \frac{x - x_0}{x_1 - x_0}f(x_1)$.

Note that

$$L_0(x_0) = 1, \quad L_0(x_1) = 0, \quad L_1(x_0) = 0, \quad \text{and} \quad L_1(x_1) = 1,$$

which implies that

$$f(x_0) = P_1(x_0) = y_0, \quad f(x_1) = P_1(x_1) = y_1.$$

So $P_1(x)$ is the unique polynomial of degree at most one that passes through (x_0, y_0) and (x_1, y_1) .

Example 1 Determine the linear Lagrange interpolating polynomial that passes through the points $(2, 4)$ and $(5, 1)$.

Solution In this case we have

$$L_0(x) = \frac{x - 5}{2 - 5} = -\frac{1}{3}(x - 5) \quad \text{and} \quad L_1(x) = \frac{x - 2}{5 - 2} = \frac{1}{3}(x - 2),$$

so

$$P(x) = -\frac{1}{3}(x - 5) \cdot 4 + \frac{1}{3}(x - 2) \cdot 1 = -\frac{4}{3}x + \frac{20}{3} + \frac{1}{3}x - \frac{2}{3} = -x + 6.$$

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

$$(x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_n, f(x_n)).$$

In this case we first construct, for each $k = 0, 1, \dots, n$, a function $L_{n,k}(x)$ with the property that $L_{n,k}(x_i) = 0$ when $i \neq k$ and $L_{n,k}(x_k) = 1$. To satisfy $L_{n,k}(x_i) = 0$ for each $i \neq k$ requires that the numerator of $L_{n,k}(x)$ contain the term

$$(x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n).$$

To satisfy $L_{n,k}(x_k) = 1$, the denominator of $L_{n,k}(x)$ must be this same term but evaluated at $x = x_k$. Thus

$$L_{n,k}(x) = \frac{(x - x_0) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_n)}.$$

Theorem 2:

If x_0, x_1, \dots, 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

$$f(x_k) = P(x_k), \quad \text{for each } k = 0, 1, \dots, n.$$

This polynomial is given by

$$P(x) = f(x_0)L_{n,0}(x) + \cdots + f(x_n)L_{n,n}(x) = \sum_{k=0}^n f(x_k)L_{n,k}(x), \quad (3.1)$$

where, for each $k = 0, 1, \dots, n$,

$$\begin{aligned} L_{n,k}(x) &= \frac{(x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0)(x_k - x_1) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_n)} \\ &= \prod_{\substack{i=0 \\ i \neq k}}^n \frac{(x - x_i)}{(x_k - x_i)}. \end{aligned} \quad \blacksquare \quad (3.2)$$

- Example 2**
- (a) Use the numbers (called *nodes*) $x_0 = 2$, $x_1 = 2.75$, and $x_2 = 4$ to find the second Lagrange interpolating polynomial for $f(x) = 1/x$.
 - (b) Use this polynomial to approximate $f(3) = 1/3$.

Solution (a) We first determine the coefficient polynomials $L_0(x)$, $L_1(x)$, and $L_2(x)$. In nested form they are

$$\begin{aligned} L_0(x) &= \frac{(x - 2.75)(x - 4)}{(2 - 2.75)(2 - 4)} = \frac{2}{3}(x - 2.75)(x - 4), \\ L_1(x) &= \frac{(x - 2)(x - 4)}{(2.75 - 2)(2.75 - 4)} = -\frac{16}{15}(x - 2)(x - 4), \end{aligned}$$

and

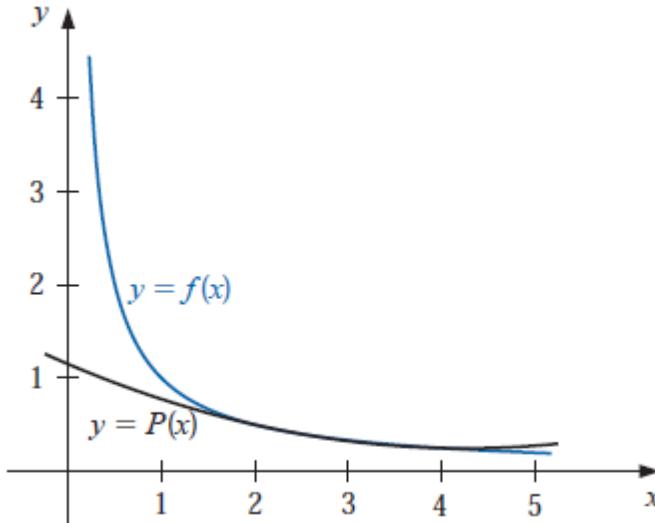
$$L_2(x) = \frac{(x - 2)(x - 2.75)}{(4 - 2)(4 - 2.75)} = \frac{2}{5}(x - 2)(x - 2.75).$$

Also, $f(x_0) = f(2) = 1/2$, $f(x_1) = f(2.75) = 4/11$, and $f(x_2) = f(4) = 1/4$, so

$$\begin{aligned} P(x) &= \sum_{k=0}^2 f(x_k)L_k(x) \\ &= \frac{1}{3}(x - 2.75)(x - 4) - \frac{64}{165}(x - 2)(x - 4) + \frac{1}{10}(x - 2)(x - 2.75) \\ &= \frac{1}{22}x^2 - \frac{35}{88}x + \frac{49}{44}. \end{aligned}$$

(b) An approximation to $f(3) = 1/3$ (see Figure 3.6) is

$$f(3) \approx P(3) = \frac{9}{22} - \frac{105}{88} + \frac{49}{44} = \frac{29}{88} \approx 0.32955.$$



The next step is to calculate a remainder term or bound for the error involved in approximating a function by an interpolating polynomial.

Theorem 3:

Suppose x_0, x_1, \dots, x_n are distinct numbers in the interval $[a, b]$ and $f \in C^{n+1}[a, b]$. Then, for each x in $[a, b]$, a number $\xi(x)$ (generally unknown) between x_0, x_1, \dots, x_n , and hence in (a, b) , exists with

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} (x - x_0)(x - x_1) \cdots (x - x_n), \quad (3.3)$$

where $P(x)$ is the interpolating polynomial given in Eq. (3.1). ■

Example 3 In Example 2 we found the second Lagrange polynomial for $f(x) = 1/x$ on $[2, 4]$ using the nodes $x_0 = 2$, $x_1 = 2.75$, and $x_2 = 4$. Determine the error form for this polynomial, and the maximum error when the polynomial is used to approximate $f(x)$ for $x \in [2, 4]$.

Solution Because $f(x) = x^{-1}$, we have

$$f'(x) = -x^{-2}, \quad f''(x) = 2x^{-3}, \quad \text{and} \quad f'''(x) = -6x^{-4}.$$

As a consequence, the second Lagrange polynomial has the error form

$$\frac{f'''(\xi(x))}{3!}(x-x_0)(x-x_1)(x-x_2) = -(\xi(x))^{-4}(x-2)(x-2.75)(x-4), \quad \text{for } \xi(x) \text{ in } (2, 4).$$

The maximum value of $(\xi(x))^{-4}$ on the interval is $2^{-4} = 1/16$. We now need to determine the maximum value on this interval of the absolute value of the polynomial

$$g(x) = (x-2)(x-2.75)(x-4) = x^3 - \frac{35}{4}x^2 + \frac{49}{2}x - 22.$$

Because

$$D_x \left(x^3 - \frac{35}{4}x^2 + \frac{49}{2}x - 22 \right) = 3x^2 - \frac{35}{2}x + \frac{49}{2} = \frac{1}{2}(3x-7)(2x-7),$$

the critical points occur at

$$x = \frac{7}{3}, \text{ with } g\left(\frac{7}{3}\right) = \frac{25}{108}, \quad \text{and} \quad x = \frac{7}{2}, \text{ with } g\left(\frac{7}{2}\right) = -\frac{9}{16}.$$

Hence, the maximum error is

$$\begin{aligned} \frac{f'''(\xi(x))}{3!}|(x-x_0)(x-x_1)(x-x_2)| &\leq \\ \frac{1}{16} * \left| \frac{-9}{16} \right| &\approx \mathbf{0.035156}. \end{aligned}$$

The next example illustrates how the error formula can be used to prepare a table of data that will ensure a specified interpolation error within a specified bound.

Example 4 Let function $f(x) = e^x$, for x in $[0,1]$. Assume that the difference between adjacent x -values, the step size, is h . What step size h will ensure that linear interpolation gives an absolute error of at most 10^{-6} for all x in $[0,1]$?

Solution Let x_0, x_1, \dots be the numbers at which f is evaluated, x be in $[0,1]$, and suppose j satisfies $x_j \leq x \leq x_{j+1}$. Eq. (3.3) implies that the error in linear interpolation is

$$|f(x) - P(x)| = \left| \frac{f^{(2)}(\xi)}{2!} (x - x_j)(x - x_{j+1}) \right| = \frac{|f^{(2)}(\xi)|}{2} |(x - x_j)|(x - x_{j+1})|.$$

The step size is h , so $x_j = jh$, $x_{j+1} = (j+1)h$, and

$$|f(x) - P(x)| \leq \frac{|f^{(2)}(\xi)|}{2!} |(x - jh)(x - (j+1)h)|.$$

Hence

$$\begin{aligned} |f(x) - P(x)| &\leq \frac{\max_{\xi \in [0,1]} e^\xi}{2} \max_{x_j \leq x \leq x_{j+1}} |(x - jh)(x - (j+1)h)| \\ &\leq \frac{e}{2} \max_{x_j \leq x \leq x_{j+1}} |(x - jh)(x - (j+1)h)|. \end{aligned}$$

Consider the function $g(x) = (x - jh)(x - (j+1)h)$, for $jh \leq x \leq (j+1)h$. Because

$$g'(x) = (x - (j+1)h) + (x - jh) = 2 \left(x - jh - \frac{h}{2} \right),$$

the only critical point for g is at $x = jh + h/2$, with $g(jh + h/2) = (h/2)^2 = h^2/4$.

Since $g(jh) = 0$ and $g((j+1)h) = 0$, the maximum value of $|g'(x)|$ in $[jh, (j+1)h]$ must occur at the critical point which implies that

$$|f(x) - P(x)| \leq \frac{e}{2} \max_{x_j \leq x \leq x_{j+1}} |g(x)| \leq \frac{e}{2} \cdot \frac{h^2}{4} = \frac{eh^2}{8}.$$

Consequently, to ensure that the the error in linear interpolation is bounded by 10^{-6} , it is sufficient for h to be chosen so that

$$\frac{eh^2}{8} \leq 10^{-6}. \quad \text{This implies that } h < 1.72 \times 10^{-3}.$$

Because $n = (1 - 0)/h$ must be an integer, a reasonable choice for the step size is $h = 0.001$. ■

Newton Divided Difference:

Suppose that $P_n(x)$ is the n th Lagrange polynomial that agrees with the function f at the distinct numbers x_0, x_1, \dots, x_n . Although this polynomial is unique, there are alternate algebraic representations that are useful in certain situations. The divided differences of f with respect to x_0, x_1, \dots, x_n are used to express $P_n(x)$ in the form

$P_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \dots + a_n(x - x_0) \cdots (x - x_{n-1}), \quad (3.5)$ for appropriate constants a_0, a_1, \dots, a_n . To determine the first of these constants, a_0 , note that if $P_n(x)$ is written in the form of Eq. (3.5), then evaluating $P_n(x)$ at x_0 leaves only the constant term a_0 ; that is,

$$a_0 = P_n(x_0) = f(x_0).$$

Similarly, when $P(x)$ is evaluated at x_1 , the only nonzero terms in the evaluation of $P_n(x_1)$ are the constant and linear terms,

$$f(x_0) + a_1(x_1 - x_0) = P_n(x_1) = f(x_1);$$

so

$$a_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}. \quad (3.6)$$

We now introduce a divided-difference notation. The zeroth divided difference of the function f with respect to x_i , denoted by $f[x_i]$ i.e.

$$f[x_i] = f(x_i). \quad (3.7)$$

The remaining divided differences are defined recursively; the *first divided difference* of f with respect to x_i and x_{i+1} is denoted $f[x_i, x_{i+1}]$ and defined as

$$f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}. \quad (3.8)$$

The *second divided difference*, $f[x_i, x_{i+1}, x_{i+2}]$, is defined as

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}.$$

Similarly, after the $(k - 1)$ st divided differences,

$$f[x_i, x_{i+1}, x_{i+2}, \dots, x_{i+k-1}] \quad \text{and} \quad f[x_{i+1}, x_{i+2}, \dots, x_{i+k-1}, x_{i+k}],$$

have been determined, the k th divided difference relative to $x_i, x_{i+1}, x_{i+2}, \dots, x_{i+k}$ is

$$f[x_i, x_{i+1}, \dots, x_{i+k-1}, x_{i+k}] = \frac{f[x_{i+1}, x_{i+2}, \dots, x_{i+k}] - f[x_i, x_{i+1}, \dots, x_{i+k-1}]}{x_{i+k} - x_i}. \quad (3.9)$$

The process ends with the single n th divided difference,

$$f[x_0, x_1, \dots, x_n] = \frac{f[x_1, x_2, \dots, x_n] - f[x_0, x_1, \dots, x_{n-1}]}{x_n - x_0}.$$

Because of Eq. (3.6) we can write $a_1 = f[x_0, x_1]$, just as a_0 can be expressed as $a_0 = f(x_0) = f[x_0]$. Hence the interpolating polynomial in Eq. (3.5) is

$$\begin{aligned} P_n(x) &= f[x_0] + f[x_0, x_1](x - x_0) + a_2(x - x_0)(x - x_1) \\ &\quad + \cdots + a_n(x - x_0)(x - x_1) \cdots (x - x_{n-1}). \end{aligned}$$

$P_n(x)$ can be rewritten in a form of Newton's Divided Difference

$$P_n(x) = f[x_0] + \sum_{k=1}^n f[x_0, x_1, \dots, x_k](x - x_0) \cdots (x - x_{k-1}). \quad (3.10)$$

The generation of the divided differences is outlined in Table 3.9. Two fourth and one fifth difference can also be determined from these data.

Table 3.9

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

Example 1 Complete the divided difference table for the following data and construct the interpolating table that uses all the data and hence intrepolate at $x = 1.5$.

x	$f(x)$
1.0	0.7651977
1.3	0.6200860
1.6	0.4554022
1.9	0.2818186
2.2	0.1103623

Solution The first divided difference involving x_0 and x_1 is

$$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0} = \frac{0.6200860 - 0.7651977}{1.3 - 1.0} = -0.4837057.$$

The remaining first divided differences are found in a similar manner and we get the following table:

i	x_i	$f[x_i]$	$f[x_{i-1}, x_i]$	$f[x_{i-2}, x_{i-1}, x_i]$	$f[x_{i-3}, \dots, x_i]$	$f[x_{i-4}, \dots, x_i]$
0	1.0	0.7651977		-0.4837057		
1	1.3	0.6200860		-0.1087339		
2	1.6	0.4554022		-0.0494433	0.0658784	
3	1.9	0.2818186		0.0118183	0.0680685	0.0018251
4	2.2	0.1103623		-0.5715210		

The coefficients of the Newton forward divided-difference form of the interpolating polynomial are along the diagonal in the table. This polynomial is

$$\begin{aligned} P_4(x) = & 0.7651977 - 0.4837057(x - 1.0) - 0.1087339(x - 1.0)(x - 1.3) \\ & + 0.0658784(x - 1.0)(x - 1.3)(x - 1.6) \\ & + 0.0018251(x - 1.0)(x - 1.3)(x - 1.6)(x - 1.9). \end{aligned}$$

the value $P_4(1.5) = 0.5118200$

Theorem

Suppose that $f \in C^n[a, b]$ and x_0, x_1, \dots, x_n are distinct numbers in $[a, b]$. Then a number ξ exists in (a, b) with

$$f[x_0, x_1, \dots, x_n] = \frac{f^{(n)}(\xi)}{n!}. \quad \blacksquare$$

Further, we can write interpolating divided difference polynomial in terms of forward and backward difference.

Newton's divided-difference formula can be expressed in a simplified form when the nodes are arranged consecutively with equal spacing. In this case, we introduce the notation $h = x_{i+1} - x_i$, for each $i = 0, 1, \dots, n - 1$ and let $x = x_0 + sh$. Then the difference $x - x_i$ is $x - x_i = (s - i)h$. So Eq. (3.10) becomes

$$\begin{aligned} P_n(x) = P_n(x_0 + sh) &= f[x_0] + sh f[x_0, x_1] + s(s - 1)h^2 f[x_0, x_1, x_2] \\ &\quad + \dots + s(s - 1) \cdots (s - n + 1)h^n f[x_0, x_1, \dots, x_n] \\ &= f[x_0] + \sum_{k=1}^n s(s - 1) \cdots (s - k + 1)h^k f[x_0, x_1, \dots, x_k]. \end{aligned}$$

Using binomial-coefficient notation,

$$\binom{s}{k} = \frac{s(s - 1) \cdots (s - k + 1)}{k!},$$

we can express $P_n(x)$ compactly as

$$P_n(x) = P_n(x_0 + sh) = f[x_0] + \sum_{k=1}^n \binom{s}{k} k! h^k f[x_0, x_1, \dots, x_k]. \quad (3.11)$$

Forward Differences

The **Newton forward-difference formula**, is constructed by making use of the forward difference notation Δ introduced in Aitken's Δ^2 method. With this notation,

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{1}{h}(f(x_1) - f(x_0)) = \frac{1}{h}\Delta f(x_0)$$

$$f[x_0, x_1, x_2] = \frac{1}{2h} \left[\frac{\Delta f(x_1) - \Delta f(x_0)}{h} \right] = \frac{1}{2h^2}\Delta^2 f(x_0),$$

and, in general,

$$f[x_0, x_1, \dots, x_k] = \frac{1}{k!h^k}\Delta^k f(x_0).$$

Since $f[x_0] = f(x_0)$, Eq. (3.11) has the following form.

Newton Forward-Difference Formula

$$P_n(x) = f(x_0) + \sum_{k=1}^n \binom{s}{k} \Delta^k f(x_0) \quad (3.12)$$

Forward Difference table

i	x_i	f_i	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
0	x_0	f_0				
1	x_1	f_1	Δf_0	$\Delta^2 f_0$	$\Delta^3 f_0$	$\Delta^4 f_0$
2	x_2	f_2	Δf_1	$\Delta^2 f_1$	$\Delta^3 f_1$	$\Delta^4 f_1$
3	x_3	f_3	Δf_2	$\Delta^2 f_2$	$\Delta^3 f_2$	
4	x_4	f_4				

Note: If the data size is big then the divided difference table will be too long. Suppose the desired intermediate value at which one needs to estimate the function falls towards the end or say in the second half of the data set then it may be better to start the estimation process from the last data set point. For this we need to use backward-differences and backward difference table.

Backward Differences

If the interpolating nodes are reordered from last to first as x_n, x_{n-1}, \dots, x_0 , we can write the interpolatory formula as

$$P_n(x) = f[x_n] + f[x_n, x_{n-1}](x - x_n) + f[x_n, x_{n-1}, x_{n-2}](x - x_n)(x - x_{n-1}) \\ + \dots + f[x_n, \dots, x_0](x - x_n)(x - x_{n-1}) \dots (x - x_1).$$

If, in addition, the nodes are equally spaced with $x = x_n + sh$ and $x = x_i + (s + n - i)h$, then

$$P_n(x) = P_n(x_n + sh) \\ = f[x_n] + sh f[x_n, x_{n-1}] + s(s+1)h^2 f[x_n, x_{n-1}, x_{n-2}] + \dots \\ + s(s+1) \dots (s+n-1)h^n f[x_n, \dots, x_0].$$

This is used to derive a commonly applied formula known as the **Newton backward-difference formula**. To discuss this formula, we need the following definition.

Newton Backward-Difference Formula

$$P_n(x) = f[x_n] + \sum_{k=1}^n (-1)^k \binom{-s}{k} \nabla^k f(x_n) \quad (3.13)$$

Backward Difference table						
i	x_i	f_i	∇f_i	$\nabla^2 f_i$	$\nabla^3 f_i$	$\nabla^4 f_i$
0	x_0	f_0	∇f_1	$\nabla^2 f_2$	$\nabla^3 f_3$	$\nabla^4 f_4$
1	x_1	f_1	∇f_2	$\nabla^2 f_3$	$\nabla^3 f_4$	
2	x_2	f_2	∇f_3	$\nabla^2 f_4$		
3	x_3	f_3	∇f_4			
4	x_4	f_4				

Example 1 Given the following data, estimate $f(1.83)$, using Newton forward difference interpolating polynomial:

i	0	1	2	3	4
x_i	1.0	3.0	5.0	7.0	9.0
f_i	0	1.0986	1.6094	1.9459	2.1972

Solution:

Here we have five data points i.e $i = 0, 1, 2, 3, 4$. Let us first generate the forward difference table.

i	x_i	f_i	Δf_i	$\Delta^2 f_i$	$\Delta^3 f_i$	$\Delta^4 f_i$
0	1.0	0				
1	3.0	1.0986	1.0986	-0.5878	0.4135	
2	5.0	1.6094	0.5108	-0.1743	-0.3244	
3	7.0	1.9459	0.3365	-0.0852	0.0891	
4	9.0	2.1972	0.2513			

$$h = 2, \quad x = 1.83, \quad x_0 = 1.0, \quad s = \frac{x - x_0}{h} = 0.415$$

By putting the above values in the following Newton forward difference interpolating formula:

$$P_n(x) = f(x_0) + \sum_{k=1}^n \binom{s}{k} \Delta^k f(x_0)$$

We get, $P_4(1.83) = 0.567602$. Thus approximate value of $f(1.83) = 0.567602$.

Example 2 Given the following data estimate $f(4.12)$ using Newton backward difference interpolation polynomial:

i	0	1	2	3	4	5
x_i	0	1	2	3	4	5
f_i	1	2	4	8	16	32

Solution:

Here

$$x_n = 5, \quad x = 4.12, \quad h = 1$$

$$\therefore s = \frac{x - x_n}{h} = \frac{4.12 - 5}{1} = -0.88$$

Let us first generate backward difference table:

i	x_i	f_i	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$	$\nabla^5 f$
0	0	1					
1	1	2	1	1	1	1	
2	2	4	2	2	1	1	1
3	3	8	4	4	2	2	
4	4	16	8	8	4		
5	5	32	16				

By putting the above values in the following Newton backward difference interpolating formula:

$$P_n(x) = f[x_n] + \sum_{k=1}^n (-1)^k \binom{-s}{k} \nabla^k f(x_n)$$

We get, $P_5(4.12) = 17.39135$. Thus approximate value of $f(4.12) = 17.39135$.

Curve Fitting or Method of Least Square

The method of least squares is a widely used method of fitting curve for a given data. Curve fitting is the process of constructing a curve, or mathematical function, that has the best fit to a given set of data.

Suppose that the data points are $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$, where x_i are the independent variable and y_i are the dependent variable. The fitting curve $f(x)$ has the deviation (error) e_i from each data point, as follows:

$$\begin{aligned}e_1 &= y_1 - f(x_1) \\e_2 &= y_2 - f(x_2) \\&\vdots \\e_n &= y_n - f(x_n).\end{aligned}$$

According to the method of least squares, the best fitting curve has the property that $\sum_{i=0}^n e_i^2 = \sum_{i=0}^n [y_i - f(x_i)]^2$ is minimum.

We now introduce the method of least squares using polynomials in the following.

Least square fit of a straight line: Suppose given data set is $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$. We are interested in fitting a straight line of the form $f(x) = a + bx$, where a and b are the constant to be determined to the given data. Now residuals is given by

$$e_i = y_i - (a + b x_i) \Rightarrow E = \sum_{i=0}^n e_i^2 = \sum_{i=0}^n [y_i - (a + b x_i)]^2,$$

We need to find a and b such that E is minimum.

The necessary condition for minimum is

$$\begin{aligned}\frac{\partial E}{\partial a} &= 0, \quad \frac{\partial E}{\partial b} = 0 \\ \Rightarrow \frac{\partial E}{\partial a} &= 2 \sum_{i=1}^n [y_i - (a + b x_i)](-1) = 0 = \sum_{i=1}^n [y_i - (a + b x_i)] = 0\end{aligned}$$

and

$$\frac{\partial E}{\partial b} = 2 \sum_{i=1}^n [y_i - (a + b x_i)](-x_i) = 0 \Rightarrow \sum_{i=1}^n [y_i - (a + b x_i)](x_i) = 0.$$

Thus, we get the following equations (are also called normal equations):

$$-an + \sum_{i=1}^n y_i - b \sum_{i=1}^n x_i = 0 \text{ and } \sum_{i=1}^n y_i x_i - a \sum_{i=1}^n x_i - b \sum_{i=1}^n x_i^2 = 0.$$

Solve these equations to get the desired values of a and b .

Example: Obtain the least square straight line fit to the following data:

x	5	10	15	20
$f(x)$	16	19	23	26

Solution: Given that $n = 4$.

Let the straight line be $y = ax + b$.

The normal equations are

$$-an + \sum_{i=0}^n y_i - b \sum_{i=0}^n x_i = 0 \Rightarrow -4a + \sum_{i=1}^4 y_i - b \sum_{i=1}^4 x_i = 0$$

and

$$\begin{aligned} \sum_{i=0}^n y_i x_i - a \sum_{i=0}^n x_i - b \sum_{i=0}^n x_i^2 &= 0 \\ \Rightarrow \sum_{i=1}^4 y_i x_i - a \sum_{i=1}^4 x_i - b \sum_{i=0}^4 x_i^2 &= 0. \end{aligned}$$

To calculate $\sum_{i=1}^4 y_i x_i$, $\sum_{i=1}^4 x_i$, $\sum_{i=0}^4 x_i^2$, we form the below table:

i	x_i	y_i	$x_i y_i$	x_i^2
1	5	16	80	25
2	10	19	190	100
3	15	23	345	225
4	20	26	520	400
Total	$\sum_{i=1}^4 x_i = 50$	$\sum_{i=1}^4 y_i = 84$	$\sum_{i=1}^4 y_i x_i = 1135$	$\sum_{i=0}^4 x_i^2 = 750$

Thus, equations become

$$-4a + 84 - 50b = 0 \Rightarrow 4a + 50b = 84$$

$$1135 - 50a - 750b = 0 \Rightarrow 50a + 750b = 1135.$$

By solving these equations, we get $a = 0.68$, $b = 12.5$.

Hence, the best fitting line is $y = f(x) = 0.68x + 12.5$.

Least square fit of a quadratic polynomial: Suppose given data set is $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$. We are interested in fitting a quadratic polynomial of the form $f(x) = a + bx + cx^2$, where a, b and c are the constant to be determined to the given data. Now residuals is given by

$$e_i = y_i - (a + bx_i + cx_i^2) \Rightarrow E = \sum_{i=0}^n e_i^2 = \sum_{i=0}^n [y_i - (a + bx_i + cx_i^2)]^2,$$

We need to find a and b such that E is minimum.

The necessary condition for minimum is

$$\frac{\partial E}{\partial a} = 0, \quad \frac{\partial E}{\partial b} = 0, \quad \frac{\partial E}{\partial c} = 0$$

$$\Rightarrow \frac{\partial E}{\partial a} = 2 \sum_{i=1}^n [y_i - (a + bx_i + cx_i^2)](-1) = 0$$

$$\Rightarrow \sum_{i=1}^n [y_i - (a + bx_i + cx_i^2)] = 0 ,$$

$$\frac{\partial E}{\partial b} = 2 \sum_{i=1}^n [y_i - (a + bx_i + cx_i^2)](-x_i) = 0$$

$$\Rightarrow \sum_{i=1}^n [y_i - (a + bx_i + cx_i^2)](x_i) = 0$$

and

$$\frac{\partial E}{\partial c} = 2 \sum_{i=1}^n [y_i - (a + bx_i + cx_i^2)](-x_i^2) = 0$$

$$\Rightarrow \sum_{i=1}^n [y_i - (a + bx_i + cx_i^2)](x_i^2) = 0.$$

Thus, we get the following equations (are also called normal equations):

$$-an + \sum_{i=1}^n y_i - b \sum_{i=1}^n x_i - c \sum_{i=1}^n x_i^2 = 0 ,$$

$$\sum_{i=1}^n y_i x_i - a \sum_{i=1}^n x_i - b \sum_{i=1}^n x_i^2 - c \sum_{i=1}^n x_i^3 = 0$$

and

$$\sum_{i=1}^n y_i x_i^2 - a \sum_{i=1}^n x_i^2 - b \sum_{i=1}^n x_i^3 - c \sum_{i=1}^n x_i^4 = 0.$$

Solve these equations to get the desired values of a and b and c .

Example: Obtain the least square quadratic polynomial fit to the following data:

x	5	10	15	20
$f(x)$	16	19	23	26

Solution: Given that $n = 4$.

Let the quadratic polynomial be $y = a + bx + cx^2$.

The normal equations are

$$\begin{aligned} -an + \sum_{i=1}^n y_i - b \sum_{i=1}^n x_i - c \sum_{i=1}^n x_i^2 &= 0 \\ \Rightarrow -4a + \sum_{i=1}^4 y_i - b \sum_{i=1}^4 x_i - c \sum_{i=1}^4 x_i^2 &= 0 \\ \sum_{i=1}^n y_i x_i - a \sum_{i=1}^n x_i - b \sum_{i=1}^n x_i^2 - c \sum_{i=1}^n x_i^3 &= 0 \\ \Rightarrow \sum_{i=1}^4 y_i x_i - a \sum_{i=1}^4 x_i - b \sum_{i=1}^4 x_i^2 - c \sum_{i=1}^4 x_i^3 &= 0 \end{aligned}$$

and

$$\begin{aligned} \sum_{i=1}^n y_i x_i^2 - a \sum_{i=1}^n x_i^2 - b \sum_{i=1}^n x_i^3 - c \sum_{i=1}^n x_i^4 &= 0 \\ \Rightarrow \sum_{i=1}^4 y_i x_i^2 - a \sum_{i=1}^4 x_i^2 - b \sum_{i=1}^4 x_i^3 - c \sum_{i=1}^4 x_i^4 &= 0. \end{aligned}$$

To calculate $\sum_{i=1}^4 y_i x_i$, $\sum_{i=1}^4 y_i x_i^2$, $\sum_{i=1}^4 x_i$, $\sum_{i=1}^4 x_i^2$, $\sum_{i=1}^4 x_i^3$, $\sum_{i=1}^4 x_i^4$, we form the below table:

i	x_i	y_i	$x_i y_i$	x_i^2	x_i^3	x_i^4	$y_i x_i^2$
1	5	16	80	25	125	1875	400
2	10	19	190	100	1000	10000	1900
3	15	23	345	225	3375	50625	5175
4	20	26	520	400	8000	160000	10400
Total	$\sum_{i=1}^4 x_i = 50$	$\sum_{i=1}^4 y_i = 84$	$\sum_{i=1}^4 y_i x_i = 1135$	$\sum_{i=1}^4 x_i^2 = 750$	$\sum_{i=1}^4 x_i^3 = 12500$	$\sum_{i=1}^4 x_i^4 = 222500$	$\sum_{i=1}^4 y_i x_i^2 = 17875$

Thus, equations become

$$\begin{aligned} -4a + 84 - 50b - 750c &= 0, \\ 1135 - 50a - 750b - 12500c &= 0, \\ \text{and } 17875 - 750a - 12500b - 222500c &= 0. \end{aligned}$$

By solving these equations, we can get the values of a , b and c .

Least square fit of a general function: Suppose given data set is $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$. We are interested in fitting a general function

$f(x, a, b, \dots)$, where a, b, \dots are the constant to be determined to the given data.
Now residuals is given by

$$e_i = y_i - (f(x_i, a, b, \dots)) \Rightarrow E = \sum_{i=0}^n e_i^2 = \sum_{i=0}^n [y_i - (f(x_i, a, b, \dots))]^2,$$

We need to find a and b such that E is minimum.

The necessary condition for minimum is

$$\frac{\partial E}{\partial a} = 0, \quad \frac{\partial E}{\partial b} = 0, \dots .$$

Thus, we get the values of constants from the normal equations obtained from the above conditions.

Example: Use the method of least square to fit the curve $f(x) = c_0 x + \frac{c_1}{\sqrt{x}}$ to the following data:

x	0.2	0.4	0.6	0.8	1.0
$f(x)$	16	14	11	6	3

Solution: Given that $n = 5$.

Let the function be $y = c_0 x + \frac{c_1}{\sqrt{x}}$.

By least square method, we minimize the error

$$E(c_0, c_1) = \sum_{i=1}^5 \left(y_i - \left(c_0 x_i + \frac{c_1}{\sqrt{x_i}} \right) \right)^2.$$

The normal equations are given by $\frac{\partial E}{\partial c_0} = 0, \quad \frac{\partial E}{\partial c_1} = 0,$

$$\begin{aligned} \sum_{i=1}^5 y_i x_i - c_0 \sum_{i=1}^5 x_i^2 - c_1 \sum_{i=1}^5 \frac{x_i}{\sqrt{x_i}} &= 0 \\ \Rightarrow \sum_{i=1}^5 y_i x_i - c_0 \sum_{i=1}^5 x_i^2 - c_1 \sum_{i=1}^5 \sqrt{x_i} &= 0 \end{aligned}$$

and

$$\begin{aligned} \sum_{i=1}^5 \frac{y_i}{\sqrt{x_i}} - c_0 \sum_{i=1}^5 \sqrt{x_i} - c_1 \sum_{i=1}^5 \frac{1}{\sqrt{x_i} \cdot \sqrt{x_i}} &= 0 \\ \Rightarrow \sum_{i=1}^5 \frac{y_i}{\sqrt{x_i}} - c_0 \sum_{i=1}^5 \sqrt{x_i} - c_1 \sum_{i=1}^5 \frac{1}{x_i} &= 0 \end{aligned}$$

To calculate $\sum_{i=1}^5 \frac{1}{x_i}$, $\sum_{i=1}^5 \sqrt{x_i}$, $\sum_{i=1}^5 y_i x_i$, $\sum_{i=1}^5 \frac{y_i}{\sqrt{x_i}}$, $\sum_{i=1}^5 x_i^2$, we form the below table:

i	x_i	y_i	$y_i x_i$	$\sqrt{x_i}$	$\frac{1}{x_i}$	$\frac{y_i}{\sqrt{x_i}}$	x_i^2
1	0.2	16	3.2	0.4472	5	$\frac{35.778}{2}$	0.04
2	0.4	14	5.6	0.6325	2.5	$\frac{22.134}{4}$	0.16
3	0.6	11	6.6	0.7746	1.6667	$\frac{14.200}{9}$	0.36
4	0.8	6	4.8	0.8944	1.25	6.7084	0.64
5	1.0	3	3.0	1	1	3	1.0
Total	$\sum_{i=1}^5 x_i = 3$	$\sum_{i=1}^5 y_i = 50$	$\sum_{i=1}^5 y_i x_i = 23.2$	$\sum_{i=1}^5 \sqrt{x_i} = 3.7487$	$\sum_{i=1}^5 \frac{1}{x_i} = 11.4167$	$\sum_{i=1}^5 \frac{y_i}{\sqrt{x_i}} = 81.8219$	$\sum_{i=0}^5 x_i^2 = 2.2$

Thus, equations become $23.2 - 2.2c_0 - 3.7487c_1 = 0$
and $81.8219 - 3.7487c_0 - 11.4167c_1 = 0$

By solving these equations, we can get the values of c_0 and c_1 .

Example: Use the method of least square to fit the curve $f(x) = a b^x$ to the following data:

x	0.2	0.4	0.6	0.8	1.0
$f(x)$	16	14	11	6	3

Solution: Given that $n = 5$.

After taking log on both sides of the given curve $y = a b^x$, we get the form $= A + Bx$, where $Y = \log y$, $A = \log a$ and $B = \log b$.

Hence the normal equations are given by

$$-5a + \sum_{i=1}^5 Y_i - b \sum_{i=1}^5 x_i = 0 \text{ and } \sum_{i=1}^5 Y_i x_i - a \sum_{i=1}^5 x_i - b \sum_{i=1}^5 x_i^2 = 0.$$

To calculate $\sum_{i=1}^5 Y_i x_i$, $\sum_{i=1}^5 x_i$, $\sum_{i=0}^5 x_i^2$, $\sum_{i=1}^5 Y_i$ we form the below table:

i	x_i	y_i	$Y_i = \log y_i$	$Y_i x_i$	x_i^2
1	0.2	16	1.2041	0.2408	0.04
2	0.4	14	1.1461	0.4584	0.16
3	0.6	11	1.0414	0.6248	0.36
4	0.8	6	0.7782	0.6226	0.64
5	1.0	3	0.4771	0.4771	1.0
Total	$\sum_{i=1}^5 x_i = 3$	$\sum_{i=1}^5 y_i = 50$	$\sum_{i=0}^5 Y_i = 4.6469$	$\sum_{i=0}^5 Y_i x_i = 2.4237$	$\sum_{i=0}^5 x_i^2 = 2.2$

Thus, equations become

$$-5a + 4.6469 - 3b = 0$$

$$2.4237 - 3a - 2.2b = 0.$$

By solving these equations, we get the values of A and B . So, we can get the values of a and b by taking antilog in $A = \log a$ and $B = \log b$.