CHAPTER 2

simultaneous Non-Linear Equations

2.1 Introduction

In this chapter, we consider the problem of finding roots of simultaneous nonlinear equations. For the sake of simplicity, we shall consider only the case of two equations in two unknowns. We take the equations in the forms:

$$\left.\begin{aligned} f(x,y) &= 0 \\ g(x,y) &= 0 \end{aligned}\right\} . \tag{2.1}$$

2.2 Numerical Methods

We shall study three numerical methods to solve system (2.1):

2.2.1 Fixed-Point Iteration

As a first step in applying fixed-point iteration, we rewrite these equations in the following equivalent forms:

$$\left.\begin{aligned} x &= F(x,y) \\ y &= G(x,y) \end{aligned}\right\} . \tag{2.2}$$

so that any solution of (2.2) is a solution of (2.1), and conversely. Let (λ,μ) be a solution of (2.1), i.e.

$$\left.\begin{aligned} f(\lambda,\mu) &= 0 \\ g(\lambda,\mu) &= 0 \end{aligned}\right\} .$$

Let (x_0,y_0) be an approximation to (λ,μ). Generate successive approximations from the recursion:

$$\left.\begin{aligned} x_{i+1} &= F(x_i,y_i) \\ y_{i+1} &= G(x_i,y_i) \end{aligned}\right\} , \ i = 0,1,2,\cdots . \tag{2.3}$$

Stop iteration if $|x_{i+1} - x_i| < \epsilon$ and $|y_{i+1} - y_i| < \epsilon$ for any i.

Note 2.1. It is shown in the above analysis that this iteration will converge under the following (but not necessary) conditions:

(a). F and G and their first partial derivatives be continuous in a neighborhood $\Re$ of the roots (λ, μ), where $\Re$ consists of all (x, y) with $|x - \lambda| \leq \epsilon$, $|y - \mu| \leq \epsilon$, for some positive ϵ.

(b). The following inequalities are satisfied:

$$\left.\begin{array}{l}|F_x|+|G_x|\leqslant K\\ |F_y|+|G_y|\leqslant K\end{array}\right\}\text{ for all points }(x,y)\text{ in }\Re\text{ and some }K<1.$$

(c). The initial approximations (x_0, y_0) is chosen in $\Re$.

Note 2.2. When this iteration does converge it converges linearly.

To proof Note 2.1(b):
Let

$$\begin{array}{l}x_1=F(x_0,y_0)\\ y_1=G(x_0,y_0)\end{array}\quad\text{and}\quad\begin{array}{l}\lambda=F(\lambda,\mu)\\ \mu=G(\lambda,\mu)\end{array}.$$

Hence
$\lambda-x_1=F(\lambda,\mu)-F(x_0,y_0)$

$\mu-y_1=G(\lambda,\mu)-G(x_0,y_0)$.
By suing **Taylor series expansion** of $F(\lambda,\mu)$ and $G(\lambda,\mu)$ about x_0 and y_0, we get:

$$F(\lambda,\mu)=F(x_0,y_0)+(\lambda-x_0)(F_x)_{(x_0,y_0)}+(\mu-y_0)\left(F_y\right)_{(x_0,y_0)}+\cdots$$
$$G(\lambda,\mu)=G(x_0,y_0)+(\lambda-x_0)(G_x)_{(x_0,y_0)}+(\mu-y_0)\left(G_y\right)_{(x_0,y_0)}+\cdots.$$

Let

$$K=\max\left\{|F_x|_{(x_0,y_0)}+|G_x|_{(x_0,y_0)},\ \ |F_y|_{(x_0,y_0)}+|G_y|_{(x_0,y_0)}\right\}.$$

$$\begin{aligned}\therefore |\lambda-x_1|+|\mu-y_1| &\leqslant |\lambda-x_0|\left\{|F_x|_{(x_0,y_0)}+|G_x|_{(x_0,y_0)}\right\}\\ &\quad+|\mu-y_0|\left\{\ |F_y|_{(x_0,y_0)}+|G_y|_{(x_0,y_0)}\right\}\\ &\leq K\left\{|\lambda-x_0|+|\mu-y_0|\right\}.\end{aligned}$$

Similarly,

$$\begin{aligned}|\lambda-x_2|+|\mu-y_2| &\leqslant K\left\{|\lambda-x_1|+|\mu-y_1|\right\}\\ &\leq K^2\left\{|\lambda-x_0|+|\mu-y_0|\right\}.\end{aligned}$$

Finally, we get:

$$|\lambda-x_n|+|\mu-y_n|\leqslant K^n\left\{|\lambda-x_0|+|\mu-y_0|\right\}.$$

The value of $|\lambda-x_n|$ and $|\mu-y_n|$ must approach to zero and this happens, when $K<1$; $K_n\longrightarrow 0$ as $n\longrightarrow\infty$. Hence, the condition $K<1$ is sufficient to force the convergence.

2.2.2 Newton-Raphson Method

To adapt Newton-Raphson method to simultaneous equations, we proceed as follows:
Let (x_0, y_0) be an approximation to the solution (λ,μ) of (2.1). Assuming that f and g

are sufficiently differentiable, expand $f(x,y)$, $g(x,y)$ about $(x_0,\, y_0)$ using Taylor series for functions of two variables:

$$0 = f(x,y) = f(x_0,y_0) + f_x(x_0,y_0)(x-x_0) + f_y(x_0,y_0)(y-y_0) + \cdots$$
$$0 = g(x,y) = g(x_0,y_0) + g_x(x_0,y_0)(x-x0) + g_y(x_0,y_0)(y-y_0) + \cdots .$$

Assuming that (x_0,y_0) sufficiently closed to (λ,μ) so that higher order terms can be neglected, we, therefore, equate the expansion through linear terms to zero. This gives us the system:

$$\left.\begin{aligned} f_x(x-x_0) + f_y(y-y_0) &\approx -f(x_0,y_0) \\ g_x(x-x_0) + g_y(y-y_0) &\approx -g(x_0,y_0) \end{aligned}\right\}, \tag{2.4}$$

where it is understood that all functions and derivatives in (2.4) are to be evaluated at (x_0,y_0). We might then expect that the solution (x_1,y_1) of (2.4) will be closer to the solution of (λ,μ) than (x_0,y_0). The solution of (2.4) by **Cramer's rule** yields

$$x_1 - x_o = \frac{\begin{vmatrix} -f & f_y \\ -g & g_y \end{vmatrix}_{(x_0,y_0)}}{\begin{vmatrix} f_x & f_y \\ g_x & g_y \end{vmatrix}_{(x_0,y_0)}} = \left[\frac{-fg_y + gf_y}{J(f,g)}\right]_{(x_0,y_0)},$$

$$y_1 - y_o = \frac{\begin{vmatrix} f_x & -f \\ g_x & -g \end{vmatrix}_{(x_0,y_0)}}{\begin{vmatrix} f_x & f_y \\ g_x & g_y \end{vmatrix}_{(x_0,y_0)}} = \left[\frac{-gf_x + fg_x}{J(f,g)}\right]_{(x_0,y_0)},$$

provided that $J(f,g) = f_xg_y - g_xf_y \neq 0$ at (x_0,y_0). The function $J(f,g)$ is called the **Jacobian** of the functions f and g. The solution (x_1,y_1) of this system now provides a new approximation to (λ,μ). Repetition of this process leads to Newton-Raphson method for systems

$$\left.\begin{aligned} x_{i+1} &= x_i - \left[\frac{fg_y - gf_y}{J(f,g)}\right]_{(x_i,y_i)} \\ y_{i+1} &= y_i - \left[\frac{gf_x - fg_x}{J(f,g)}\right]_{(x_i,y_i)} \end{aligned}\right\}, \text{ for } i = 0,1,\cdots .$$

where $J(f,g) = f_xg_y - g_xf_y$ and where all functions involved are to be evaluated at (x_i,y_i).

Also, the iteration formula can be written as follows:

$$\begin{bmatrix} x_{i+1} \\ y_{i+1} \end{bmatrix} = \begin{bmatrix} x_i \\ y_i \end{bmatrix} - \left(J(f,g)_{(x_i,y_i)}\right)^{-1} \begin{bmatrix} f(x_i,y_i) \\ g(x_i,y_i) \end{bmatrix}; i = 0,1,2,\cdots .$$

Stop iteration if $|x_{i+1} - x_i| < \epsilon$ and $|y_{i+1} - y_i| < \epsilon$ for any i.

When this iteration converges, it converges quadratically.

Note 2.3. A set of conditions sufficient to ensure convergence is the following:

i f, g and all their derivatives through second order are continuous and bounded in a region $\Re$ containing (λ, μ).

ii The Jacobian $J(f, g)$ does not vanish in $\Re$.

iii The initial approximation (x_0, y_0) is chosen sufficiently close to the root (λ, μ).

Example 2.1. Solve the system

$$\begin{aligned} x^2 + y^2 &= 1 \\ x^2 - y^2 &= -0.5, \end{aligned}$$

at $(x_0, y_0) = (0.5, 0.5)$.
Solution: Let

$$\begin{aligned} f(x,y) &= x^2 + y^2 - 1 = 0 \\ g(x,y) &= x^2 - y^2 + 0.5 = 0. \end{aligned}$$

$\therefore f_x = 2x,\ \ f_y = 2y,\ \ g_x = 2x,\ \ g_y = -2y$. At $(x_0, y_0) = (0.5, 0.5)$, we see that

$$\begin{aligned} &f(0.5, 0.5) = -0.5, \quad f_x(0.5, 0.5) = 1, \quad f_y(0.5, 0.5) = 1, \\ &g(0.5, 0.5) = 0.5, \quad g_x(0.5, 0.5) = 1, \quad g_y(0.5, 0.5) = -1. \end{aligned}$$

Hence

$$\begin{aligned} x_1 &= x_0 - \left[\frac{fg_y - gf_y}{J(f,g)}\right]_{(x_0,y_0)} = 0.5 - \left[\frac{(-0.5 \times -1) - (0.5 \times 1)}{(1 \times -1) - (1 \times 1)}\right] \\ &= 0.5 + \frac{0}{2} = 0.5, \end{aligned}$$

and

$$\begin{aligned} y_1 &= y_0 - \left[\frac{gf_x - fg_x}{J(f,g)}\right]_{(x_0,y_0)} = 0.5 - \left[\frac{(0.5 \times 1) - (-0.5 \times 1)}{(1 \times -1) - (1 \times 1)}\right] \\ &= 0.5 + \frac{1}{2} = 1. \end{aligned}$$

Similarly, at $(x_1, y_1) = (0.5, 1)$, we see that

$$\begin{aligned} &f(0.5, 1) = 0.25, \quad f_x(0.5, 1) = 1, \quad f_y(0.5, 1) = 2, \\ &g(0.5, 1) = -0.25, \quad g_x(0.5, 1) = 1, \quad g_y(0.5, 1) = -2. \end{aligned}$$

Hence

$$x_2 = x_1 - \left[\frac{fg_y - gf_y}{J(f,g)}\right]_{(x_1,y_1)} = 0.5 - \left[\frac{(0.25 \times -2) - (-0.25 \times 2)}{(1 \times -2) - (2 \times 1)}\right] = 0.5$$

and

$$y_2 = y_1 - \left[\frac{gf_x - fg_x}{J(f,g)}\right]_{(x_1,y_1)} = 1 - \left[\frac{(-0.25 \times 1) - (0.25 \times 1)}{(1 \times -2) - (2 \times 1)}\right] = 0.875.$$

For the other values, we obtain:

i	x_i	y_i	$f(x_i, y_i)$	$g(x_i, y_i)$
3	0.5	0.8660714	0.000079706	-0.000079713
4	0.5	0.8660254	0.000000007	0.000000007
5	0.5	0.866254	0.000000007	0.000000007

Example 2.2. Use two iterations of the Newton-Raphson method to approximate the solution to

$$x^2 + y^2 = 5$$
$$y - x^2 = -1.$$

Use $x_0 = y_0 = 1.5$ as an initial guess.
Solution: Let

$$f(x,y) = x^2 + y^2 - 5 \text{ and } g(x,y) = -x^2 + y + 1.$$

Thus:

$$f_x = 2x, \quad f_y = 2y, \quad g_x = -2x, \quad \text{and} \quad g_y = 1.$$

Hence, when $x = y = 1.5$, we find that:

$$f_x(x_0,y_0) = 2(1.5) = 3, \quad f_y(x_0,y_0) = 2(1.5) = 3,$$
$$g_x(x_0,y_0) = -2(1.5) = -3, \quad g_y(x_0,y_0) = 1.$$

Also

$$f(x_0,y_0) = (1.5)^2 + (1.5)^2 - 5 = -0.5,$$
$$g(x_0,y_0) = -(1.5)^2 + 1.5 + 1 = 0.25,$$
$$(f_x g_y - f_y g_x)_{(x_0,y_0)} = (3)(1) - (3)(-3) = 12.$$

So, for the first iteration, we see that:

$$x_1 = 1.5 - \frac{(-0.5)(1) - (0.25)(3)}{12} \approx 1.604,$$
$$y_1 = 1.5 - \frac{(0.25)(3) - (-0.5)(-3)}{12} \approx 1.5625.$$

Now we find that iteration 2 produces:

$$f_x(x_1,y_1) = 2(1.604) = 3.208, \quad f_y(x_1,y_1) = 2(1.5625) = 3.125,$$
$$g_x(x_1,y_1) = -2(1.604) = -3.208, \quad g_y(x_1,y_1) = 1.$$

Also,

$$\begin{aligned}
f(x_1, y_1) &= (1.604)^2 + (1.5625)^2 - 5 = 0.1422, \\
g(x_1, y_1) &= -(1.604)^2 + 1.5625 + 1 = -0.0103, \\
(f_x g_y - f_y g_x)_{(x_1,y_1)} &= (3.208)(1) - (3.125)(-3.208) = 13.233.
\end{aligned}$$

So for the second iteration we see that:

$$\begin{aligned}
x_2 &= 1.604 - \frac{(0.1422)(1) - (-0.0103)(3.125)}{13.233} \approx 1.591, \\
y_2 &= 1.5625 - \frac{(-0.0103)(3.208) - (0.1422)(-3.208)}{13.233} \approx 1.5623.
\end{aligned}$$

2.2.3 Modified Newton-Raphson Method

Newton-Raphson method is not very easy in general for n simultaneous equations in n unknowns. But in Modified Newton-Raphson method for (2.1), we use the idea of Newton-Raphson method for single variable as follows:

$$\left.\begin{aligned}
x_{i+1} &= x_i - \left[\frac{f(x,y)}{f_x(x,y)}\right]_{(x_i,y_i)} \\
y_{i+1} &= y_i - \left[\frac{g(x,y)}{g_y(x,y)}\right]_{(x_{i+1},y_i)}
\end{aligned}\right\}, \text{ for } i = 0, 1, \cdots . \tag{2.5}$$

Stop iteration if $|x_{i+1} - x_i| < \epsilon$ and $|y_{i+1} - y_i| < \epsilon$ for any i. Also, for nonlinear system:

$$\begin{aligned}
f(x,y,z) &= 0 \\
g(x,y,z) &= 0 \\
h(x,y,z) &= 0,
\end{aligned}$$

we have:

$$\begin{aligned}
x_{i+1} &= x_i - \left[\frac{f(x,y,z)}{f_x(x,y,z)}\right]_{(x_i,y_i,z_i)}, \\
y_{i+1} &= y_i - \left[\frac{g(x,y,z)}{g_y(x,y,z)}\right]_{(x_{i+1},y_i,z_i)}, \\
z_{i+1} &= z_i - \left[\frac{h(x,y,z)}{h_z(x,y,z)}\right]_{(x_{i+1},y_{i+1},z_i)},
\end{aligned}$$

for $i = 0, 1, \cdots$.
Stop iteration if $|x_{i+1} - x_i| < \epsilon$, $|y_{i+1} - y_i| < \epsilon$ and $|z_{i+1} - z_i| < \epsilon$ for any i.

Example 2.3. Solve nonlinear system

$$\begin{aligned}
f(x,y) &= e^x + xy - 1 = 0 \\
g(x,y) &= \sin(xy) + x + y - 1 = 0.
\end{aligned}$$

By using modified Newton-Raphson method with $x_0 = 0.1,\ \ y_0 = 0.5$, carry out two iterations only. It is easily verified that $x = 0,\ \ y = 1$ is a solution of the above system.

Solution: We compute the first partial derivatives

$$f_x(x,y) = e^x + y \ \text{ and } \ g_y(x,y) = x\cos(xy) + 1.$$

Then, the iteration (2.5) becomes:

$$\left.\begin{aligned} x_{i+1} &= x_i - \frac{e^{x_i} + x_i y_i - 1}{e^{x_i} + y_i} \\ y_{i+1} &= y_i - \frac{\sin(x_{i+1}\ y_i) + x_{i+1} + y_i - 1}{x_{i+1}\cos(x_{i+1}\ \ y_i) + 1} \end{aligned}\right\}. \tag{2.6}$$

We obtain from (**??**) for the next two approximations:

$$x_1 = -0.02, \quad y_1 = 1.34,$$

and

$$x_2 = 0.00009, \quad y_2 = 0.99979.$$

2.3 Exercises

1. Find an approximate solution of the following system, using Newton-Rahpson method:

$$\begin{aligned} x^2\,y + y^3 &= 10 \\ x\,y^2 - x^2 &= 3, \end{aligned}$$

with $(x_0\ ,\ y_0) = (0.8\,,\,2.2)$ and $\varepsilon = 10^{-2}$.

2. A solution of the system

$$\begin{aligned} x^2\ + y^2 &= 1 \\ xy &= 0 \end{aligned}$$

is $x = 1,\ \ y = 0$. Use Fixed-point method with $x_0 = 0.5,\ \ y_0 = 0.1$ to solve the system, carry out three iterations only.

3. Find an approximate solution of the following system, using modified Newton-Rahpson method:

$$\begin{aligned} x^2 + xy^3 &= 9 \\ 3x^2\,y - y^3 &= 4, \end{aligned}$$

with $(x_0\ ,\ y_0) = (1.2\,,\,2.5)$ and $\varepsilon = 10^{-1}$.

CHAPTER 3

Interpolation and Numerical Differentiation

3.1 Introduction

In this chapter, we discuss the problem of approximating a given function by polynomials. There are two main uses of these approximating polynomials. The ***first use*** is to reconstruct the function $f(x)$ when it is not given explicitly and only values of $f(x)$ and/or its certain order derivatives are given at a set of distinct points called nodes or tabular points. The ***second use*** is to perform the required operations which were intended for $f(x)$, like determination of roots, differentiation and integration, etc. can be carried out using the approximating polynomial $P(x)$. The approximating polynomial $P(x)$ can be used to predict the value of at a non-tabular point. The deviation of $P(x)$ from $f(x)$, that is $f(x) - P(x)$, is called the error of approximation. And also various industrial, business and research organizations routinely collect and analyze data. We shall investigate the collected data in the form of two variables which we label x and y.

3.2 The finite difference calculus

Given a discrete function $f(x_k) = y_k$, $k = 0, 1, \cdots, n$, that is, each argument x_k has a mate y_k and suppose that the arguments (nodes) are equally spaced so that $x_{k+1} = x_k + h$, $k = 0, 1, \cdots, n-1$ where h is the subinterval widths. Then, we define the following difference operators of the y_k.

3.2.1 Shifting Operator (E)

This operator is defined as:
$Ef(x) = f(x+h)$, i.e. $Ey_0 = y_1$,
$E^2 f(x) = f(x+2h)$, i.e. $E^2 y_0 = y_2$,
$\vdots$
$E^k f(x) = f(x+kh)$, i.e. $E^k y_0 = y_k$.
In general,
$E^k y_i = y_{i+k}$ for $i = 0, 1, \cdots$ and $k = 1, 2, \cdots$.

3.2.2 Forward Difference Operator (Δ)]

This operator is defined as follows:
$\Delta f(x_0) = f(x_0 + h) - f(x_0)$ or $\Delta y_k = y_{k+1} - y_k$ where $k = 0, 1, 2, \cdots$ i.e. $\Delta y_0 = y_1 - y_0$ or $\Delta y_0 = Ey_0 - y_0 = (E-1)y_0$ which implies that $\Delta = E - 1$.
The difference $\Delta y_k = y_{k+1} - y_k$ is called first difference and the second difference is

denoted by

$$\Delta^2 y_k = \Delta(\Delta y_k) = \Delta(y_{k+1} - y_k) = \Delta y_{k+1} - \Delta y_k = y_{k+2} - 2y_{k+1} + y_k.$$

In general,

$$\Delta^n y_i = \sum_{j=0}^{n} (-1)^j \left(\begin{array}{c} n \\ j \end{array} \right) y_{i+n-j} \quad \text{or} \quad \Delta^n f(x) = \sum_{j=0}^{n} (-1)^j \left(\begin{array}{c} n \\ j \end{array} \right) f(x+jh),$$

where

$$\left(\begin{array}{c} n \\ j \end{array} \right) = \frac{n!}{j!(n-j)!}.$$

Example 3.1. Prove the following concepts

(i) If $f(x) = c$, then $\Delta f(x) = 0$.

(ii) If $f(x) = ax^2 + bx + c$, then $\Delta^2 f(x) = 2ah^2$ and $\Delta^3 f(x) = 0$.

(iii) if $p(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$, then $\Delta^n p(x) = n! a_n h^n$ and $\Delta^{n+1} p(x) = 0$.

Solution:
(i) $\Delta f(x) = f(x+h) - f(x) = c - c = 0$.
(ii) $\Delta f(x) = f(x+h) - f(x) = a(x+h)^2 + b(x+h) + c - ax^2 - bx - c$
$= 2axh + ah^2 + bh.$
$\Delta^2 f(x) = \Delta f(x+h) - \Delta f(x) = (2a(x+h)h + ah^2 + bh)$
$-(2axh - ah^2 - bh) = 2ah^2.$
$\Delta^3 f(x) = \Delta(\Delta^2 f(x)) = \Delta^2 f(x+h) - \Delta^2 f(x) = 2ah^2 - 2ah^2 = 0.$
(iii) Left to the reader as an exercise.

Example 3.2. show that
$\Delta(u(x)v(x)) = u(x)\Delta v(x) + v(x+h)\Delta u(x)$ Or $\Delta u_i v_i = u_i \Delta v_i + v_{i+1}\Delta u_i$.

Solution:

$$\begin{aligned}
\Delta(u(x)v(x)) &= u(x+h)v(x+h) - u(x)v(x) \\
&= u(x+h)v(x+h) - u(x)v(x) - v(x+h)u(x) + v(x+h)u(x) \\
&= v(x+h)[u(x+h) - u(x)] + u(x)[v(x+h) - v(x)] \\
&= u(x)\Delta v(x) + v(x+h)\Delta u(x).
\end{aligned}$$

From the above, we can form the following forward difference table:

i	$f(x)$	Δ	Δ^2	Δ^3	Δ^4
$\vdots$	$\vdots$				
x_{-2}	y_{-2}				
		Δy_{-2}			
x_{-1}	y_{-1}		$\Delta^2 y_{-2}$		
		Δy_{-1}		$\Delta^3 y_{-2}$	
x_0	y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$
		Δy_0		$\Delta^3 y_{-1}$	
x_1	y_1		$\Delta^2 y_0$		$\Delta^4 y_{-1}$
		Δy_1		$\Delta^3 y_0$	
x_2	y_2		$\Delta^2 y_1$		
		Δy_2			
x_3	y_3				
$\vdots$	$\vdots$				

Example 3.3. Construct the forward difference table for the following values:

(*i*) (0, 1), (1, 5), (2, 31), (3, 121) and (4, 341). (*ii*) (1, 0), (2, 5), (3, 22), (4, 57), (5, 116), (6, 205).

Solution:

(*i*)

x	$f(x)$	Δ	Δ^2	Δ^3	Δ^4
0	1				
		4			
1	5		22		
		26		42	
2	31		64		24
		90		66	
3	121		130		
		220			
4	341				

(*ii*)

x	$f(x)$	Δ	Δ^2	Δ^3	Δ^4
1	0				
		5			
2	5		12		
		17		6	
3	22		18		0
		35		6	
4	57		24		0
		59		6	
5	116		30		
		89			
6	205				

3.2.3 Backward Difference Operator (∇)]

This operator is defined as follows:

$\nabla y_i = y_i - y_{i-1}; \quad i = 1, 2, \cdots$

$$\nabla^2 y_i = \nabla(\nabla y_i) = \nabla(y_i - y_{i-1}) = \nabla y_i - \nabla y_{i-1}$$
$$= (y_i - y_{i-1}) - (y_{i-1} - y_{i-2}) = y_i - 2y_{i-1} + y_{i-2}.$$

In general, $\nabla^n y_i = \sum\limits_{j=0}^{n} (-1)^j \begin{pmatrix} n \\ j \end{pmatrix} y_{i-j}$, for any i and any natural number n. From the above, we can form the following backward difference table:

i	$f(x)$	∇	∇^2	∇^3	∇^4
$\vdots$	$\vdots$				
x_{-2}	y_{-2}				
		∇y_{-1}			
x_{-1}	y_{-1}		$\nabla^2 y_0$		
		∇y_0		$\nabla^3 y_1$	
x_0	y_0		$\nabla^2 y_1$		$\nabla^4 y_2$
		∇y_1		$\nabla^3 y_2$	
x_1	y_1		$\nabla^2 y_2$		$\nabla^4 y_3$
		∇y_2		$\nabla^3 y_3$	
x_2	y_2		$\nabla^2 y_3$		
		∇y_3			
x_3	y_3				
$\vdots$	$\vdots$				

Example 3.4. Show that $\nabla^i y_0 = \Delta^i y_{-1}$.
Solution: It is left to the reader as an exercise.

3.2.4 Divided Difference Operator

Given a discrete function $f(x_k) = y_k$, that is, each argument x_k has a mate y_k and supposing that the arguments x_k, $k = 0, 1, \cdots$ are equally or unequally spaced points. Then we define the divided difference table $f[.,.]$ as follows:

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

$$\begin{aligned} f[x_i, x_{i+1}, x_{i+2}] &= \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i} \\ &= \frac{\frac{f[x_{i+2}] - f[x_{i+1}]}{x_{i+2} - x_{i+1}} - \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}}{x_{i+2} - x_i} \\ &= \frac{\frac{y_{i+2} - y_{i+1}}{x_{i+2} - x_{i+1}} - \frac{y_{i+1} - y_i}{x_{i+1} - x_i}}{x_{i+2} - x_i}. \end{aligned}$$

In general,

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

Note 3.1.

$$f[x_i, x_{i+1}] = f[x_{i+1}, x_i],$$
$$f[x_i, x_j, x_k] = f[x_j, x_i, x_k] = f[x_j, x_k, x_i] \cdots .$$

From the above, we can form the following divided difference table:

i	$f(x)$	$f[.,.]$	$f[.,.,.]$	$f[.,.,.,.]$	$f[.,.,.,.,.]$
x_0	y_0				
		$f[x_0, x_1]$			
x_1	y_1		$f[x_0, x_1, x_2]$		
		$f[x_1, x_2]$		$f[x_0, x_1, x_2, x_3]$	
x_2	y_2		$f[x_1, x_2, x_3]$		$f[x_0, x_1, x_2, x_3, x_4]$
		$f[x_2, x_3]$		$f[x_1, x_2, x_3, x_4]$	
x_3	y_3		$f[x_2, x_3, x_4]$		
		$f[x_3, x_4]$			
x_4	y_4				
$\vdots$	$\vdots$				

3.3 Interpolation

Interpolation is a method used in numerical analysis to approximate functions or to estimate the value of a function $f(x)$ for arguments between x_0, x_1, $\cdots$, x_n at which the values y_0, y_1, $\cdots$, y_n are known.

3.3.1 Interpolation Problem

Let x_0, x_1, $\cdots$, x_n be $(n+1)$ distinct points on the x-axis, and $f(x)$ be a real-valued function defined on $[a, b]$ such that

$$a = x_0 < x_1 < \cdots < x_n = b. \tag{3.1}$$

Suppose we know the values of f at these points. Let

$$y_i = f(x_i), \quad i = 0, 1, \cdots, n. \tag{3.2}$$

We want to prove the existence and uniqueness of a polynomial $p_n(x)$ of degree$\leq n$ which interpolates (takes the same values as) $f(x)$ at the given $(n+1)$ distinct points. That is, it satisfies:

$$p_n(x_i) = y_i = f(x_i), \quad i = 0, 1, \cdots, n. \tag{3.3}$$

This polynomial will be constructed and called the **interpolation polynomial**.

Lagrange Interpolation Polynomial

Suppose that a polynomial

$$p_n(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0, \tag{3.4}$$

of degree n satisfies (3.3). Then, the condition that this polynomial must pass through this $(n+1)$ points leads to $(n+1)$ equations for the $(n+1)$ unknown's ai as follows:

$$\begin{aligned}
f(x_0) &= a_n x_0^n + a_{n-1}x_0^{n-1} + \cdots + a_1 x_0 + a_0\\
f(x_1) &= a_n x_1^n + a_{n-1}x_1^{n-1} + \cdots + a_1 x_1 + a_0\\
&\vdots\\
f(x_n) &= a_n x_n^n + a_{n-1}x_n^{n-1} + \cdots + a_1 x_n + a_0.
\end{aligned}$$

We find the values of a_i's by solving the above linear system of equations. Then, put the value of a_i's in (3.4) and add the coefficients, we get:

$$p_n(x) = \sum_{k=0}^{n} L_n^k(x) f(x_k), \tag{3.5}$$

where,

$$\begin{aligned}
L_n^k(x) &= \frac{(x-x_0)(x-x_1)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)}{(x_k-x_0)(x_k-x_1)\cdots(x_k-x_{k-1})(x_k-x_{k+1})...(x_k-x_n)}\\
&= \prod_{\substack{i=0\\ i\neq k}}^{n}\left(\frac{x-x_i}{x_k-x_i}\right),
\end{aligned} \tag{3.6}$$

such that

$$L_n^k(x_i) = \delta_{ki} = \begin{cases} 0 \text{ if } k \neq i\\ 1 \text{ if k = i.}\end{cases} \tag{3.7}$$

The polynomials in (3.6) are called **Lagrange polynomial** and (3.5) is of degree$\leq n$ and is ***called Lagrange interpolation polynomial***.
For $n = 1$:

$$p_1(x) = \sum_{k=0}^{1} L_1^k(x) f(x_k) = L_1^0(x) f(x_0) + L_1^1(x) f(x_1),$$

where $l_1^0(x) = \frac{x-x_1}{x_0-x_1}$ and $l_1^1(x) = \frac{x-x_0}{x_1-x_0}$.
For $n = 2$:

$$p_2(x) = \sum_{k=0}^{2} L_2^k(x) f(x_k) = L_2^0(x) f(x_0) + L_2^1(x) f(x_1) + L_2^2(x) f(x_2),$$

where

$$
\begin{aligned}
l_2^0(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \\
l_2^1(x) &= \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \\
l_2^2(x) &= \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_1-x_1)}.
\end{aligned}
$$

And so on, ...

To explain the procedure for deriving Lagrange interpolation polynomial, we derive Lagrange interpolation polynomial of degree one as follows:

Suppose we have two distinct points (x_0, y_0) and (x_1, y_1). Let $P_(x) = ax + b$ interpolation polynomial interpolating $f(x)$ at x_0 and x_1, *i.e.* $P(x_i) = fff(x_i) = y_i$, for i =0, 1. Hence

$$
\begin{aligned}
y_0 &= f(x_0) = P_1(x_0) = ax_0 + b \\
y_1 &= f(x_1) = P_1(x_1) = ax_1 + b.
\end{aligned}
$$

Solve the above two equations for a, we get $a = \frac{y_1 - y_0}{x_1 - x_0}$. Substitute the value of a in the first equation to find b, yields:

$$
b = y_0 - ax_0 = y_0 - \frac{y_1 - y_0}{x_1 - x_0}x_0 = \frac{y_0x_1 - y_1x_0}{x_1 - x_0}.
$$

Hence

$$
\begin{aligned}
P_1(x) = ax + b &= \frac{y_1 - y_0}{x_1 - x_0}x + \frac{y_0x_1 - y_1x_0}{x_1 - x_0} \\
&= \frac{y_1x - y_0x + y_0x_1 - y_1x_0}{x_1 - x_0} = \frac{x_1 - x}{x_1 - x_0}y_0 + \frac{x - x_0}{x_1 - x_0}y_1 \\
&= \frac{x - x_1}{x_0 - x_1}y_0 + \frac{x - x_0}{x_1 - x_0}y_1.
\end{aligned}
$$

This is Lagrange interpolation polynomial of degree one.

The interpolation polynomial of a given set of data points is **unique**.

To prove the uniqueness of interpolation polynomial:

Suppose $p_n(x)$ and $q_n(x)$ are two polynomials of degree$\leq n$, interpolating f at the $(n+1)$ distinct points given by (3.1), then $p_n(x_i) = y_i = q_n(x_i),\ \ i = 0, 1, 2, \cdots, n$. It follows then that the polynomial $d_n(x) = p_n(x) - q_n(x)$ which is of degree$\leq n$ has $(n+1)$ distinct roots (because $d_n(x_i) = p_n(x_i) - q_n(x_i) = y_i - y_i = 0$ for $i = 0, 1, \cdots, n$). This is impossible unless $d_n(x)$ vanishes identically, but if $d_n(x)$ vanishes identically, then $p_n(x) = q_n(x)$.

We have proved the existence and uniqueness of a polynomial $p_n(x)$, given by (3.5) and (3.6) of degree$\leq n$ which interpolates $f(x)$ at $(n+1)$ distinct points (i.e. it satisfies (3.3)).

Example 3.5. Find the interpolating polynomial $p_2(x)$ which interpolating the function f as:

x	-1	0	2
$y = f(x)$	2	-1	5

Solution: From (3.5) and (3.6) we have

$$\begin{aligned} P_2(x) &= \sum_{k=0}^{2} L_2^k(x) f(x_k) = L_2^0(x) f(x_0) + L_2^1(x_1) f(x_1) + L_2^2(x) f(x_2) \\ &= 2L_2^0(x) - L_2^1(x_1) + 5L_2^2(x), \end{aligned}$$

where

$$\begin{aligned} L_2^0(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-0)(x-2)}{(-1-0)(-1-2)} = \frac{1}{3}(x^2-2x). \\ L_2^1(x) &= \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x+1)(x-2)}{(0+1)(0-2)} = -\frac{1}{2}(x^2-x-2). \\ L_2^2(x) &= \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x+1)(x-0)}{(2+1)(2-0)} = \frac{1}{6}(x^2+x). \end{aligned}$$

Hence, $P_2(x) = x^2 - x - 1$.
To estimate the value of $f(x)$ at 0.5 i.e. $f(0.5)$ from the above table, we put this value in $P_2(x)$ we get

$$f(0.5) \approx p_2(x) = 2(0.5)^2 - (0.5) - 1 = -0.5.$$

Error of the Polynomial Interpolation

Theorem 3.1. Let $f \in C^n[a,b]$ such that $f^{(n+1)}$ exists in (a,b). If $p_n(x)$ is the interpolating polynomial (3.5) of f at the $(n+1)$ distinct points $a = x_0 < x_1 < \cdots < x_n = b$, then for any x in $[a,b]$, there exists $c \in (a,b)$ with

$$E_n(x) = f(x) - p_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(c)\ w(x), \tag{3.8}$$

where $w(x) = \prod_{i=0}^{n}(x - x_i)$.

Proof: If $x = x_i$, then $f(x_i) = p_n(x_i)$, $w(x_i) = 0$ and (3.8) holds. Fix $x \in [a,b]$, $x \neq x_i$ for $i = 0, 1, 2, \cdots, n$. Consider the function:

$$k(x) = \frac{f(x) - p_n(x)}{w(x)}. \tag{3.9}$$

And the real-values function $g : [a,b] \to R$ of the variable t

$$g(t) = f(t) - p_n(t) - (t - x_0)(t - x_1)...(t - x_n)k(x).$$

We have $g \in C^n[a,b]$ and $g^{(n+1)}$ exists in (a,b), and g has at least the $(n+2)$ distinct roots $x_0, x_1, \cdots, x_n, x$. It follows then by successive applications of **Generalized Rolle's Theorem** on g and its derivatives that $g^{(n+1)}$ has at least one root, say $c \in (a,b)$. Therefore,

$$g^{(n+1)}(c) = f^{(n+1)}(c) - (n+1)!k(x) = 0.$$

Hence

$$k(x) = \frac{f^{(n+1)}(c)}{(n+1)!}. \tag{3.10}$$

The above equation, together with (3.9) implies (3.8)■.

Hint: **Generalized Rolle's Theorem** said the (Suppose $f \in C[a,\ b]$ and n times differentiable on$(a,\ b)$. If $f(x) = 0$ at the $n+1$ distinct numbers $a = x+0 < x_1 < \cdots < x_n = b$, then the numbers c in $(x_0,\ x_n)$, and hence in $(a,\ b)$ there exists$f^{(n)}(c) = 0$)

Note 3.2. The error in linear interpolation is given by:

$$E_1(x) = f(x) - \left[\frac{x-b}{a-b}f(a) + \frac{x-a}{b-a}f(b)\right] = \frac{(x-a)(x-b)}{2!}f''(c), \tag{3.11}$$

where $a < c < b$.

To see how this error can be used, take the probability integral

$$\varphi(x) = \frac{1}{\sqrt{2\pi}}\int_0^x e^{-\frac{t^2}{2}}dt. \tag{3.12}$$

In the below table, we have

x	1.2	1.3
$\varphi(x)$	0.3849	0.4032

If linear interpolation (3.5) is used to approximate $\varphi(1.22)$, we get:

$$P_1(1.22) = \frac{1.22-1.3}{1.2-1.3}(0.3849) + \frac{1.22-1.2}{1.3-1.2}(0.4032).$$

That is,

$$P_1(1.22) = 0.3886.$$

Now, using (3.11), we have:

$$E_1(1.22) = \varphi(1.22) - p_1(1.22) = \frac{(1.22-1.2)(1.22-1.3)}{2}\varphi''(c),$$

where $1.2 < c < 1.3$.

Hence, $|E_1(1.22)| = 0.0008|\varphi''(c)|$.

But $\varphi'(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}$ and $\varphi''(x) = -x\frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}$.

Hence, $|\varphi''(x)| \leqslant \frac{1}{\sqrt{2\pi}}(1.2)e^{-\frac{(1.2)^2}{2}} \approx 0.25$.
Therefore, $|E_1(1.22)| \leqslant 0.0002$.
That is, $P_1(1.22) = 0.3886$, is correct to at least 3-decimal places. This is conformed since $\varphi(1.22) = 0.3888$ as it is clear from the tables.

Of course in (3.11), c is unknown and in practice we should try to find an upper bound for $\left|f^{(n+1)}(x)\right|$ in [a, b]. If for example $f \in C^{n+1}[a,\ b]$, then we use:

$$\left|f^{(n+1)}(c)\right| \leqslant M = \max_{a \leqslant \zeta \leqslant b}\left|f^{(n+1)}(\zeta)\right|. \tag{3.13}$$

Example 3.6. Let $f(x) = \ln(1+x)$, $x_0 = 1$ and $x_1 = 1.1$. Use linear interpolation to calculate an approximate value of $f(1.04)$ and obtain a bound on the truncation error.
Solution: We have $f(x) = ln(1+x)$, $f(1) = \ln(2) = 0.693147$ and $f(1.1) = \ln(2.1) = 0.741937$.
The Lagrange interpolating polynomial is obtained as:

$$P_1(x) = \frac{x-1.1}{1-1.1}(0.693147) + \frac{x-1}{1.1-1}(0.741937,$$

which gives $f(1.04) \approx P_1(1.04) = 0.712663$.
The error in linear interpolation is given by:

$$E = \frac{1}{2!}(x-x_0)(x-x_1)f''(\xi),\ \ x_0 < \xi < x_1.$$

Hence, we obtain the bound on the error as:

$$|E| \leqslant \frac{1}{2}\max_{1 \leqslant x \leqslant 1.1}|(x-x_0)(x-x_1)| \max_{1 \leqslant x \leqslant 1.1}\left|f''(x)\right|.$$

Since the maximum of $(x-x_0)(x-x_1)$ is obtained at $x = \frac{x_0-x_1}{2}$ and $f''(x) = -\frac{1}{(1+x)^2}$, we get:

$$|E| \leq \frac{1}{2}\frac{(x_1-x_0)^2}{4}\max_{1 \leqslant x \leqslant 1.1}\left|\frac{1}{(1+x)^2}\right| \leq \frac{(0.1)^2}{8} \times \frac{1}{4} = 0.0003125.$$

Example 3.7. Determine an appropriate step size to use, in the construction of a table of $f(x) = (1+x)^6$ on $[0,1]$. The truncation error for linear interpolation is to be bounded by 5×10^{-5}.
Solution: The maximum error in linear interpolation is given by $\frac{h^2 M_2}{8}$, where

$$M_2 = \max_{0 \leqslant x \leqslant 1}\left|f''(x)\right| = \max_{0 \leqslant x \leqslant 1}\left|30(1+x)^4\right| = 480.$$

We choose h so that $\frac{h^2 M_2}{8} = 60h^2 \leq 0.00005$ which gives $h \leqslant 0.00091$.

Divided Difference Interpolation Formula

The divided difference interpolation formula which interpolates f at $x_0,\ x_1, \cdots, x_n$ can be derived as follows::

$$f[x_0, x] = \frac{f[x] - f[x_0]}{(x - x_0)} \implies f(x) = f[x] = f[x_0] + (x - x_0)f[x_0, x].$$

$$f[x_0, x_1, x] = f[x_1, x_0, x] = \frac{f[x_0, x] - f[x_1, x_0]}{(x - x_1)} \implies f[x_0, x] = f[x_0, x_1] + (x - x_1)f[x_0, x_1, x].$$

$\therefore\ \ f(x) = f[x_0] + (x - x_0)f[x_0, x_1] + (x - x_0)(x - x_1)f[x_0, x_1, x].$

$$f[x_0, x_1, x_2, x] = f[x_2, x_0, x_1, x] = \frac{f[x_0, x_1, x] - f[x_2, x_0, x_1]}{(x - x_2)} \implies$$
$$f[x_0, x_1, x] = f[x_0, x_1, x_2] + (x - x_2)f[x_0, x_1, x_2, x].$$

Hence

$$\begin{aligned} f(x) &= f[x_0] + (x - x_0)f[x_0, x_1] + (x - x_0)(x - x_1)f[x_0, x_1, x_2] \\ &\quad + (x - x_0)(x - x_1)(x - x_2)f[x_0, x_1, x_2, x], \end{aligned}$$

and so on. Finally we get

$$\begin{aligned} P_n(x) &= f[x_0] + (x - x_0)f[x_0, x_1] + (x - x_0)(x - x_1)f[x_0, x_1, x_2] + \cdots \\ &\quad + (x - x_0)(x - x_1)\cdots(x - x_{n-1})f[x_0, x_1, \cdots, x_n]. \end{aligned} \tag{3.14}$$

Equation (3.14) is known as **divided difference interpolation formula**.

Theorem 3.2. Suppose that $f \in C^n[a, b]$ and $x_0, x_1, \cdots, x_n$ are distinct numbers in $[a, b]$. Then, a number ζ in (a, b) exists with:

$$f[x_0, x_1, \cdots, x_n] = \frac{f^{(n)}(\zeta)}{n!}.$$

Proof: Let $g(x) = f(x) - P_n(x)$. Since $f(x_i) - P_n(x_i) = 0$ for each $i = 0, 1, \cdots, n$, g has $n+1$ distinct zeros in $[a, b]$. The **generalized Rolle's theorem** (Assume that $f \in [a, b]$ and that f', f'', $\cdots$, $f^{(n)}$ exists over (a, b) and x_0, x_1, $\cdots$, $x_n \in [a, b]$. If $f(x_j) = 0$ for $j = 0,\ 1,\ 2, \cdots, n$ there exists $c \in (a, b)$ such that $f^{(n)}(x_j)$.) implies that a number ζ in (a, b) exists with $g^{(n)}(\zeta) = 0$, so:

$$f^{(n)}(\zeta) - p_n^{(n)}(\zeta) = 0.$$

Since $P_n(x)$ is a polynomial of degree n whose leading coefficient is $f[x_0, x_1, \cdots, x_n]$,

$$P_n^{(n)}(x) = f[x_0, x_1, ..., x_n]n!.$$

As a consequence,

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

When $x_0, x_1, \cdots, x_n$ are arranged consequently with equal spacing, equation (3.14) can be expressed in a simplified form. Introducing the notation $h = x_{i+1} - x_i$ for each $i = 0, 1, \cdots, n-1$ and $x = x_0 + sh$, the difference $x - x_i$ can be written as $x - x_i = (s-i)h$; so equation (3.14) becomes

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

Using binomial-coefficient notation

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

we can express $P_n(x)$ compactly as:

$$P_n(x) = P_n(x_0 + sh) = f[x_0] + \sum_{k=1}^{n} \begin{pmatrix} s \\ k \end{pmatrix} k! h^k f[x_0, x_1, \cdots, x_k]. \tag{3.15}$$

Example 3.8. Approximate $f(1.1)$ using the following data and the divided difference interpolation formula:

x	1	1.3	1.6	1.9	2.2
$f(x)$	0.751977	0.200860	0.4554022	0.2818186	0.1103623

Solution: The divided difference table corresponding to this data is given below:

x	$f(x)$	$f[.,.]$	$f[.,.,.]$	$f[.,.,.,.]$	$f[.,.,.,.,.]$
1	0.751977				
		-0.4837057			
1.3	0.200860		-0.1087339		
		-0.5489460		0.0658784	
1.6	0.4554022		-0.0494433		0.0018251
		,-0.5786120		0.068085	
1.9	0.2818186		-0.0118183		
		-0.5715210			
2.2	0.1103623				

From (3.15) for $n=4$, we obtain

$$\begin{aligned}P_4(x) &= f(x_0)+\sum_{k=1}^{4}\begin{pmatrix} s \\ k\end{pmatrix} k!h^k f[x_0,x_1,\cdots,x_k]\\ &= f(x_0)+shf[x_0,x_1]+s(s-1)h^2f[x_0,x_1,x_2]\\ &+s(s-1)(s-2)h^3f[x_0,x_1,x_2,x_3]\\ &+s(s-1)(s-2)(s-3)h^4f[x_0,x_1,x_2,x_3,x_4].\end{aligned}$$

If $x=1.1$, this implies that $h=0.3$ and $s=\frac{1}{3}$. Hence,

$$\begin{aligned}P_4(x) &= 0.7651997+\frac{1}{3}(0.3)(-0.4837057)+\frac{1}{3}(-\frac{2}{3})(0.3)2(-0.1087339)\\ &+\frac{1}{3}(-\frac{2}{3})(-\frac{5}{3})(0.3)3(0.0658784)\\ &+\frac{1}{3}(-\frac{2}{3})(-\frac{5}{3})(-\frac{8}{3})(0.3)4(0.0018251)=0.7196480.\end{aligned}$$

3.4 Interpolation at Equally Spaced Points

3.4.1 Newton Forward Difference Interpolation Formula

We suppose the $(n+1)$ points $x_0,x_1,\cdots,x_n$ to be equally spaced points, with

$$x_{i+1}-x_i=h;\ \ i=0,1,\cdots,n-1. \tag{3.16}$$

That is,

$$x_i=x_0+ih;\ \ i=0,1,\cdots,n. \tag{3.17}$$

The Newton forward-difference interpolation formula, is constructed by making use of the forward difference operator Δ. With this notation,

$$\begin{aligned}f[x_0,x_1] &= \frac{f(x_1)-f(x_0)}{x_1-x_0}=\frac{1}{h}\Delta f(x_0),\\ f[x_0,x_1,x_2] &= \frac{f[x_1,x_2]-f[x_0,x_1}{x_2-x_0}=\frac{\frac{1}{h}\Delta f(x_1)-\frac{1}{h}\Delta f(x_0)}{2h}\\ &= \frac{1}{2h^2}\Delta^2 f(x_0),\end{aligned}$$

and, in general,

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

Since $f[x_0]=f(x_0)$, Equation (3.15) has the following form:

$$\begin{aligned}P_n(x) &= f(x_0)+\sum_{k=1}^{n}\begin{pmatrix} s \\ k\end{pmatrix}\Delta^k f(x_0)\\ &= f(x_0)+s\Delta f(x_0)+\frac{s(s-1)}{2!}\Delta^2 f(x_0)+\cdots+\frac{s(s-1)(s-2)\cdots(s-n+1)}{n!}\Delta^n f(x_0),\end{aligned} \tag{3.18}$$

The corresponding error becomes

$$E_n(x) = f(x) - P_n(x) = \frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}h^{n+1}f^{(n+1)}(c), \qquad (3.19)$$

where $a < c < b$.
Also we can able to derive Newton forward difference interpolation formula as follows:

$$\begin{aligned}
\Delta y_0 &= y_1 - y_0 \;\Rightarrow\; y_1 = (1+\Delta)y_0. \\
\Delta y_1 &= y_2 - y_1 \;\Rightarrow\; y_2 = (1+\Delta)y_1 = (1+\Delta)(1+\Delta)y_0 = (1+\Delta)^2 y_0.
\end{aligned}$$

In general,

$$\begin{aligned}
y_s &= (1+\Delta)^s y_0 \\
&= f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \cdots + \frac{s(s-1)(s-2)\cdots(s-n+1)}{n!}\Delta^n f(x_0),
\end{aligned}$$

Notes 3.1.

i This formula is used for interpolation near the beginning of a difference table, but it may also be applied in the other parts of the table by suitable shifting the origin. Shifting the origin does not affect the result, but on the other hand it may result in a simpler formula, which less prone to zero.

ii This formula is applicable for $0 \le s < 1$. When working with differences, we can select any values of x in the tabular points to be x_0. This mostly done to keep s within the range.

Example 3.9. Use Newton forward difference interpolation formula to interpolate the value of $f(1.75)$ fro the following data:

x	0.5	1	1.5	2	2.5
$f(x)$	0	1.376	2	2.625	4

Solution:

x	$f(x)$	Δ	Δ^2	Δ^3	Δ^4
0.5	0				
		1.375			
1	1.375		-0.750		
		0.625		0.750	
1.5	2		0		0
		0.625		0.750	
2	2.625		0.750		
		1.375			
2.5	4				

$x_s = 1.75$, $x_0 = 0.5$ and $h = 0.5$. $s = \frac{x_s - x_0}{h} = \frac{1.75-0.5}{0.5} = 2.5$.
As s(=2.5) does not lies between 0 and 1, we cannot use the origin to be $x_0 = 0.5$. Let us shift the origin to $x_0 = 1$. Then, $s = \frac{1.75-1}{0.5} = 1.5$. We cannot use 1 as the origin because still $s > 1$. Let as shift the origin to $x_0 = 1.5$. $s = \frac{1.75-1.5}{0.5} = 0.5$. So we can use $x_0 = 1.5$ as the origin because the calculated value of $s < 1$. Hence $y_0 = 2$, $\Delta y_0 = 0.625$ and $\Delta^2 y_0 = 0.750$ and

$$y_s = y_0 + s\Delta y_0 + \frac{s(s-1)}{2}\Delta^2 y_0.$$

Inserting the values in the above formula, we get

$$f(1.75) = 2 + 0.5(0.625) + \frac{0.5(0.5-1)}{2}(0.750) = 2.219.$$

Example 3.10. From the following table

x	1	2	3	4	5	6
$f(x)$	0	5	22	57	116	205

find $f(2.3)$ and $f(3.5)$ by Newton forward difference interpolation formula.
Solution:

x	$f(x)$	Δ	Δ^2	Δ^3	Δ^4
1	0				
		5			
2	5		12		
		17		6	
3	22		18		0
		35		6	
4	57		24		
		59			
5	116		30		
		89			
6	205				

For f(2.3), $x_0 = 2$, $h = 1$, hence $s = \frac{x-x_0}{h} = \frac{2.3-2}{1} = 0.3$, $y_0 = 5$, $\Delta y_0 = 17$, $\Delta^2 y_0 = 18$, $\Delta^3 y_0 = 6$ and $\Delta^4 y_0 = 0$. Form (3.18) we have:

$$P_3(x) = f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0).$$

Hence,

$$\begin{aligned} f(2.3) \cong P_3(2.3) &= 5 + (0.3)(17) + \frac{0.3(0.3-1)}{2!}18 \\ &+ \frac{0.3(0.3-1)(0.3-2)}{3!}6 = 8.567. \end{aligned}$$

For $f(3.5)$, $x_0 = 3$, $h = 1$, hence $s = \frac{x-x_0}{h} = \frac{3.5-3}{1} = 0.5$, $y_0 = 22$, $\Delta y_0 = 35$, $\Delta^2 y_0 = 24$, $\Delta^3 y_0 = 6$ and $\Delta^4 y_0 = 0$. Also, form (3.18) we have:

$$P_3(x) = f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0).$$

Hence,

$$\begin{aligned} f(3.5) \cong P_3(3.5) &= 22 + (0.5)(35) + \frac{(0.5)(0.5-1)}{2!}24 \\ &+ \frac{(0.5)(0.5-1)(0.5-2)}{3!}6 = 36.875. \end{aligned}$$

If $s = 0.3$:

$$\begin{aligned}|E_3(x)| = |f(x) - P_3(x)| &= \left|\frac{s(s-1)(s-2)(s-3)}{4!}h^4 f^{(4)}(c)\right| \\ &= \frac{|s(s-1)(s-2)(s-3)|}{4!}h^4\left|f^{(4)}(c)\right| \\ &= \frac{|0.3(0.3-1)(0.3-2)(0.3-3)|}{24}M_4 = 0.0402\ M_4,\end{aligned}$$

where $M_4 = \max\limits_{1<c<6}\left|f^{(4)}(c)\right|$.

To show that equation (3.18) is valid when s **is rational number:**

Let f is continuously differentiable function for any order, then

$$\begin{aligned}f(x_0+h) &= f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \cdots = \\ &= \left\{1 + hd + \frac{h^2D^2}{2!} + \cdots\right\} f(x_0) = e^{hd}f(x_0),\end{aligned} \tag{3.20}$$

where $D = \frac{d}{dx}$.
But

$$\Delta f(x_0) = f(x_0+h) - f(x_0),$$

hence,

$$f(x_0+h) = f(x_0) + \Delta f(x_0) = (1+\Delta)f(x_0). \tag{3.21}$$

From (3.20) and (3.21), we get $1 + \Delta = e^{hd}$. Also,

$$\begin{aligned}f(x_0+sh) &= f(x_0) + shf'(x_0) + \frac{s^2h^2}{2!}f''(x_0) + \cdots \\ &= \left\{1 + shd + \frac{s^2h^2D^2}{2!} + \cdots\right\} f(x_0) = e^{shd}f(x_0) \\ &= \left(e^{hd}\right)^s f(x_0) = (1+\Delta)^s f(x_0).\end{aligned} \tag{3.22}$$

The formula (3.22) is the Newton forward difference interpolation formula converges when $|s| < 1$.

3.4.2 Newton Backward Difference Interpolation Formula

If the interpolating nodes are reordered from last to first as $x_n, x_{n-1}, \ldots, x_0$, we can write rewrite Equation (3.14) as follows:

$$\begin{aligned}P_n(x) = f[x_n] &+ (x-x_n)f[x_n, x_{n-1}] + (x-x_n)(x-x_{n-1})f[x_n, x_{n-1}, x_{n-2}] + \cdots \\ &+ (x-x_n)(x-x_{n-1})\cdots(x-x_1)f[x_n, x_{n-1}, \cdots, x_0].\end{aligned}$$

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

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

Since

$$\begin{aligned} f[x_n, x_{n-1}] &= \frac{1}{h}\nabla f(x_n), \\ f[x_n, x_{n-1}, x_{n-2}] &= \frac{1}{2h^2}\nabla^2 f(x_n), \end{aligned}$$

and, in general,

$$f[x_n, x_{n-1}, \dots, x_{n-k}] = \frac{1}{k!h^k}\nabla^k f(x_n).$$

Consequently, we can obtain the following Newton backward difference interpolation formula:

$$\begin{aligned} P_n(x) &= f(x_n) + s\nabla f(x_n) + \frac{s(s+1)}{2!}\nabla^2 f(x_n) + \dots \\ &+ \frac{s(s+1)\dots(s+n-1)}{n!}\nabla^n f(x_n). \end{aligned} \tag{3.23}$$

The corresponding error:

$$E_n(x) = f(x) - P_n(x) = \frac{s(s+1)(s+2)...(s+n)}{(n+1)!}h^{n+1} f^{(n+1)}(c). \tag{3.24}$$

where $a < c < b$. Also, Newton backward difference interpolation formula, can be derived as follows:

$$\begin{aligned} \nabla y_1 = y_1 - y_0 \;\Rightarrow\; (1-\nabla)y_1 = y_0 \;\Rightarrow\; y_1 = (1-\nabla)^{-1}y_0. \\ \nabla y_2 = y_2 - y_1 \;\Rightarrow\; y_1 = (1-\nabla)y_2 \;\Rightarrow\; y_2 = (1-\nabla)^{-1}y_1 \\ = (1-\nabla)^{-1}(1-\nabla)^{-1}y_0 = (1-\nabla)^{-2}y_0. \end{aligned}$$

In general,

$$\begin{aligned} y_s &= (1-\nabla)^{-s}y_0 \\ &= f(x_n) + s\nabla f(x_n) + \frac{s(s+1)}{2!}\nabla^2 f(x_n) + \dots \\ &+ \frac{s(s+1)\dots(s+n-1)}{n!}\nabla^n f(x_n). \end{aligned}$$

Notes 3.2.

i This formula is used toward the end of the difference table, but it may also be applied in the other parts of the table by suitable shifting the origin.

ii This formula is applicable for $0 \leq s < 1$. When working with differences, we can select any values of x in the tabular points to be x_n. This mostly done to keep s within the range.

Example 3.11. From Example 3.10, find $f(2.5)$ and $f(5.5)$ by using (3.23).
Solution: For $f(2.5)$, $x_n = 3$, h=1, hence $s = \frac{x-x_n}{h} = \frac{2.5-3}{1} = -0.5$, $y_n = 22$, $\nabla y_n = 17$ and $\nabla^2 y_n = 12$.
From (3.23), we have:

$$P_2(x) = f(x_n) + s\nabla f(x_n) + \frac{s(s+1)}{2!}\nabla^2 f(x_n).$$

Hence

$$f(2.5) \cong P_2(2.5) = 22 + (-0.5)(17) + \frac{(-0.5)(-0.5+1)}{2}12 = 12.$$

Similarly, for $f(5.5)$, $x_n = 6$, $s = -0.5$, $y_n = 205$, $\nabla y_n = 89$, $\nabla^2 y_n = 30$, $\nabla^3 y_n = 6$ and $\nabla^4 y_n = 0$.

$$\begin{aligned}
P_3(x) &= y_n + s\nabla y_n + \frac{s(s+1)}{2!}\nabla^2 y_n + \frac{s(s+1)(s+2)}{3!}\nabla^3 y_n \\
&+ \frac{s(s+1)(s+2)(s+3}{4!}\nabla^y_n \\
&= 205 + (-0.5)89 + \frac{-0.5(-0.5+1)}{2!}30 + \frac{-0.5(-0.5+1)(-0.5+2)}{3!}6 \\
&+ \frac{-0.5(-0.5+1)(-0.5+2)(-0.5+2)}{4!}0 = 156.375.
\end{aligned}$$

If s=-0.5:

$$\begin{aligned}
|E_2(x)| = |f(x) - P_2(x)| &= \left|\frac{s(s+1)(s+2)}{3!}h^3 f^{(3)}(c)\right| \\
&= \frac{|s(s+1)(s+2)|}{4!}h^3 \left|f^{(3)}(c)\right| \\
&= \frac{|-0.5(-0.5+1)(-0.5+2)|}{6}M_3 = 0.0625\ M_3,
\end{aligned}$$

where $M_3 = \max\limits_{1<c<6} \left|f^{(3)}(c)\right|$.

3.5 Numerical Differentiation

Numerical differentiation deals with the following problem: We are given the function $y = f(x)$ and wish to obtain one of its derivatives at the point $x = x_i$. The term ″given″ means that we either have an algorithm for computing the function or possess a set of discrete data points (x_i, y_i), $i = 0, 1, \cdots, n$. In either case, we have access to a finite number of (x, y) data pairs from which to compute the derivative. If you suspect by now that numerical differentiation is related to interpolation, you are right-one means of finding the derivative is to approximate the function locally by a polynomial and then differentiate it. An equally effective tool is the Taylor series expansion of $f(x)$ about the point $x = x_i$, which has the advantage of providing us with information about the error involved in the approximation.

3.5.1 Differentiation of Continuous Functions

The derivative of a function at x is defined as:

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

To be able to find a derivative numerically, one could make Δx finite to give:

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

Knowing the value of x at which you want to find the derivative of $f(x)$, we choose a value of Δx to find the value of $f'(x)$. To estimate the value of $f'(x)$, three such approximations are suggested as follows.

3.5.2 Forward Difference Approximation of the First Derivative

From differential calculus, we know that:

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

For a finite Δx,

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

The above is the forward divided difference approximation of the first derivative. It is called forward because you are taking a point ahead of x. To find the value of $f'(x)$ at $x = x_i$, we may choose another point Δx ahead as $x = x_{i+1}$. This gives:

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{\Delta x} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}, \quad \text{where } \Delta x = x_{i+1} - x_i.$$

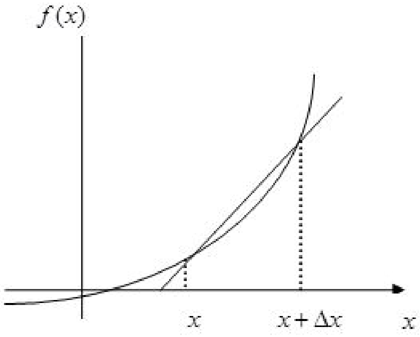


Figure 3.1: *Graphical representation of forward difference approximation of the first derivative.*

Example 3.12. The velocity of a rocket is given by:

$$\nu(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t, \;\; 0 \leqslant t \leqslant 30,$$

where ν is given in m/s and t is given in seconds. At $t = 16\,\text{s}$,
a) Use the forward difference approximation of the first derivative of $\nu(t)$ to calculate the acceleration. Use a step size of $\Delta t = 2\,\text{s}$.
b) Find the exact value of the acceleration of the rocket.
c) Calculate the absolute relative true error for part (b).
Solution:
(a)

$$a(t_i) \approx \frac{\nu(t_{i+1}) - \nu(t_i)}{\Delta t}, \;\; t_i = 16, \;\; \Delta t = 2, \;\; t_{i+1} = t_i + \Delta t = 16 + 2 = 18.$$

$$a(16) \approx \frac{\nu(18) - \nu(16)}{2}.$$

$$\nu(18) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)} \right] - 9.8(18) = 453.02 \text{ m/s},$$

$$\nu(16) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)} \right] - 9.8(16) = 392.07 \text{ m/s}.$$

Hence,

$$a(16) \approx \frac{\nu(18) - \nu(16)}{2} = \frac{453.02 - 392.07}{2} = 30.474\,\text{m/s}^2.$$

(b) The exact value of $a(16)$ can be calculated by differentiating

$$\nu(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t,$$

as

$$a(t) = \frac{d}{dt}\left[\nu(t)\right].$$

Knowing that:

$$\frac{d}{dt}\left[\ln(t)\right] = \frac{1}{t} \quad \text{and} \quad \frac{d}{dt}\left[\frac{1}{t}\right] = -\frac{1}{t^2}.$$

$$\begin{aligned}
a(t) &= 2000\left(\frac{14\times10^4 - 2100t}{14\times10^4}\right)\frac{d}{dt}\left(\frac{14\times10^4}{14\times10^4 - 2100t}\right) - 9.8\\
&= 2000\left(\frac{14\times10^4 - 2100t}{14\times10^4}\right)(-1)\left(\frac{14\times10^4}{\left(14\times10^4 - 2100t\right)^2}\right)(-2100) - 9.8\\
&= \frac{-4040 - 29.4t}{-200 + 3t}.\\
a(16) &= \frac{-4040 - 29.4(16)}{-200 + 3(16)} = 29.674\,\text{m/s}^2.
\end{aligned}$$

(c) The absolute relative true error is

$$\begin{aligned}
|\in_t| &= \left|\frac{\text{True Value} - \text{Approximate Value}}{\text{True Value}}\right| \times 100\\
&= \left|\frac{29.674 - 30.474}{29.674}\right| \times 100 = 2.6967\%.
\end{aligned}$$

3.5.3 Backward Difference Approximation for the First Derivative

We know

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

For a finiteΔx,

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

If Δx is chosen as a negative number,

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x} = \frac{f(x) - f(x - \Delta x)}{\Delta x}.$$

This is a backward difference approximation as you are taking a point backward from . To find the value of $f'(x)$ at $x = x_i$, we may choose another point Δx behind as $x = x_{i-1}$. This gives:

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{\Delta x} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}},$$

where $\Delta x = x_i - x_{i-1}$.

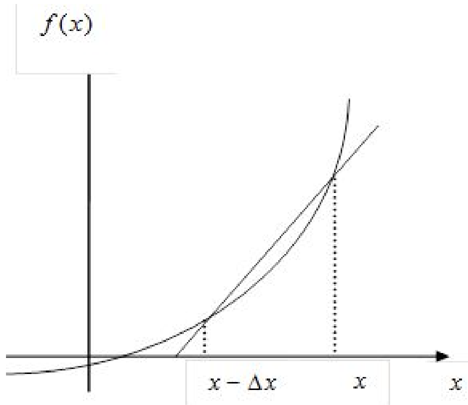


Figure 3.2: *Graphical representation of backward difference approximation of first derivative.*

Example 3.13. The velocity of a rocket is given by:

$$\nu\left(t\right) = 2000\ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100t}\right] - 9.8t,\quad 0\leqslant t\leqslant 30.$$

(a) Use the backward difference approximation of the first derivative of $\nu\left(t\right)$ to calculate the acceleration at $t = 16s$. Use a step size of $\Delta t = 2$ s.
(b) Find the absolute relative true error for part (a).
Solution:

$$\begin{aligned}
a\left(t\right) &\approx \frac{\nu(t_i) - \nu(t_{i-1})}{\Delta t},\quad t_i = 16,\quad \Delta = 2\;\; t_{i-1} = t_i - \Delta t = 16 - 2 = 14.\\
a(16) &\approx \frac{\nu(16) - \nu(14)}{2},\\
\nu(16) &= 2000\ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100\times 16}\right] - 9.8\times 16 = 392.07\,\mathrm{m/s},\\
\nu(14) &= 2000\ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100\times 14}\right] - 9.8\times 14 = 334.24\,\mathrm{m/s},\\
a(16) &\approx \frac{\nu(16) - \nu(14)}{2} = \frac{392.07 - 334.24}{2} = 28.915\mathrm{m/s}^2.
\end{aligned}$$

(b) The exact value of the acceleration at $t = 16\,$s from Example 3.15 is:

$$a\left(16\right) = 29.674\ \mathrm{m/s}^2.$$

The absolute relative true error for the answer in part (a) is:

$$\left|\in_t\right| = \left|\frac{29.674 - 28.915}{29.674}\right|\times 100 = 2.5584\%$$

.

3.5.4 Forward Difference Approximation from Taylor Series

Taylor's theorem says that if you know the value of a function $f(x)$ at a point x_i and all its derivatives at that point, provided, the derivatives are continuous between x_i and x_{i+1}, then:

$$f\left(x_{i+1}\right)=f\left(x_i\right)+f'\left(x_i\right)\left(x_{i+1}-x_i\right)+\frac{f''\left(x_i\right)}{2!}\left(x_{i+1}-x_i\right)^2+\ldots.$$

Substituting for convenience $\Delta x=x_{i+1}-x_i$, we get:

$$\begin{aligned}
f\left(x_{i+1}\right)&=f\left(x_i\right)+f'\left(x_i\right)\Delta x+\frac{f''\left(x_i\right)}{2!}(\Delta x)^2+\ldots,\\
f'\left(x_i\right)&=\frac{f\left(x_{i+1}\right)-f\left(x_i\right)}{\Delta x}-\frac{f''\left(x_i\right)}{2!}(\Delta x)+\ldots,\\
f'\left(x_i\right)&=\frac{f\left(x_{i+1}\right)-f\left(x_i\right)}{\Delta x}+O(\Delta x).
\end{aligned}$$

The $O(\Delta x)$ term shows that the error in the approximation is of the order of Δx.

Can you now derive from the Taylor series the formula for the backward divided difference approximation of the first derivative?

As you can see, both forward and backward divided difference approximations of the first derivative are accurate on the order of $O(\Delta x)$. Can we get better approximations? Yes, another method to approximate the first derivative is called the **central difference approximation of the first derivative**.
From the Taylor series

$$f\left(x_{i+1}\right)=f\left(x_i\right)+f'\left(x_i\right)\Delta x+\frac{f''\left(x_i\right)}{2!}(\Delta x)^2+\frac{f'''\left(x_i\right)}{3!}(\Delta x)^3+\cdots \tag{3.25}$$

And

$$f\left(x_{i-1}\right)=f\left(x_i\right)-f'\left(x_i\right)\Delta x+\frac{f''\left(x_i\right)}{2!}(\Delta x)^2-\frac{f'''\left(x_i\right)}{3!}(\Delta x)^3+\cdots. \tag{3.26}$$

Subtracting Equation (3.29) from Equation (3.28), we get:

$$f\left(x_{i+1}\right)-f\left(x_{i-1}\right)=f'\left(x_i\right)(2\Delta x)+\frac{2f'''\left(x_i\right)}{3!}(\Delta x)^3+\cdots.$$

Hence

$$\begin{aligned}
f'\left(x_i\right)&=\frac{f\left(x_{i+1}\right)-f\left(x_{i-1}\right)}{2\Delta x}-\frac{f'''\left(x_i\right)}{3!}(\Delta x)^2+\cdots\\
&=\frac{f\left(x_{i+1}\right)-f\left(x_{i-1}\right)}{2\Delta x}+O(\Delta x)^2,
\end{aligned}$$

hence showing that we have obtained a more accurate formula as the error is of the order of $O(\Delta x)^2$.

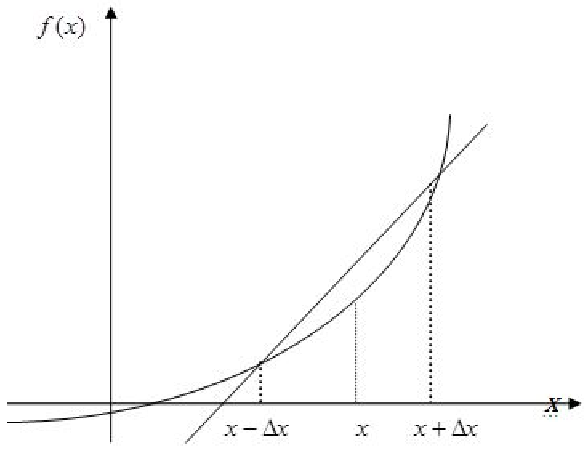


Figure 3.3: *Graphical representation of central difference approximation of first derivative.*

Example 3.14. The velocity of a rocket is given by

$$\nu(t) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100t}\right] - 9.8t,\ \ 0 \leqslant t \leqslant 30.$$

(a) Use the central difference approximation of the first derivative of $\nu(t)$ to calculate the acceleration at $t = 16$ s. Use a step size of $\Delta t = 2s$.
(b) Find the absolute relative true error for part (a).
Solution:

$$a(t_i) \approx \frac{\nu(t_{i+1}) - \nu(t_{i-1})}{2\Delta t},\ \ t_i = 16,\ \Delta t = 2,\ t_{i+1} = t_i + \Delta t = 16 + 2 = 18,$$
$$t_{i-1} = t_i - \Delta t = 16 - 2 = 14,$$
$$a(16) \approx \frac{\nu(18) - \nu(14)}{2(2)},$$
$$\nu(18) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100(18)}\right] - 9.8(18) = 453.02\,\mathrm{m/s},$$
$$\nu(14) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100(14)}\right] - 9.8(14) = 334.24\,\mathrm{m/s}.$$

Hence,
$$a(16) \approx \frac{\nu(18) - \nu(14)}{4} = \frac{453.02 - 334.24}{4} = 29.694\ \mathrm{m/s^2}.$$

(b) The exact value of the acceleration at $t = 16s$ from Example 3.15 is

$$a(16) = 29.674\ \mathrm{m/s^2}.$$

The absolute relative true error for the answer in part (a) is

$$|\in_t| = \left|\frac{29.674 - 29.694}{29.674}\right| \times 100 = 0.069157\%.$$

The results from the three difference approximations are given in Table (3.1).

Table (3.1) *Summary of $a(16)$ using different approximations.*

Type of difference approximation	$a(16)\text{m/s}^2$	$\lvert\in_t\rvert$ %
Forward	30.475	2.6967
Backward	28.915	2.5584
Central	29.695	0.069157

Clearly, the central difference scheme is giving more accurate results because the order of accuracy is proportional to the square of the step size. In real life, one would not know the exact value of the derivative-so how would one know how accurately they have found the value of the derivative? A simple way would be to start with a step size and keep on halving the step size until the absolute relative approximate error is within a pre-specified tolerance. Take the example of finding $\nu'(t)$ for

$$\nu(t) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right] - 9.8t,$$

at $t = 16$ using the backward difference scheme. Given in Table (3.2) are the values obtained using the backward difference approximation method and the corresponding absolute relative approximate errors.

Table (3.2) *First derivative approximations and relative errors for different Δt values of backward difference scheme.*

Δt	$\nu'(t)$	$\lvert\in_a\rvert$ %
2	28.915	
1	29.289	1.2792
0.5	29.480	0.64787
0.25	29.577	0.32604
0.125	29.625	0.16355

From the above table, one can see that the absolute relative approximate error decreases as the step size is reduced. At $\Delta t = 0.125$, the absolute relative approximate error is 0.16355%, meaning that at least 2 significant digits are correct in the answer.

3.5.5 Finite Difference Approximation of Higher Derivatives

One can also use the Taylor series to approximate a higher order derivative. For example, to approximate $f''(x)$, the Taylor series is

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2\Delta x) + \frac{f''(x_i)}{2!}(2\Delta x)^2 + \frac{f'''(x_i)}{3!}(2\Delta x)^3 + \cdots, \tag{3.27}$$

where $x_{i+2} = x_i + 2\Delta x$, and

$$f(x_{i+1}) = f(x_i) + f'(x_i)(\Delta x) + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 \cdots, \tag{3.28}$$

where $x_{i-1} = x_i - \Delta x$. Subtracting 2 times Equation (3.31) from Equation (3.30) gives

$$\begin{aligned} f(x_{i+2}) - 2f(x_{i+1}) &= -f(x_i) + f''(x_i)(\Delta x)^2 + f'''(x_i)(\Delta x)^3 \cdots, \\ f''(x_i) &= \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2} - f'''(x_i)(\Delta x) + \cdots, \\ f''(x_i) &\approx \frac{f(x_{i+2}) - 2f(x_{i+1}) - f(x_i)}{(\Delta x)^2} + O(\Delta x). \end{aligned} \tag{3.29}$$

Example 3.15. The velocity of a rocket is given by:

$$\nu(t) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right] - 9.8t, \ \ 0 \le t \le 30$$

Use the forward difference approximation of the second derivative of $\nu(t)$ to calculate the jerk at $t = 16s$. Use a step size of $\Delta t = 2$s.

Solution: let

$$\begin{aligned} j(t_i) &\approx \frac{\nu(t_{i+2}) - 2\nu(t_{i+1}) + \nu(t_i)}{(\Delta t)^2}, \ \ t_i = 16, \ \ \Delta t = 2, \\ t_{i+1} &= t_i + \Delta t = 16 + 2 = 18, \ \ t_{i+2} = t_i + 2\Delta t = 16 + 2(2) = 20, \\ j(16) &\approx \frac{\nu(20) - 2\nu(18) + \nu(16)}{(2)^2}, \\ \nu(20) &= 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(20)}\right] - 9.8(20) = 517.35\,\mathrm{m/s}, \\ \nu(18) &= 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)}\right] - 9.8(18) = 453.02\,\mathrm{m/s}, \\ \nu(16) &= 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)}\right] - 9.8(16). \end{aligned}$$

Hence,

$$j(16) \approx \frac{517.35 - 2(453.02) + 392.07}{4} = 0.84515\mathrm{m/s^3}.$$

The exact value of $j\left(16\right)$ can be calculated by differentiating

$$\nu\left(t\right) = 2000\ln\left[\frac{14\times10^4}{14\times10^4-2100t}\right] - 9.8t,$$

twice as:

$$a\left(t\right) = \frac{d}{dt}\left[\nu\left(t\right)\right] \quad \text{and} \quad j\left(t\right) = \frac{d}{dt}\left[a\left(t\right)\right].$$

Knowing that:

$$\frac{d}{dt}\left[\ln\left(t\right)\right] = \frac{1}{t} \text{ and } \frac{d}{dt}\left[\frac{1}{t}\right] = -\frac{1}{t^2},$$

$$\begin{aligned}
a\left(t\right) &= 2000\left(\frac{14\times10^4-2100t}{14\times10^4}\right)\frac{d}{dt}\left(\frac{14\times10^4}{14\times10^4-2100t}\right) - 9.8\\
&= 2000\left(\frac{14\times10^4-2100t}{14\times10^4}\right)\left(-1\right)\left(\frac{14\times10^4}{\left(14\times10^4-2100t\right)^2}\right)\left(-2100\right) - 9.8\\
&= \frac{-4040-29.4t}{-200+3t}.
\end{aligned}$$

Similarly, it can be shown that:

$$j\left(t\right) = \frac{d}{dt}\left[a\left(t\right)\right] = \frac{18000}{\left(-200+3t\right)^2},$$

$$j(16) = \frac{18000}{\left(-200+3(16)\right)^2} = 0.77909 m/s^3.$$

The absolute relative true error is:

$$\left|\in_t\right| = \left|\frac{0.77909-0.84515}{0.77909}\right| \times 100 = 8.4797\%.$$

The formula given by Equation (**??**) is a forward difference approximation of the second derivative and has an error of the order of $O\left(\Delta x\right)$. Can we get a formula that has a better accuracy? Yes, we can derive the central difference approximation of the second derivative. The Taylor series is:

$$\begin{aligned}
f\left(x_{i+1}\right) &= f\left(x_i\right) + f'\left(x_i\right)\Delta x + \frac{f''\left(x_i\right)}{2!}(\Delta x)^2 + \frac{f'''\left(x_i\right)}{3!}(\Delta x)^3\\
&\quad + \frac{f''''\left(x_i\right)}{4!}(\Delta x)^4 + \cdots,
\end{aligned} \tag{3.30}$$

where $x_{i+1} = x_i + \Delta x$, and

$$\begin{aligned}
f\left(x_{i-1}\right) &= f\left(x_i\right) - f'\left(x_i\right)\Delta x + \frac{f''\left(x_i\right)}{2!}(\Delta x)^2 - \frac{f'''\left(x_i\right)}{3!}(\Delta x)^3\\
&\quad + \frac{f''''\left(x_i\right)}{4!}(\Delta x)^4 - \cdots,
\end{aligned} \tag{3.31}$$

where $x_{i-1} = x_i - \Delta x$. Adding Equations (3.33) and (3.34), gives

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + f''(x_i)(\Delta x)^2 + f'''(x_i)\frac{(\Delta x)^4}{12} + \cdots,$$
$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2} - \frac{f''''(x_i)(\Delta x)^2}{12} + \cdots,$$
$$= \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2} + O(\Delta x)^2.$$

Example 3.16. The velocity of a rocket is given by:

$$\nu(t) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30,$$

Use the central difference approximation of the second derivative of $\nu(t)$ to calculate the jerk at $t = 16$s. Use a step size of $\Delta t = 2$s.

Solution: The second derivative of velocity with respect to time is called jerk. The second order approximation of jerk then is:

$$j(t_i) \approx \frac{\nu(t_{i+1}) - 2\nu(t_i) + \nu(t_{i-1})}{(\Delta t)^2}, \ \ t_i = 16, \ \ \Delta t = 2,$$
$$t_{i+1} = t_i + \Delta t = 16 + 2 = 18, \ \ t_{i-1} = t_i - \Delta t = 16 - 2 = 14,$$
$$j(16) \approx \frac{\nu(18) - 2\nu(16) + \nu(14)}{(2)^2},$$
$$\nu(18) = 2000\ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100(18)}\right] - 9.8(18) = 453.02\,\mathrm{m/s},$$
$$\nu(16) = 2000\ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100(16)}\right] - 9.8(16) = 392.07\,\mathrm{m/s},$$
$$\nu(14) = 2000\ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100(14)}\right] - 9.8(14) = 334.24\,\mathrm{m/s},$$

Hence,

$$j(16) \approx \frac{\nu(18) - 2\nu(16) + \nu(14)}{(2)^2}$$
$$= \frac{453.02 - 2(392.07) + 334.24}{4} = 0.77969\mathrm{m/s}^3.$$

The absolute relative true error is:

$$|\in_t| = \left|\frac{0.77908 - 0.77969}{0.77908}\right| \times 100 = 0.077992\%.$$

3.5.6 Differentiation of Discrete Functions

If we are given this set of distinct points (x_i, y_i), $i = 0, 1, 2, \cdots, n$, determine the interpolation polynomial passing through these points. We then differentiate this polynomial to obtain $p^{(j)}(x)$, $j = 1, 2, \cdots$ whose values for any given x are taken as an approximation to $f^{(j)}(x)$. Construct a polynomial $p_n(x)$ which is best approximate polynomial to f(x) by any methods given in interpolation.

Notes 3.3.

(1) For unequally space points, we must use Lagrange interpolation polynomial, divided difference interpolation formula or spline function.

(2) For equally space points, we are able to use all available methods in interpolation.

(3) If we find $p_n(x)$ by Lagrange interpolation polynomial, divided difference interpolation formula or spline function, differentiate $p_n(x)$ with respect to x directly.

(4) If we find $p_n(x)$ by **NFDIF**, **NBDIF** and **Bessel's interpolation formula**, we differentiate $p_n(x)$ with respect to x as follows:

$$
\begin{aligned}
\frac{df(x)}{dx} &\cong \frac{dp_n(x)}{dx} = \frac{dp_n(x)}{ds}\frac{ds}{dx} = \frac{1}{h}\frac{dp_n(x)}{ds} \\
&= \frac{1}{h}\frac{d}{ds}\left\{y_0 + s\Delta y_0 + \frac{s(s-1)}{2!}\Delta^2 y_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 y_0 + \cdots\right\} \\
&= \frac{1}{h}\left\{\Delta y_0 + (s-\frac{1}{2})\Delta^2 y_0 + (\frac{s^2}{2} - s + \frac{1}{3})\Delta^3 y_0 + \cdots\right\}. \\
\frac{d^2 f(x)}{dx^2} &\cong \frac{d^2 p_n(x)}{dx^2} = \frac{d}{dx}\left[\frac{1}{h}\left\{\Delta y_0 + (s-\frac{1}{2})\Delta^2 y_0 + (\frac{s^2}{2} - s + \frac{1}{3})\Delta^3 y_0 + \cdots\right\}\right] \\
&= \frac{d}{ds}\left[\frac{1}{h}\left\{\Delta y_0 + (s-\frac{1}{2})\Delta^2 y_0 + (\frac{s^2}{2} - s + \frac{1}{3})\Delta^3 y_0 + \cdots\right\}\right]\frac{ds}{dx} \\
&= \frac{1}{h^2}\left\{\Delta^2 y_0 + (s-1)\Delta^3 y_0 + \cdots\right\}.
\end{aligned}
$$

In general,

$$\frac{d^j f(x)}{dx^j} \cong \frac{d^j p_n(x)}{dx^j} = \frac{1}{h^j}\frac{d^j p_n(x)}{ds^j}, j = 1, 2, \cdots.$$

Similarly, we obtain $\frac{d^j f(x)}{dx^j} \cong \frac{d^j p_n(x)}{dx^j}$ for Newton backward difference interpolation and Bessel's interpolation formula.

Note 3.3. If $x = x_i$ (interpolation point), we get $s = 0$.

Example 3.17. Find an approximate value to $f'(0.7)$ where $f(x) = \sin(x)$ and $x_0 = 0.4$, $x_1 = 0.6$, $x_2 = 0.8$, $x_3 = 1$.

Solution:

x	0.4	0.6	0.8	1
$f(x)$	0.389418	0.564642	0.717356	0.841471

By using Lagrange interpolation polynomial,

$$\begin{aligned}
&x_0 = 0.4, \ \ x_1 = 0.6, \ \ x_2 = 0.8, \ \ x_3 = 1, \\
&y_0 = 0.389418, \ \ y_1 = 0.564642, \ \ y_2 = 0.717356, \ \ y_2 = .0.841471. \\
P_3(x) = &\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}y_0 + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}y_1 \\
&+ \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_1-x_3)}y_2 + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}y_3 \\
&= -0.12683772x^3 - 0.05307353x^2 + 1.02559085x - 0.00420862.
\end{aligned}$$

Hence,

$$P_3'(x) = -0.38051316x^2 - 0.10614706x + 1.02559085$$

and

$$f'(0.7) \cong p_3'(0.7) = 0.7648346.$$

Exact value=cos(0.7)=0.76484219 and the error=0.00000573.

Example 3.18. Given the set of data as follows

x	4	2	0	3
y	63	11	7	28

Find $f'(x)$ at $x = 1$ by using divided difference interpolation formula.

Solution:

x	$f(x)$	$f[,]$	$f[,,]$	$f[,,,]$
4	63			
		$\frac{11-63}{2-4} = 26$		
2	11		$\frac{2-26}{0-4} = 6$	
		$\frac{7-11}{0-2} = 2$		$\frac{5-6}{3-4} = 1$
0	7		$\frac{7-2}{3-2} = 5$	
		$\frac{28-7}{3-0} = 7$		
3	28			

$$\begin{aligned}
P(x) &= 63 + 26(x-4) + 6(x-4)(x-2) + 1(x-4)(x-2)(x-0) \\
&= x^3 - 2x + 7.
\end{aligned}$$

Hence, $P'(x) = 3x^2 - 2$. Thus, $f'(1) \cong P'(1) = 3(1)^2 - 2 = 1$.

Example 3.19. Find an approximate value to $f'(2.31)$and $f'(1)$ by using Newton forward difference interpolation formula where $f(x) = x^3 + 2$ and x =0, 1, 2, 3, 4, 5.

Solution:

x	$f(x)$	Δ	Δ^2	Δ^3	Δ^4
0	2				
		1			
1	3		6		
		7		6	
2	10		12		0
		19		6	
3	29		18		0
		37		6	
4	66		24		
		61			
5	127				

If $x = 2.31$, and $h = 1$, then $s = \frac{x-x_0}{h} = \frac{2.31-2}{1} = 0.31$, and

$$P_3(x) = y_0 + s\Delta y_0 + \frac{s(s-1)}{2!}\Delta^2 y_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 y_0.$$

Hence

$$P_3'(x) = \frac{1}{h}\left\{\Delta y_0 + \left(s - \frac{1}{2}\right)\Delta^2 y_0 + \left(\frac{s^2}{2} - s + \frac{1}{3}\right)\Delta^3 y_0\right\},$$

and

$$\begin{aligned} f'(2.31) \cong P_3'(2.31) &= 19 + (0.31 - 0.5)(18) + (\frac{(0.31)^2}{2} - 0.31 + \frac{1}{3})(6) \\ &= 16.008. \end{aligned}$$

To find the exact value of $f'(x)$, differentiate $f(x)$directly with respect to x, we get $f'(x) = 3x^2$.
Hence $f'(2.31) = 3(2.31)^2 = 16.0083$(exactvalue).
Error=exact value-approximate value=16.0083-16.008=0.0003.
If $x = 1$, and $h = 1$, then $s = \frac{x-x_0}{h} = \frac{1-1}{1} = 0$. Hence,

$$P_3(x) = y_0 + s\Delta y_0 + \frac{s(s-1)}{2!}\Delta^2 y_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 y_0.$$

Thus

$$\begin{aligned} P_3'(x) &= \frac{1}{h}\left\{\Delta y_0 + (s-\frac{1}{2})\Delta^2 y_0 + (\frac{s^2}{2} - s + \frac{1}{3})\Delta^3 y_0\right\} \\ &= \frac{1}{h}\left\{\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0\right\}. \end{aligned}$$

and

$$f'(1) \cong P_3'(1) = 7 - \frac{1}{2}(12) + \frac{1}{3}(6) = 3.$$

Since $f'(x) = 3x^2$, implies that $f'(1) = 3(1)^2 = 3(\text{exactvalue})$
Error=exact value-approximate value=3-3=0.

Theorem 3.3. Let $f(x)$ is continuously differentiable $(n+1)$ times on $[a,b]$, then,

$$f'(x_j) - P_n'(x_j) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{\substack{i=0\\ i\neq j}}(x_j - x_i), \quad j = 0,1,\cdots,n.$$

Proof: From errors in interpolation, we have:

$$f(x) - P_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x - x_i).$$

Let $g(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}$ and $w(x) = \prod\limits_{i=0}^{n}(x - x_i)$. This implies that

$$f(x) - p_n(x) = g(x)w(x).$$

Hence,

$$\begin{aligned} f'(x) - P_n'(x) &= g(x)w'(x) + g'(x)w(x) \\ f'(x_j) - P_n'(x_j) &= g(x_j)w'(x_j) + g'(x_j)w(x_j). \end{aligned}$$

But $w(x_j) = 0, \text{for} j = 0,1,2,...,n$. Therefore

$$f'(x_j) - p_n'(x_j) = g(x_j)w'(x_j).$$

We now that

$$w'(x_j) = \prod_{\substack{i=0\\ i\neq j}}(x_j - x_i).$$

Hence

$$f'(x_j) - P_n'(x_j) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{\substack{i=0\\ i\neq j}}(x_j - x_i).\blacksquare$$

We can use **forward difference** for discrete functions as follows:
We know

$$f'(x) = \lim_{\Delta x\to 0}\frac{f(x+\Delta x) - f(x)}{\Delta x}.$$

For a finite Δx,

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}.$$

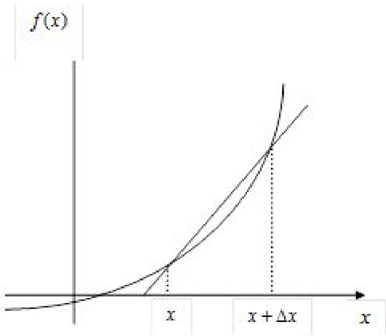


Figure 3.4: *Graphical representation of forward difference approximation of first derivative.*

So given $n+1$ data points $(x_0, y_0), (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, the value of $f'(x)$ for $x_i \leq x \leq x_{i+1}$, $i = 0, ..., n-1$, is given by:

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}.$$

Example 3.20. The upward velocity of a rocket is given as a function of time in Table (**??**).

Table (3.3) *Velocity as a function of time.*

$t\,(s)$	0	10	15	20	22.5	30
$v(t)$ (m/s)	0	227.04	362.78	517.35	602.97	901.67

By using forward divided difference, find the acceleration of the rocket at $t = 16\,\text{s}$.
Solution: To find the acceleration at $t = 16s.$, we need to choose the two values of velocity closest to $t = 16\,\text{s}$, that also bracket $t = 16\,\text{s}$ to evaluate it. The two points are $t = 15\,\text{s}$ and $t = 20\,\text{s}$

$$\begin{aligned} a(t_i) &\approx \frac{v(t_{i+1}) - v(t_i)}{\Delta t}, \quad t_i = 15, \quad t_{i+1} = 20, \quad \Delta t = t_{i+1} - t_i = 20 - 15 = 5, \\ a(16) &\approx \frac{v(20) - v(15)}{5} = \frac{517.35 - 362.78}{5} = 30.914 \text{m/s}^2. \end{aligned}$$

3.6 EXERCISES

1. Show that

(a) $\Delta\left(\frac{u(x)}{v(x)}\right) = \frac{v(x)\Delta u(x) - u(x)\Delta v(x)}{v(x+h)v(x)}$.

(b) $\sum_{i=0}^{n-1} \Delta y_i = y_n - y_0$.

(c) $\sum_{i=0}^{n-1} u_i \Delta v_i = u_n v_n - u_0 v_0 - \sum_{i=0}^{n-1} v_{i+1}\Delta u_i$.

(d) $y_k = \sum_{i=0}^{k} \binom{k}{i} \Delta^i y_0$.

(e) $\nabla = \delta E^{-\frac{1}{2}} = 1 - E^{-1} = 1 - (1+D)^{-1}$.

(f) $\Delta^n f(x_0) = h^n f^{(n)}(x_0)$.

(g) $\Delta(\alpha u_i + \beta v_i) = \alpha \Delta u_i + \beta \Delta v_i$.

(h) $\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}}$.

(i) $\nabla = 1 - E^{-1}$.

(j) $E\Delta = \Delta E$

(k) $E\nabla = \nabla E = \Delta$.

2. Given the following pairs of values of x and y

x	1	2	4	8	10
y	0	1	5	21	27

Determine the value y at $x = 0.4$, use Divided difference interpolation polynomial.

3. Use mathematical induction to prove that $f[x_0, x_1, \cdots, x_n] = \frac{\Delta^n f(x_0)}{n!h^n}$.

4. Show that: If a function $g(x)$ interpolates the function $f(x)$ at $x_1, x_2, \ldots, x_{n-1}$, and $h(x)$ interpolates the function $f(x)$ at $x_2, x_3, \ldots, x_n$, then, $T(x) = g(x) + \frac{(x_1 - x)}{(x_n - x_1)}[g(x) - h(x)]$; Interpolate $f(x)$ at x_1, x_2,..., x_{n-1}, x_n.

5. If the following values (a, s), $(a+h, t)$, $(a+2h, u)$ and $(a+3h, v)$ are obtained from polynomial of degree two. Prove that $f(a+1.5h) = \frac{(t+u)}{2} + \frac{1}{24}[\frac{3}{2}(t+u-s-v)]$ by using Newton forward difference interpolation formula.

6. Use the definition of central difference operator to show that $\Delta^n y_k = \delta^n{}_{k+\frac{n}{2}}$.

7. Use the divided difference method to obtain a polynomial of least degree that fits the following values:

x	1	0	3	-1	5
y	1	-1	8	3	1

8. From the following values:

x	0	0.5	1	1.5	2
y	-1	-2	1	2	3

Find $f(0.6)$ by using Newton forward difference interpolation formula and Bessel interpolation formula.

9. If we interpolate the function $f(x) = e^{x-1}$ with a polynomial p of degree 12 using 13 nodes in $[-1, 1]$, what is a good upper bound for $|f(x) - p(x)|$ on $[-1, 1]$?

10. Compute a divided difference table for these function values: (3,1), (1,-3), (5,2) and (6,4) and also find $f(1.2)$ and $f(5.5)$ by using divided difference interpolation formula.

11. Suppose we know the values of $cos(x)$ at $x = -h$, $x = 0$, $x = h$, $(h > 0)$, write the interpolation polynomial $P(x)$ which interpolates $cos(x)$ at these points. Prove the error bound $|E_n(x)| = |\cos(x) - P(x)| \leq 0.065h^3$,for all $x \in [-h, h]$. Determine h such that the previous interpolation gives 4 exact decimals for any $x \in [-h, h]$.

12. Determine the maximum step size that can be used in tabular of $f(x) = e^x$ in $[0, 1]$, so that the error in the linear interpolation will be less than 5×10^{-4}. Find also the step size if quadratic interpolation is used.

13. Find the unique polynomial of degree 2 or less such that $P(1) = 1$, $P(3) = 27$, and $P(4) = 64$ by using each of the following methods: (i) Lagrange interpolating formula and (ii) Divided difference interpolating formula.

14. Calculate the n^{th} divided difference of $f(x) = \frac{1}{x}$.

15. If $f(x) = U(x)V(x)$, show that $f[x_0, x_1] = U[x_0]V[x_0, x_1] + U[x_0, x_1]V[x_1]$.

16. Use the Lagrange interpolation polynomial and Divided difference interpolation formula to estimate $f(3)$ from the following values:

x	0	1	2	3	5	6
$f(x)$	1	14	15	5	6	19

17. Find $\frac{dy}{dx}$ at $x = 0.6$ of the function $y = f(x)$ where

x	0.4	0.5	0.6	0.7	0.8
$f(x)$	1. 5836494	1. 7974426	2 .0442376	2.3275054	2. 6510818

18. Given the following pairs of values of x and y.

x	1	2	4	8	10
$f(x)$	0	1	5	21	27

Determine the first derivative at $x = 0.4$, use divided difference interpolation.

19. Find the first and second derivative at $x = 0.6$ for the following data: (0.4, 1.5836), (0.5,1.7974), (0.6,2.0442), (0.7, 2.3275) and (0.8, 2.6511).

20. A rod is moving in a plane, the following table given the angle θ in radian through which the rod has turned for various values of t seconds.

t	0	0.2	0.4	0.6	0.8	1	1.2
θ	0	0.12	0.49	1.12	2.02	3.2	4.67

Calculate the angular velocity=$\frac{d\theta}{dt}$ and angular accuracy=$\frac{d^2\theta}{dt^2}$ of the rod, when $x = 0.6$.

CHAPTER 4

Spline Approximations

4.1 Introduction

In practice, many of the constructed curves or surfaces have a sufficiently complex shape which does not permit a universal analytic description at large with the help of the elementary functions. For this reason, the objects are assembled out of the relatively simple smooth fragments (segments for curves) and (patches for surfaces), each being represented as a graph of the elementary function of one or two variables.

4.2 Interpolation by Spline Function

Definition 4.1. A function S is called a spline of degree k if:

(i) The domain of S is an interval $[a, b]$.

(ii) S, S', S'', $\cdots$, $S^{(k-1)}$ are all continuous functions on $[a, b]$.

(iii) There are points x_j (The notes of S), where $a = x_0 < x_1 < \cdots < x_n = b$ and such that S is a polynomial of degree at most k on each subinterval [x_j, x_{j+1}].

Definition 4.2. A spline function is a function consisting of polynomial pieces joined together with certain smooth conditions. We are forced to write:

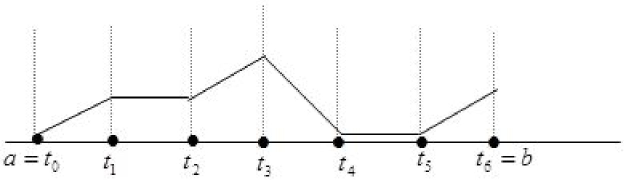
$$S(x) = \begin{cases} s_0(x), & x \in [x_0, x_1] \\ s_1(x), & x \in [x_1, x_2] \\ \vdots \\ s_{n-1}(x), & x \in [x_{n-1}, x_n]. \end{cases} \tag{4.1}$$

Note 4.1. The function $S(x)$ that we wish to construct consists of $(n-1)$ polynomial pieces. The interpolation conditions are $S(x_i) = y_i$, $1 \le i \le n$. The continuity conditions are imposed only at the interior knots x_2, x_3, …, x_{n-1}, these conditions are written as

$$\lim_{x \to x_i^-} S^{(j)}(x) = \lim_{x \to x_i^+} S^{(j)}(x), \quad i = 1, 2, \ldots, n-1; \quad j = 0, 1, \ldots, k-1.$$

4.2.1 First Degree Spline

A first degree spline is a function whose pieces are linear polynomials joined together to achieve continuity.

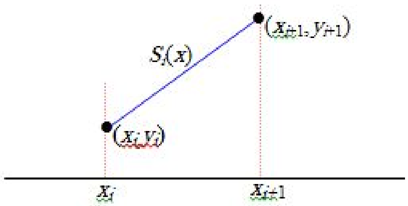


The points $t_0, t_1, t_2, t_3, t_4, t_5, t_6$ at which the function changes its character are termed ***knots***, in the theory of spline. Thus, the above spline function has seven knots.
For first degree spline, in equation (4.1)

$$S_i(x) = a_i x + b_i = m_i(x - x_i) + y_i$$

where

$$m_i = \frac{y_{i+1} - y_i}{x_{i+1} - x_i} \quad \text{for} \quad i = 0, 1, \ldots, n-1.$$



Example 4.1. Determine a spline function of degree one which interpolates the following data:

x	0	1	3
$f(x)$	2	4	5

Solution: since

$$S(x) = \begin{cases} s_0(x), x \in [0,1] \\ s_1(x), x \in [1,3]. \end{cases}$$

Hence

$$\begin{aligned} S_0(x) &= \frac{y_1 - y_0}{x_1 - x_0}(x - x_0) + y_0 \\ &= \frac{4-2}{1-0}(x-0) + 2 = 2x + 2, \end{aligned}$$

and

$$\begin{aligned} s_1(x) &= \frac{y_2 - y_1}{x_2 - x_1}(x - x_1) + y_1 \\ &= \frac{5-4}{3-1}(x-1) + 4 = \frac{1}{2}x + \frac{7}{2}. \end{aligned}$$

Note 4.2. To find $S(c)$, where c is any numbers:

(1) If $c \in [x_i, x_{i+1}]$, then $S(c) = s_i(c)$ for $i = 0, 1, \ldots, n-1$.

(2) If $c \notin [a = x_0, b = x_n]$, then

$$S(c) = s_0(c) \quad \text{if} \quad c < a$$
$$S(c) = s_{n-1}(c) \quad \text{if} \quad c \geq b.$$

Example 4.2. Determine whether

$$S(x) = \begin{cases} x, x \in [-1, 0] \\ 1 - x,\ x \in (0, 1) \\ 2x - 2,\ \ x \in [1, 2] \end{cases}$$

is a first degree spline?

Solution: The function $S(x)$ is not a spline of degree one because $\lim_{x \to 0^+} S(x) = \lim_{x \to 0^+} (1 - x) = 1$, but $\lim_{x \to 0^-} S(x) = \lim_{x \to 0^-} (x) = 0$ and $1 \neq 0$.

4.2.2 Spline of Degree Two (Quadratic Spline)

A function $S(x)$ in the equation (4.1) is a spline of degree two if $S(x)$ is piecewise quadratic polynomial such that S and S' are continuous. $s_i(x)$ must satisfy the interpolation conditions $s_i(x_i) = y_i$ and $s_i(x_{i+1}) = y_{i+1}$, $i = 0, 1, \ldots, n-1$.

We derive the equations for the interpolating quadratic spline $S(x)$ as follows: Seek a piecewise quadratic function $S(x)$ in the equation (4.1) which is continuously differentiable on $[x_0,\ x_n] = [a,\ b]$ and interpolates the table that is$s_i(x_i) = y_i$, $i = 0,\ 1,\ \ldots,\ n$. Since $S'(x)$ is continuous, we can put $m_i = s_i'(x_i)$ and $m_{i+1} = s_i'(x_{i+1})$. From Lagrange interpolation of degree one, we get:

$$s_i'(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} m_i + \frac{x - x_i}{x_{i+1} - x_i} m_{i+1}. \tag{4.2}$$

Integrating both sides of (4.2) with respect to x, we get

$$s_i(x) = \frac{(x - x_{i+1})^2}{2(x_i - x_{i+1})} m_i + \frac{(x - x_i)^2}{2(x_{i+1} - x_i)} m_{i+1} + c,$$

where c is the constant of integration. To find c, use the interpolation condition $s_i(x_i) = y_i$, we obtain $c = y_i - \frac{(x_i - x_{i+1})}{2} m_i$. Substituting the value of c in the above equation, we get:

$$s_i(x) = \frac{m_{i+1} - m_i}{2(x_{i+1} - x_i)} (x - x_i)^2 + (x - x_i) m_i + y_i, \quad i = 0, 1, \ldots, n-1, \tag{4.3}$$

where $s_i(x_i) = y_i$, $s_i'(x_i) = m_i$ and $s_i'(x_{i+1}) = m_{i+1}$. These three conditions defined the function $s_i(x)$ uniquely on $[x_i, x_{i+1}]$ as given in the equation (4.3) where

$$m_{i+1} = -m_i + 2\left(\frac{y_{i+1} - y_i}{x_{i+1} - x_i}\right), \quad i = 0, 1, \ldots, n-1, \tag{4.4}$$

where m_0 is arbitrary.

Note 4.3. To derive (4.4) from (4.3), put $x = x_{i+1}$, we get (4.4) directly.

Example 4.3. Determine whether the following function is a quadratic spline.

$$(x) = \begin{cases} x^2, & -\infty < x \leq 0 \\ -x^2, & 0 \leq x \leq 1 \\ 1 - 2x, & x < \infty. \end{cases}$$

Solution: Since $\lim\limits_{x \to 0^-} S(x) = \lim\limits_{x \to 0^-} x^2 = 0$, and also $\lim\limits_{x \to 0^+} S(x) = \lim\limits_{x \to 0^+} (-x^2) = 0$, hence S(x) is continuous at 0.
$\lim\limits_{x \to 1^-} S(x) = \lim\limits_{x \to 1^-}(-x^2) = -1$, and also $\lim\limits_{x \to 1^+} S(x) = \lim\limits_{x \to 1^+} (1 - 2x) = -1$, hence $S(x)$ is continuous at 1.
Therefore $S(x)$ is continuous. From $S(x)$ we find $S'(x)$ by differentiating $S(x)$ directly with respect to x we get:

$$S'(x) = \begin{cases} 2x, & -\infty < x \leq 0 \\ -2x, & 0 \leq x \leq 1 \\ -2, & 1 \leq x < \infty. \end{cases}$$

Since $\lim\limits_{x \to 0^-} S'(x) = \lim\limits_{x \to 0^-} 2x = 0$ and $\lim\limits_{x \to 0^+} S(x) = \lim\limits_{x \to 0^+} (-2x) = 0$,
hence S′(x) is continuous at 0.

Since $\lim\limits_{x \to 1^-} S'(x) = \lim\limits_{x \to 1^-} (-2x) = -2$ and $\lim\limits_{x \to 1^+} S'(x) = \lim\limits_{x \to 1^+} (-2) = -2$,
hence $S'(x)$ is continuous at 1.
$\therefore$ $S'(x)$ is continuous.
Hence, $S(x)$ is a spline function of degree two.

Example 4.4. Find a quadratic spline **interplant** for these data:

x	-1	0	0.5	1
$f(x)$	2	1	0	1

Solution: Let

$$S(x) = \begin{cases} s_0(x), & x \in [-1, 0] \\ s_1(x), & x \in [0, 0.5] \\ s_2(x), & x \in [0.5, 1], \end{cases} ,$$

where $s_i(x) = \frac{m_{i+1} - m_i}{2(x_{i+1} - x_i)}(x - x_i)^2 + (x - x_i)m_i + y_i$ for i =0, 1, 2.
To find m_0, m_1, m_2 and m_3, let $m_0 = 0$. From equation (**??**)

$$m_1 = -m_0 + 2\left(\frac{y_1 - y_0}{x_1 - x_0}\right) = 2\left(\frac{1 - 2}{0 - (-1)}\right) = -2,$$

$$m_2 = -m_1 + 2\left(\frac{y_2 - y_1}{x_2 - x_1}\right) = 2 + 2\left(\frac{0-1}{0.5-0}\right) = -2,$$

and

$$m_3 = -m_2 + 2\left(\frac{y_3 - y_2}{x_3 - x_2}\right) = 2 + 2\left(\frac{1-0}{1-0.5}\right) = 6.$$

Thus,

$$\begin{aligned}
s_0(x) &= \frac{m_1 - m_0}{2(x_1 - x_0)}(x - x_0)^2 + (x - x_0)m_0 + y_0 \\
&= \frac{-2-0}{2(0-(-1))}(x+1)^2 + 2 = -(x+1)^2 + 2 \\
s_1(x) &= \frac{m_2 - m_1}{2(x_2 - x_1)}(x - x_1)^2 + (x - x_1)m_1 + y_1 \\
&= \frac{-2+2}{2(0.5-0)}x^2 - 2x + 1 = -2x + 1. \\
s_2(x) &= \frac{m_3 - m_2}{2(x_3 - x_2)}(x - x_2)^2 + (x - x_2)m_2 + y_2 \\
&= \frac{6+2}{2(1-0.5)}(x-0.5)^2 - 2(x-0.5) = 8(x-0.5)^2 - 2(x-0.5).
\end{aligned}$$

Hence

$$S(x) = \begin{cases} -(x+1)^2 + 2, & x \in [-1, 0] \\ -2x + 1, & x \in [0, 0.5] \\ 8(x-0.5)^2 - 2(x-0.5), & x \in [0.5, 1]. \end{cases}$$

4.3 EXERCISES

1. Find the value of a and b such that

$$f(x) = \begin{cases} x^2 - ax + 1, & 1 \le x \le 2 \\ 3x - b, & 2 \le x \le 3. \end{cases}$$

   is a quadratic spline.

2. IS $f(x) = \begin{cases} -x^2 - 2x^3, & -1 \le x \le 0 \\ x^2 + 2x^3, & 0 \le x \le 1. \end{cases}$ a cubic spline function?

3. Suppose $S(x) = \begin{cases} 1 + a_1x + b_1x^2 + c_1x^3, & 0 \le x \le 1 \\ 1 + a_2(x-1) + b_2(x-1)^2 + c_2(x-1)^3, & 1 \le x \le 2, \end{cases}$
   is the natural cubic spline approximation of f that satisfies $f(0) = 1$, $f(1) = 0$ and $f(2) = 3$. Find all constants a_1, a_2, b_1, b_2, c_1 and c_2.

CHAPTER 5

Least Square and Curve Fitting

5.1 Introduction

The experimental data $(x_1, y_1), (x_2, y_2), \ldots,$ (x_n, y_n) are plotted on a rectangular coordinate system. Such a curve is known as an approximating curve that the data appears to be approximated by a straight line and it clearly exhibits a linear relationship between the two variables. ***Curve fitting*** is the general problem of finding equations of approximating curves which best fit the given set of data. The famous method, proposed by Gauss and used to find the best fitted line, is called ***least squares methods***.

5.2 Linear Least Square

We wish to predict response to n data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ by a straight line given by:

$$y = a + bx,$$

where a and b are the constants of the least square straight lines. Let us use the least squares criterion where we minimize:

$$S_r = \sum_{i=1}^{n} E_i{}^2 = \sum_{i=1}^{n} (y_i - a - bx_i)^2,$$

where S_r is called the sum of the square of the residuals. To find a and b, we minimize S_r with respect to a and b.

$$\frac{\partial S_r}{\partial a} = 2\sum_{i=1}^{n} (y_i - a - bx_i)(-1) = 0,$$

$$\frac{\partial S_r}{\partial b} = 2\sum_{i=1}^{n} (y_i - a - bx_i)(-x_i) = 0,$$

giving

$$-\sum_{i=1}^{n} y_i + \sum_{i=1}^{n} a + \sum_{i=1}^{n} bx_i = 0.$$

$$-\sum_{i=1}^{n} y_i x_i + \sum_{i=1}^{n} ax_i + \sum_{i=1}^{n} bx_i^2 = 0.$$

Noting that

$$na + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i, \tag{5.1}$$

$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i. \tag{5.2}$$

Solving the above Equations (5.1) and (5.2) gives:

$$b = \frac{n\sum\limits_{i=1}^{n} x_i y_i - \sum\limits_{i=1}^{n} x_i \sum\limits_{i=1}^{n} y_i}{n\sum\limits_{i=1}^{n} x_i^2 - \left(\sum\limits_{i=1}^{n} x_i\right)^2}, \tag{5.3}$$

$$a = \frac{\sum\limits_{i=1}^{n} x_i^2 \sum\limits_{i=1}^{n} y_i - \sum\limits_{i=1}^{n} x_i \sum\limits_{i=1}^{n} x_i y_i}{n\sum\limits_{i=1}^{n} x_i^2 - \left(\sum\limits_{i=1}^{n} x_i\right)^2}. \tag{5.4}$$

Also a can be rewritten as follows

$$a = \left(\frac{\sum\limits_{i=1}^{n} y_i}{n}\right) - b\left(\frac{\sum\limits_{i=1}^{n} x_i}{n}\right).$$

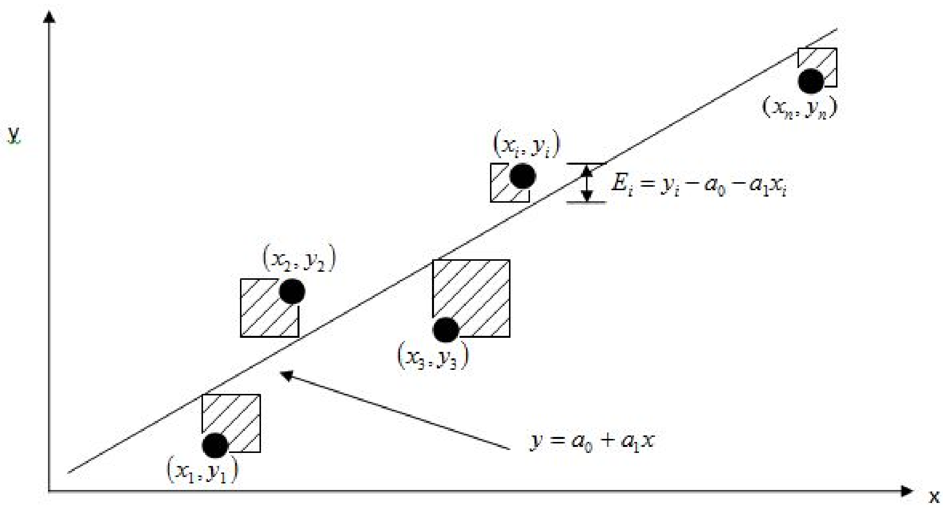


Figure 5.1: *Linear lest square of y vs. x data showing residuals and square of residual at a typical point,* x_i.

Example 5.1. Find a straight line $y = a + b\,x$ for the following data by using least square:

x	1	3	8	10	13
$f(x)$	80	100	110	120	140

Solution:

x	y	x^2	xy
1	80	1	80
3	100	9	300
8	110	64	880
10	120	100	1200
13	140	169	1820
35	550	343	4280

We are now ready to use the results of our calculations in the formula:

$$b = \frac{5 \times 4280 - 35 \times 550}{5 \times 343 - 35^2} = \frac{2150}{490} \approx 4.388,$$

$$a = \frac{550 - 4.388 \times 35}{5} = \frac{396.42}{5} \approx 79.284.$$

That means the equation of the least square line is $y = 4.388x + 79.284$.

Example 5.2. The torque T needed to turn the torsional spring of a mousetrap through an angle, θ is given in Table (5.1),

Table (5.1) *Torque versus angle for a torsion spring.*

Angle, θ (Radians)	Torque, T N. m
0.698132	0.188224
0.959931	0.209138
1.134464	0.230052
1.570796	0.250965
1.919862	0.313707

Find the constants k_1 and k_2 of the least square line $T = k_1 + k_2\theta$.

Solution: Table (5.2) shows the summations needed for the calculation of the constants of the regression model.

Table (5.2) *Tabulation of data for the calculation of the needed summations.*

I	θ	T	θ^2	$T\theta$
1	Radians	N. m	, $(Radians)^2$	N. m
2	0.698132	0.188224	4.87388×10^{-1}	1.31405×10^{-1}
3	0.959931	0.209138	9.21468×10^{-1}	$latex 2.00758 \times 10^{-1}$
4	1.134464	0.230052	1.2870	2.60986×10^{-1}
5	1.570796	0.250965	2.4674	3.94215×10^{-1}
6	1.919862	0.313707	3.6859	6.02274×10^{-1}
$\sum_{i=1}^{5}$	6.2831	1.1921	8.8491	1.5896

Since $n = 5$:

$$k_2 = \frac{n\sum_{i=1}^{5}\theta_i T_i - \sum_{i=1}^{5}\theta_i \sum_{i=1}^{5} T_i}{n\sum_{i=1}^{5}\theta_i^2 - \left(\sum_{i=1}^{5}\theta_i\right)^2} = \frac{5(1.5896) - (6.2831)(1.1921)}{5(8.8491) - (6.2831)^2}$$
$$= 9.6091 \times 10^{-2}\text{N - m/rad},$$
$$k_1 = \frac{\sum_{i=1}^{5}\theta_i^2 \sum_{i=1}^{5} T_i - \sum_{i=1}^{5}\theta_i \sum_{i=1}^{5}\theta_i T_i}{n\sum_{i=1}^{5}\theta_i^2 - \left(\sum_{i=1}^{5}\theta_i\right)^2} = \frac{(8.8491)(1.1921) - (6.2831)(1.5896)}{5(8.8491) - (6.2831)^2}$$
$$= 1.1767 \times 10^{-1}\text{N - m}.$$

Example 5.3. Find the least square lines approximating this data :

x	1	2	3	4	5
$f(x)$	1.3	3.5	4.2	5	7

Solution:

x	y	x_i^2	$x_i y_i$
1	1.3	1	1.3
2	3.5	4	7.0
3	4.2	9	12.6
4	5	16	20.0
5	7	25	35.0
15	21	55	79.9

Hence

$$b = \frac{5(79.9) - (15)(21)}{5(55) - (15)^2} = \frac{379.5 - 315}{275 - 225} = \frac{64.5}{50} = 1.29$$

$$a = \frac{(55)(21) - (75.9)(15)}{5(55) - (15)^2} = \frac{1155 - 1138.5}{275 - 225} = \frac{16.5}{50} = 0.33$$

Thus $f(x) = 1.29x + 0.33$ To find the error

$$\begin{aligned}\sum_{i=1}^{5} (y_i - 1.29x_i - 0.33)^2 &= (y_1 - 1.29x_1 - 0.33)^2 + (y_2 - 1.29x_2 - 0.33)^2 \\ &+ (y_3 - 1.29x_3 - 0.33)^2 + (y_4 - 1.29x_4 - 0.33)^2 \\ &+ (y_5 - 1.29x_5 - 0.33)^2 \\ &= 0.1042 + 0.3481 + 0 + 0.2401 + 0.0484 = 0.6868.\end{aligned}$$

Example 5.4. Fit a straight line to the following data:

x	1	2	3	4	6	8
$y = f(x)$	2.4	3	3.6	4	5	6

Solution: Let the straight line be $y = a + bx$.
The normal equations are

$$na + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i.$$

Table for calculations:

i	x	y	x^2	xy
1	1	2.4	1	2.4
2	2	3	4	6
3	3	3.6	9	10.8
4	4	4	16	16
5	6	5	36	30
6	8	6	64	48
sum	24	24	130	113.2

Since there are 6 pairs of values of x and y, hence here $n = 6$ and substitute the above values in the above normal equations, we have

$$6a + 24b = 24$$
$$24a + 130b = 113.2.$$

Solving these equations, we get $a = 1.976$ and $b = 0.5058$.
Therefore, the required least square line is $y = 1.976 + 0.5058x$, which is the line of best fit.

Example 5.5. By the method of least squares, find the straight line that best fits the following data and hence find the value of y when $x = 3$.

x	1	2	3	4	5
$y = f(x)$	12	25	40	50	65

Solution: Let the straight line be $y = a + bx$.
The normal equations are

$$na + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$
$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i.$$

Table for calculations:

i	x	y	x^2	xy
1	1	12	1	12
2	2	25	4	50
3	3	40	9	120
4	4	50	16	200
5	5	65	25	325
sum	15	192	55	707

Since there are 5 pairs of values of x and y, hence here $n = 5$ and substitute the above values in the above normal equations, we have

$$5a + 15b = 192$$
$$15a + 55b = 707.$$

Solving these equations, we get $a = -0.8$ and $b = 13.1$.
Therefore, the required least square line is $y = -0.8 + 13.1x$, which is the line of best fit.
When $x = 2$ the value of $y = -0.8 + 13.1(2) = 25.5$.

Example 5.6. Fit a least square line to the following data:

x	4	6	8	10	12
$y = f(x)$	13.72	12.90	12.01	11.14	10.31

Solution: Let the straight line be $y = a + bx$.
The normal equations are

$$na + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$
$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i.$$

Table for calculations:

i	x	y	x^2	xy
1	4	13.72	16	54.88
2	6	12.90	36	77.40
3	8	12.01	64	96.08
4	10	11.14	100	111.40
5	12	10.31	144	123.72
sum	40	60.08	360	463.48

Since there are 5 pairs of values of x and y, hence here $n = 5$ and substitute the above values in the above normal equations, we have

$$5a + 40b = 60.08$$
$$40a + 360b = 463.48.$$

Solving these equations, we get $a = 5.5171$ and $b = 0.6744$.
Therefore, the required least square line is $y = 5.5171 + 0.6744x$, which is the line of best fit.

Example 5.7. Fit a least square line to the following data:

x	1	2	3	4	5
$y = f(x)$	14	27	40	55	68

Solution: Let the straight line be $y = a + bx$.
The normal equations are

$$na + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$
$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i.$$

Table for calculations:

i	x	y	x^2	xy
1	1	14	1	14
2	2	27	4	54
3	3	40	9	120
4	4	55	16	220
5	5	68	25	340
sum	15	204	55	748

Since there are 5 pairs of values of x and y, hence here $n = 5$ and substitute the above values in the above normal equations, we have

$$5a + 15b = 204$$
$$15a + 55b = 748.$$

Solving these equations, we get $a = 0$ and $b = 13.6$.
Therefore, the required least square line is $y = 13.6x$, which is the line of best fit.

Example 5.8. Fit a straight line $y = a + bx$ from the following data:

x	0	1	2	3	4
$y = f(x)$	1	1.8	3.3	4.5	6.3

Solution: The straight line is $y = a + bx$.
The normal equations are

$$na + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$
$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i.$$

Table for calculations:

i	x	y	x^2	xy
1	0	1	0	0
2	1	1.8	1	1.8
3	2	3.3	4	6.6
4	3	4.5	9	13.5
5	4	6.3	16	25.2
sum	10	16.9	30	47.1

Since there are 5 pairs of values of x and y, hence here $n = 5$ and substitute the above values in the above normal equations, we have

$$5a + 10b = 16.9$$
$$10a + 30b = 47.1.$$

Solving these equations, we get $a = 0.72$ and $b = 1.33$.
Therefore, the required least square line is $y = 0.72 + 1.33x$, which is the line of best fit.

5.3 Transforming the data to use linear least square formulas

Examination of the nonlinear models above shows that in general iterative methods are required to estimate the values of the model parameters. It is sometimes useful to use simple linear least square formulas to estimate the parameters of a nonlinear model. This involves first transforming the given data such as to regress it to a linear model. Following the transformation of the data, the evaluation of model parameters lends itself to a direct solution approach using the least squares method. Data for nonlinear models such as exponential, power, and growth can be transformed.

5.3.1 Exponential Model

Many physical and chemical processes are governed by the exponential function:

$$y = ae^{bx}. \tag{5.5}$$

Taking natural ln of both sides of Equation (5.5) gives:

$$\ln(y) = \ln(a) + bx.$$

Let $z = \ln(y)$, $A = \ln(a)$ and $B = b$ implying $a = e^A$, $b = B$ then $z = A + Bx$.
The data z versus x is now a linear model. These equations simplify to what is known as the normal equations (see Section 5.2):

$$nA + B\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} z_i$$
$$A\sum_{i=1}^{n} x_i + B\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i z_i.$$

The solution to this system of equations is

$$B = \frac{n\sum_{i=1}^{n} x_i z_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2},$$
$$A = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} z_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i z_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}.$$

Now since A and B are found, the original constants with the model are found as:

$$A = \ln(a) \implies a = e^A \text{ and } b = B.$$

Example 5.9. Fit an exponential curve $y = ae^{bx}$ to the following data by the method of least squares:

x	2	3	4	5	6
$y = f(x)$	144	172.8	207.4	248.8	298.6

Solution: Let the given equation be $y = ae^{bx}$. Repeat the procedure in subsection 5.3.1, we get $z = A + Bx$ where $A = ln(a)$, $B = b$ and $z = ln(y)$.
The normal equations are given by

$$nA + B\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} z_i$$
$$A\sum_{i=1}^{n} x_i + B\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i z_i.$$

Table for calculations:

i	x	y	$z = ln(y)$	x^2	xz
1	2	144	4.97	4	9.94
2	3	172.8	5.15	9	15.45
3	4	207.4	5.33	16	21.32
4	5	248.8	5.52	25	27.60
5	6	298.6	5,69	36	34.14
sum	20		26.66	90	108.45

Here $n = 5$ and substitute the above values in the above normal equations, we have

$$5A + 20B = 26.66$$
$$20A + 90B = 108.45.$$

Solving these equations, we get $A = 4.608$ and $B = 0.181$.
Since $A = ln(a) = 4.608 \implies a = e^A = e^{4.608} = 100.28$ and $b = B = 0.181$.
Hence, the required equation for the given data is

$$y = 100.28e^{0.181x}.$$

Example 5.10. Find an exponential curve $y = ae^{bx}$ to the following data by the method of least squares:

x	0	2	4
$y = f(x)$	5.012	10	31.62

Solution: Let the given equation be $y = ae^{bx}$. Repeat the procedure in subsection 5.3.1, we get $z = A + Bx$ where $A = ln(a)$, $B = b$ and $z = ln(y)$.
The normal equations are given by

$$nA + B\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} z_i$$
$$A\sum_{i=1}^{n} x_i + B\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i z_i.$$

Table for calculations:

i	x	y	$z = ln(y)$	x^2	xz
1	0	5.012	1.6118	0	0
2	2	10.00	2.3026	4	4.6052
3	4	31.62	3.4538	16	13.8152
sum	6		7.3682	20	18.4204

Here $n = 3$ and substitute the above values in the above normal equations, we have

$$3A + 6B = 7.3682$$
$$6A + 20B = 18.420.$$

Solving these equations, we get $A = 1.5352$ and $B = 0.4604$.
Since $A = ln(a) = 1.5352 \implies a = e^A = e^{1.5352} = 4.6423$ and $b = B = 0.4604$.
Hence, the required equation for the given data is

$$y = 4.6423e^{0.4604x}.$$

5.3.2 Exponential Curve

An exponential curve with base b is defined by

$$y = ab^x. \tag{5.6}$$

where $a \neq 0$, $b > 0$, $b \neq 1$, and x is any real number. The base, b, is constant and the exponent, x, is a variable.

Many physical and chemical processes are governed by the exponential function: Taking natural ln of both sides of Equation (5.6) gives:

$$\ln(y) = \ln(a) + xln(b).$$

Let $z = \ln(y)$, $A = \ln(a)$ and $B = ln(b)$ implying $a = e^A, \ b = e^B$ then $z = A + Bx$. The data z versus x is now a linear model. These equations simplify to what is known as the normal equations (see Section 5.2):

$$\begin{aligned} nA + B\sum_{i=1}^{n} x_i &= \sum_{i=1}^{n} z_i \\ A\sum_{i=1}^{n} x_i + B\sum_{i=1}^{n} x_i^2 &= \sum_{i=1}^{n} x_i z_i. \end{aligned}$$

The solution to this system of equations is

$$B = \frac{n\sum\limits_{i=1}^{n} x_i z_i - \sum\limits_{i=1}^{n} x_i \sum\limits_{i=1}^{n} z_i}{n\sum\limits_{i=1}^{n} x_i^2 - \left(\sum\limits_{i=1}^{n} x_i\right)^2},$$

$$A = \frac{\sum\limits_{i=1}^{n} x_i^2 \sum\limits_{i=1}^{n} z_i - \sum\limits_{i=1}^{n} x_i \sum\limits_{i=1}^{n} x_i z_i}{n\sum\limits_{i=1}^{n} x_i^2 - \left(\sum\limits_{i=1}^{n} x_i\right)^2}.$$

Now since A and B are found, the original constants with the model are found as:

$$A = \ln(a) \implies a = e^A$$

and

$$B = \ln(b) \implies b = e^B$$

Example 5.11. Fit an equation of the form $y = ab^x$ to the following data:

x	2	3	4	5	6
$y = f(x)$	144	172.8	207.4	248.8	298.6

Solution: Let the given equation be $y = ab^x$. Repeat the procedure in subsection 5.3.2, we get $z = A + Bx$ where $A = ln(a)$, $B = ln(b)$ and $z = ln(y)$.
The normal equations are given by

$$\begin{aligned} nA + B\sum_{i=1}^{n} x_i &= \sum_{i=1}^{n} z_i \\ A\sum_{i=1}^{n} x_i + B\sum_{i=1}^{n} x_i^2 &= \sum_{i=1}^{n} x_i z_i. \end{aligned}$$

Table for calculations:

i	x	y	$z = ln(y)$	x^2	xz
1	2	144	4.97	4	9.94
2	3	172.8	5.15	9	15.45
3	4	207.4	5.33	16	21.32
4	5	248.8	5.52	25	27.60
5	6	298.6	5,69	36	34.14
sum	20		26.66	90	108.45

Here $n = 5$ and substitute the above values in the above normal equations, we have

$$5A + 20B = 26.66$$
$$20A + 90B = 108.45.$$

Solving these equations, we get $A = 4.608$ and $B = 0.181$.
Since $A = ln(a) = 4.608 \implies a = e^A = e^{4.608} = 100.28$ and $b = e^B = e^{0.181} = 1.1984$.
Hence, the required equation for the given data is

$$y = 100.28(1.1984)^x.$$

Example 5.12. Find an exponential curve $y = ab^x$ to the following data by the method of least squares:

x	0	2	4
$y = f(x)$	5.012	10	31.62

Solution: Let the given equation be $y = ab^x$. Repeat the procedure in subsection eqec7.1, we get $z = A + Bx$ where $A = ln(a)$, $B = ln(b)$ and $z = ln(y)$.
The normal equations are given by

$$nA + B\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} z_i$$
$$A\sum_{i=1}^{n} x_i + B\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i z_i.$$

Table for calculations:

i	x	y	$z = ln(y)$	x^2	xz
1	0	5.012	1.6118	0	0
2	2	10.00	2.3026	4	4.6052
3	4	31.62	3.4538	16	13.8152
sum	6		7.3682	20	18.4204

Here $n = 3$ and substitute the above values in the above normal equations, we have

$$3A + 6B = 7.3682$$
$$6A + 20B = 18.420.$$

Solving these equations, we get $A = 1.5352$ and $B = 0.4604$.
Since $A = ln(a) = 1.5352 \implies a = e^A = e^{1.5352} = 4.6423$ and $b = e^B = e^{0.4604} = 1.5847$.
Hence, the required equation for the given data is

$$y = 4.6423(1.5847)^x.$$

5.3.3 Logarithmic Functions

The form for the log models is:

$$y = \beta_0 + \beta_1 \ln(x).$$

This is a linear function between y and $ln(x)$, the usual least square method are applied in which y is the response variable and $ln(x)$ is the regresses.
Let $t = ln(x)$, we obtain: $y = \beta_0 + \beta_1 t$. This is a linear relationship between y and t, and the coefficients β_0 and β_1. These equations simplify to what is known as the normal equations (see Section 5.2):

$$n\beta_0 + \beta_1 \sum_{i=1}^{n} t_i = \sum_{i=1}^{n} y_i \quad \text{and} \quad \beta_0 \sum_{i=1}^{n} t_i + \beta_1 \sum_{i=1}^{n} t_i^2 = \sum_{i=1}^{n} t_i y_i.$$

The solution to this system of equations is

$$\beta_1 = \frac{n\sum_{i=1}^{n} t_i y_i - \sum_{i=1}^{n} t_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} t_i^2 - \left(\sum_{i=1}^{n} t_i\right)^2},$$
$$\beta_0 = \frac{\sum_{i=1}^{n} t_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} t_i \sum_{i=1}^{n} t_i y_i}{n\sum_{i=1}^{n} t_i^2 - \left(\sum_{i=1}^{n} t_i\right)^2}.$$

$b = a_1; \quad a = e^{a_0}.$

Example 5.13. Fit a logarithmic functions $y = \beta_0 + \beta_1 \ln(x)$ from the following data:

x	1	2	3	4
$y = f(x)$	1.8	3.3	4.5	6.3

Solution: The logarithmic function is $y = \beta_0 + \beta_1 t$, where $t = \ln(x)$.
The normal equations are

$$n\beta_0 + \beta_1 \sum_{i=1}^{n} t_i = \sum_{i=1}^{n} y_i$$
$$\beta_0 \sum_{i=1}^{n} t_i + \beta_1 \sum_{i=1}^{n} t_i^2 = \sum_{i=1}^{n} t_i y_i.$$

Table for calculations:

i	x	t	y	t^2	ty
1	1	0	1.8	0	0
2	2	0.6931	3.3	0.4804	2.2872
3	3	1.0986	4.5	1.2069	4.943
4	4	1.3863	6.3	1.9218	8.7337
sum		3.1780	16.9	3.6091	15.9639

Since there are 4 pairs of values of t and y, hence here $n = 4$ and substitute the above values in the above normal equations, we have

$$4\beta_0 + 3.1780\beta_1 = 16.9$$
$$3.1780\beta_0 + 3.6091\beta_1 = 15.9639.$$

Solving these equations, we get $\beta_0 = 2.3660$ and $\beta_1 = 2.3399$.
Therefore, the required least square line is $y = 2.3660 + 2.3399 \ln(x)$, which is the line of best fit.

5.3.4 Power Functions

The power function equation describes many scientific and engineering phenomena. In chemical engineering, the rate of chemical reaction is often written in power function of the form of

$$y = ax^b.$$

The method of least squares is applied to the power function by first linearizing the data (the assumption is that b is not known). If the only unknown is a, then a linear relation exists between x^b and y. The linearization of the data is as follows:

$$\ln(y) = \ln(a) + b \ln(x).$$

The resulting equation shows a linear relation between $\ln(y)$ and $\ln(x)$.

Let $z = \ln(y)$, $w = \ln(x)$, and $A = \ln a$ which imply $a = e^A$, $B = b$.

We get:

$$z = A + Bw.$$

Hence,

$$B = \frac{n\sum_{i=1}^{n} w_i z_i - \sum_{i=1}^{n} w_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} w_i^2 - \left(\sum_{i=1}^{n} w_i\right)^2},$$

$$A = \frac{\sum_{i=1}^{n} w_i^2 \sum_{i=1}^{n} z_i - \sum_{i=1}^{n} w_i \sum_{i=1}^{n} w_i z_i}{n\sum_{i=1}^{n} w_i^2 - \left(\sum_{i=1}^{n} w_i\right)^2}.$$

Since A and B can be found, the original constants of the model are: $b = B$; $a = e^A$.

Example 5.14. Fit the power curve of the form $y = ax^b$ for the following data:

x	1	2	4	6
$y = f(x)$	6	4	2	2

Solution: Let the given equation be $y = ax^b$. Repeat the procedure in subsection 5.3.4, we get $z = A + Bw$ where $A = ln(a)$, $B = b$, $w = ln(x)$ and $z = ln(y)$.
The normal equations are given by

$$nA + B\sum_{i=1}^{n} w_i = \sum_{i=1}^{n} z_i$$

$$A\sum_{i=1}^{n} w_i + B\sum_{i=1}^{n} w_i^2 = \sum_{i=1}^{n} w_i z_i.$$

Table for calculations:

i	x	y	$w = ln(x)$	$z = ln(y)$	w^2	wz
1	1	6	0	1.79	0	0
2	2	4	0.693	1.386	0.48	0.96
3	4	2	1.386	0.693	1.92	0.96
4	6	2	1.79	0.693	3.2	1.24
sum			3.87	4.56	5.6	3.16

Here $n = 4$ and substitute the above values in the above normal equations, we have

$$4A + 3.87B = 4.56$$

$$3.87A + 5.6B = 3.16.$$

Solving these equations, we get $A = 1.786$ and $B = -0.672$.
Since $A = ln(a) = 1.786 \implies a = e^A = 5.965$ and $b = B = -0.672$.
Hence, the required power curve is

$$y = 5.965x^{-0.672}.$$

Example 5.15. Fit a curve $y = ax^b$ to the following data:

x	1	2	3
$y = f(x)$	2.98	4.26	5.21

Solution: Let the given equation be $y = ax^b$. Repeat the procedure in subsection 5.3.4, we get $z = A + Bw$ where $A = ln(a)$, $B = b$, $w = ln(x)$ and $z = ln(y)$.
The normal equations are given by

$$nA + B\sum_{i=1}^{n} w_i = \sum_{i=1}^{n} z_i$$
$$A\sum_{i=1}^{n} w_i + B\sum_{i=1}^{n} w_i^2 = \sum_{i=1}^{n} w_i z_i.$$

Table for calculations:

i	x	y	$w = ln(x)$	$z = ln(y)$	w^2	wz
1	1	2.98	0	1.0919	0	0
2	2	4.26	0.6931	1.4493	0.4804	1.0045
3	3	5.21	1.0986	1.6506	1.2069	1.8133
sum			1.7917	4.1918	1.6873	2.8178

Here $n = 6$ and substitute the above values in the above normal equations, we have

$$3A + 1.7917B = 4.1918$$
$$1.7917A + 1.6873B = 2.8178.$$

Solving these equations, we get $A = 1.0931$ and $B = 0.5092$.
Since $A = ln(a) = 1.0931 \implies a = e^A = 2.9835$ and $b = B = 0.5092$.
Hence, the required power curve is

$$y = 2.9835x^{0.5092}.$$

5.4 EXERCISES

1. Find the linear lest-squares solution for the following table of values:

x	4	7	11	13	17
y	2	0	2	6	7

2. By using the method of least-squares, find the constant function that best fits the following data:

x	-1	2	3
y	$\frac{5}{4}$	$\frac{4}{3}$	$\frac{5}{12}$

3. Find an equation of the form $y = ae^{x^2} + bx^3$ that best fits the points $(-1, 0)$, $(0, 1)$ and $(1, 2)$ in the least-squares sense.

4. Find the equation of a parabola of form $y = ax^2 + b$ that best represents the following data. Use the method of least squares.

x	-1	0	1
y	3.1	0.9	2.9

5. What straight line best fits the following data

x	1	2	3	4
y	0	1	1	2

in the least-squares sense?

6. What constant c makes the expression $\sum_{k=0}^{n}[f(x_k) - ce^{x_k}]^2$ as small as possible?

7. Find an equation of the form $y = (1 + b\,e^{ax})$, $y = a\,x + b\,x^2$, $y = a\,x + \frac{b}{\sqrt{x}}$, $y = a\,e^{-3x} + b\,e^{-2x}$, $y = \frac{b}{x+a}$, $y = \frac{b}{x(x-a)}$ and $y = a + bxy$ that best fits the points (1,4), (2,6), (3,8) and (4,9) in the least-squares sense.

8. Find the power fits $y = Ax^2$, $y = Bx^3$, $y = \frac{C}{x}$ and $y = \frac{D}{x^2}$ for the following data and use the least-squares error to determine which curve fits best.

x	2	2.3	2.6	2.9	3.2
y	3	3.4	3.8	5	5.2

CHAPTER 6

Numerical Integrations

6.1 Introduction

The process of evaluating a definite integral from a set of tabulated values of the integrand $f(x)$, which is not known explicit is called numerical integration. Numerical integration, also known as **quadrature**, quadrature approximates the definite integral as follows:

$$I = \int_a^b f(x)dx = \sum_{i=0}^{n} A_i f(x_i),$$

where the nodal abscissas x_i and weights A_i depend on the particular rule used for the quadrature. All rules of quadrature can be derived from polynomial interpolation of the integrand as follows:

$$\begin{aligned} I &= \int_a^b f(x)dx \approx \int_a^b P_n(x)dx \\ &= \int_a^b \sum_{i=0}^{n} f(x_i) l_n^i(x)dx = \sum_{i=0}^{n} f(x_i) \int_a^b l_n^i(x)dx = \sum_{i=0}^{n} A_i f(x_i), \end{aligned} \tag{6.1}$$

where $A_i = \int_a^b l_n^i(x)dx; \quad i = 0, 1, \ldots, n$ and $P_n(x)$ Lagrange interpolation polynomial of degree n.

Definition 6.1. The **degree of accuracy** or **precision** of a numerical integration formula is the largest positive integer n such that the formula is exact for x^k, for each k =0, 1, 2, $\ldots, n$.

In this chapter we derive several formulas for numerical integration

6.2 Trapezoidal Rule of Integration

In this method, the known function values are joined by straight lines. The area enclosed by these lines between the given end points is computed to approximate the integral as shown in Figure 6.1.

$$I = \int_a^b f\,(x)\,dx,$$

where $f(x)$ is called the integrand, a = lower limit of integration, b = upper limit of integration.

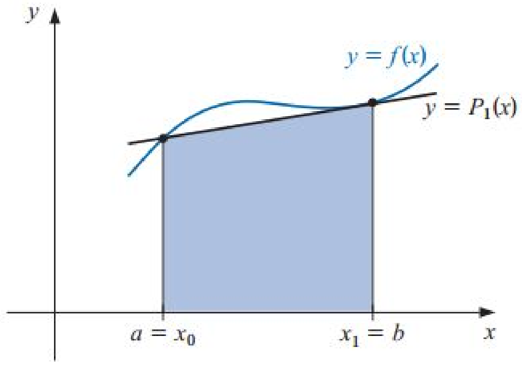


Figure 6.1: *Integration by Trapezoid rule.*

6.2.1 Derivation of the Trapezoidal Rule

In this section, trapezoidal rule is derived by two different methods as follows:

Method 1: Derived from Lagrange Interpolation Polynomial

Since we have two points $(a, f(a))$ and $(b, f(b))$, we construct Lagrange interpolation polynomial of degree one

$$f(x) \approx P_1(x) = \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b),$$

which approximate $f(x)$ between these two points (see Figure 6.1). From (6.1), we have

$$\begin{aligned}
\int_a^b f(x)dx \approx \int_a^b P_1(x)dx &= \int_a^b \left(\frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b) \right) dx \\
&= \frac{f(a)}{a-b} \int_a^b (x-b)dx + \frac{f(b)}{b-a} \int_a^b (x-a)dx \\
&= \frac{f(a)}{a-b} \frac{(x-b)^2}{2}\bigg|_a^b + \frac{f(b)}{b-a} \frac{(x-a)^2}{2}\bigg|_a^b \\
&= -\frac{f(a)}{a-b} \frac{(a-b)^2}{2} + \frac{f(b)}{b-a} \frac{(b-a)^2}{2} \\
&= -f(a)\frac{(a-b)}{2} + f(b)\frac{(b-a)}{2} \\
&= \frac{b-a}{2}[f(a) + f(b)] \\
&= \frac{h}{2}[f(a) + f(b)], \quad \text{(Trapezoid rule)} \qquad (6.2)
\end{aligned}$$

where $h = b - a$ in Trapezoid rule.

The error in the trapezoidal rule E_{tr}) is the area of the region between $f(x)$ and the straight-line interpolant, as indicated in Figure 6.2.

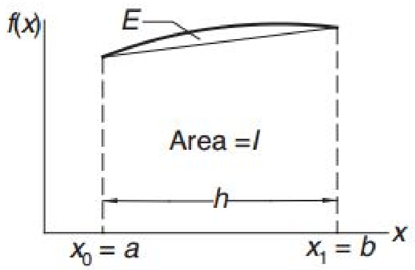


Figure 6.2: *Error in Trapezoid rule.*

It can be obtained by integrating the interpolation error

$$f(x) - P_1(x) = \frac{f''(\zeta)}{2!}(x-a)(x-b)$$

as follows:

$$\begin{aligned}
E_{tr} &= \int_a^b [f(x) - P_1(x)]dx = \frac{f''(\zeta)}{2!}\int_a^b \underbrace{(x-a)}_{u}\underbrace{(x-b)dx}_{dv} \\
&= \frac{f''(\zeta)}{2!}\left[(x-a)\frac{(x-b)^2}{2}\bigg|_a^b - \int_a^b \frac{(x-b)^2}{2}dx\right] \\
&= \frac{f''(\zeta)}{2!}\left[-\frac{(x-b)^3}{6}\bigg|_a^b\right] \\
&= -\frac{(b-a)^3}{12}f''(\zeta), \;\; a \le \zeta \le b \\
&= -\frac{h^3}{12}f''(\zeta). \qquad (6.3)
\end{aligned}$$

Method 2: Derived from Newton Forward Difference interpolation

The trapezoidal rule can also be derived from Newton forward difference interpolation polynomial

$$\begin{aligned}
P_n(x) = f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \cdots \\
+ \frac{s(s-1)(s-2)\cdots(s-n+1)}{n!}\Delta^n f(x_0). \qquad (6.4)
\end{aligned}$$

Look at Figure 6.2. The area under the curve $f(x)$ is the area of a trapezoid. Substituting $s = 1$ in Equation (6.4) and considering the curve $y = f(x)$ through the points $(a = x_0, y_0)$ and $(b = x_1, y_1)$ as a straight line (a polynomial of first degree so that the differences of order higher than first vanished), we get:

$$I_1 = \int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx = \int_{x_0}^{x_1} (y_0 + s\Delta y_0)dx = h\int_0^1 (y_0 + s\Delta y_0)ds$$
$$= h\left[y_0 + \frac{1}{2}\Delta y_0\right] = \frac{h}{2}\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}[y_0 + y_1]$$
$$= \frac{h}{2}[f(a) + f(b)] = \frac{h}{2}[f(x_0) + f(x_1)].$$

To find the error E_{tr}:
The error in approximating $f(x)$ by Newton forward difference interpolation polynomial of degree one *i.e.* $P_1(x) = y_0 + s\Delta y_0$ is equal to:

$$f(x) - P_1(x) = \frac{s(s-1)}{2!}h^2 f''(\zeta), \;\; a = x_0 \le \zeta \le b = x_1.$$

Hence

$$E_{tr} = \int_a^b [f(x) - P_1(x)]dx = \int_{x_0}^{x_1} [f(x) - P_1(x)]dx$$
$$= \int_{x_0}^{x_1} [\frac{s(s-1)}{2!}h^2 f''(\zeta)]dx = h\int_0^1 [\frac{s(s-1)}{2!}h^2 f''(\zeta)]ds$$
$$= \frac{h^3}{2}f''(\zeta)\int_0^1 [s(s-1)]ds = \frac{h^3}{2}f''(\zeta)\left[\frac{s^3}{3} - \frac{s^2}{2}\right]_0^1$$
$$= \frac{h^3}{2}f''(\zeta)\left[\frac{1}{3} - \frac{1}{2}\right]$$
$$= -\frac{h^3}{12}f''(\zeta).$$

6.3 Composite Trapezoidal Rule of Integration

Consider the integral $I = \int_a^b f(x)dx$.
Let us divide the interval (a, b) into n sub intervals of width h so that:

$$x_0 = a, \;\; x_1 = x_0 + h, \;\; x_2 = x_1 + h = x_0 + 2h, \dots, x_n = x_{n-1} + h = x_0 + nh = b,$$

where $h = \frac{b-a}{n}$; n even or odd natural number.
Now

$$I = \int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx$$
$$= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \int_{x_2}^{x_3} f(x)dx + \dots + \int_{x_{n-1}}^{x_n} f(x)dx$$
$$= \frac{h}{2}[f(x_0) + f(x_1)] + \frac{h}{2}[f(x_1) + f(x_2)] + \frac{h}{2}[f(x_2) + f(x_3)] + \dots$$
$$+ \frac{h}{2}[f(x_{n-1}) + f(x_n)] \;\; \text{by using (6.2)}$$
$$= \frac{h}{2}[f(x_0) + 2f(x_1) + 2f(x_2) + \dots + 2f(x_{n-1}) + f(x_n)].$$

Hence, the total area, representing $\int_a^b f(x)dx$, is:

$$
\begin{aligned}
I &= \int_a^b f(x)dx \\
&= \frac{h}{2}[f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n)] \\
&= \frac{h}{2}\left[f(x_0) + 2\left\{\sum_{i=1}^{n-1} f(x_i)\right\} + f(x_n)\right]. \qquad (6.5)
\end{aligned}
$$

Which is the composite trapezoidal rule (method).

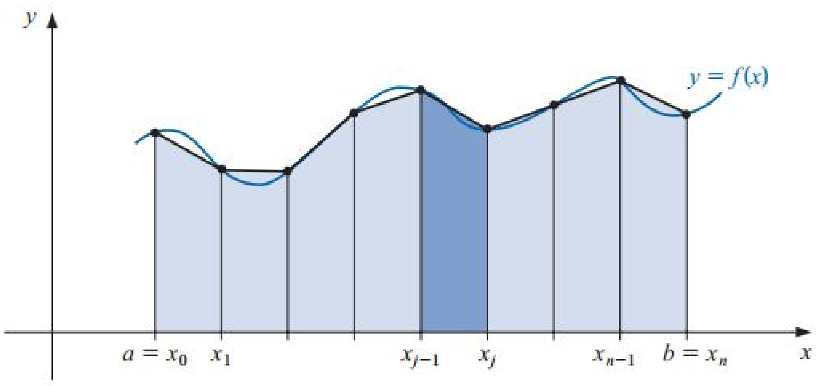


Figure 6.3: *Composite trapezoidal rule approximations.*

6.3.1 Error in Composite Trapezoidal Rule

The true error for a single segment Trapezoidal rule is given by:

$$E_t = -\frac{h^3}{12} f''(\zeta), \quad a < \zeta < b,$$

where $h = \frac{b-a}{n}$.

The error in each segment is:

$$
\begin{aligned}
E_1 &= -\frac{h^3}{12} f''(\zeta_1), \quad x_0 = a < \zeta_1 < x_1. \\
E_2 &= -\frac{h^3}{12} f''(\zeta_2), \quad x_1 < \zeta_2 < x_2. \\
&\vdots \\
E_n &= -\frac{h^3}{12} f''(\zeta_n), \quad x_{n-1} < \zeta_n < x_n = b.
\end{aligned}
$$

Hence, the total error in the composite trapezoidal rule is:

$$
\begin{aligned}
E_t &= \sum_{i=1}^{n} E_i = -\frac{h^3}{12}\sum_{i=1}^{n} f''(\zeta_i) = -\frac{h^3}{12n^3}\sum_{i=1}^{n} f''(\zeta_i) \\
&= -\frac{(b-a)^3}{12n^2}\frac{\sum_{i=1}^{n} f''(\zeta_i)}{n} = -\frac{(b-a)}{12} h^2 f''(\zeta); \;\; x_0 = a < \zeta < x_n = b.
\end{aligned}
$$

Hence

$$E_t = -\frac{(b-a)}{12}h^2 f''(\zeta); \;\; x_0 = a < \zeta < x_n = b.$$

Example 6.1. Use the trapezoidal rule to numerically integrate $\int_0^2 (0.2 + 25\,x)dx$.

Solution: Let $f(x) = 0.2 + 25\,x$, $f(a) = f(0) = 0.2$, $f(b) = f(2) = 50.2$ and $\frac{b-a}{2}$ $frac2 - 02 = 1$.

$$\begin{aligned} I &= \int_0^2 f(x)dx = \frac{h}{2}[f(a) + f(b)] \\ &= \frac{1}{2}[0.2 + 50.2] = 50.4. \end{aligned}$$

The true solution is:

$$I = \int_0^2 f(x)\,dx = \left.(0.2\,x + 12.5\,x^2)\right]_0^2 = 50.4.$$

Since $f(x)$ is a linear function, using the trapezoidal rule gets the exact solution, because $f''(x) = 0$ (see (6.3)).

Example 6.2. Use the trapezoidal rule to numerically integrate $\int_0^2 (0.2 + 25\,x + 3\,x^2)dx$.

Solution: Let $f(x) = 0.2 + 25\,x + 3\,x^2$. Hence $f(a) = f(0) = 0.2$, $f(b) = f(2) = 62.2$ and
$h = \frac{b-a}{2} = \frac{2-0}{2} = 1$. Using the Trapezoid rule, we get

$$\begin{aligned} I &= \int_0^2 f(x)dx = \frac{h}{2}[f(a) + f(b)] \\ &= \frac{1}{2}[0.2 + 62.2] = 62.4. \end{aligned}$$

The true solution is:

$$I = \int_0^2 f(x)\,dx = \left.(0.2\,x + 12.5\,x^2 + x^3)\right]_0^2 = 58.4.$$

The relative error is:

$$\left| \in_t = \left| \frac{58.4 - 62.4}{58.4} \right| \right| \times 100\,\% = 6.85\,\%.$$

Example 6.3. Approximate the integral $\int_0^\pi \sin(x)\,dx$ using composite trapezoidal rule for $n = 4$ and $n = 8$.

Solution:
The exact value of the integral is

$$\int_0^\pi \sin(x)\,dx = [-\cos(x)]_0^\pi = 2.$$

As $n = 4$, $h = \frac{b-a}{n} = \frac{\pi}{4}$,

$$\begin{aligned}\int_0^{\pi} \sin(x)\,dx &\approx \tfrac{\pi}{2\cdot 4}\left[\sin(0) + 2\sin\left(\tfrac{\pi}{4}\right) + 2\sin\left(\tfrac{2\pi}{4}\right) + 2\sin\left(\tfrac{3\pi}{4}\right) + \sin(\pi)\right] \\ &= \tfrac{\pi}{8}\left[0 + \sqrt{2} + 2 + \sqrt{2} + 0\right] = \tfrac{\pi\left(1+\sqrt{2}\right)}{4} \\ &\approx 1.896\end{aligned}$$

As $n = 8$, $h = \frac{\pi}{8}$,

$$\begin{aligned}\int_0^{\pi} \sin(x)\,dx &\approx \tfrac{\pi}{2\cdot 8}\left[\sin(0) + 2\sin\left(\tfrac{\pi}{8}\right) + \cdots + 2\sin\left(\tfrac{7\pi}{8}\right) + \sin(\pi)\right] \\ &= \tfrac{\pi}{16}\left[2 + 2\sqrt{2} + 4\sin\left(\tfrac{\pi}{8}\right) + 4\sin\left(\tfrac{3\pi}{8}\right)\right] \\ &\approx 1.974\end{aligned}$$

The question to ask: how accurate the above approximations are?
The error for the trapezoidal rule is denoted as

$$E_{tr} = \int_a^b f(x)\,dx - \left(\frac{h}{2}\right)\left[f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n)\right],$$

the accuracy of the trapezoidal rule: $\left|f''(x)\right| \le M$ for $x \in [a,b]$. Then,

$$|E_{tr}| \le M \cdot \frac{(b-a)^3}{12n^2}.$$

The above result can be used to obtain the required number of partitions, n.

Example 6.4. Determine a value of n so that the composite trapezoidal rule will approximate the value of $\int_0^1 \sqrt{1+x^2}dx$ with an error that is less than 0.01.

Solutions:

$$f(x) = \sqrt{1+x^2},\ f'(x) = x\left(1+x^2\right)^{-1/2},\ f''(x) = \left(1+x^2\right)^{-3/2}.$$

Since the maximum value of $f''(x)$ on $[0,1]$ is 1, i.e.,

$$\left|f''(x)\right| = \left(1+x^2\right)^{-3/2} \le 1,\ x \in [0,1].$$

Thus,

$$|E_{tr}| \le M \cdot \frac{(b-a)^3}{12n^2} = 1 \cdot \frac{(1-0)^3}{12n^2} = \frac{1}{12n^2}.$$

As

$$\frac{1}{12n^2} \le 0.01 \ \Leftrightarrow\ 12n^2 \ge 100 \ \Leftrightarrow\ n \ge 2.89 \ \Rightarrow\ n = 3,$$

the error is smaller than 0.01. As $n = 3$, $h = \frac{1}{3}$,

$$\begin{aligned}\int_0^1 \sqrt{1+x^2}dx &\approx \tfrac{1}{2\cdot 3}\left[\sqrt{1+0^2} + 2\sqrt{1+\left(1/3\right)^2} + 2\sqrt{1+\left(2/3\right)^2} + 2\sqrt{1+1^2}\right] \\ &= 1.154\end{aligned}$$

Thus,

$$\left|\int_0^1 \sqrt{1+x^2}dx - 1.154\right| \leq 0.01$$
$$\Leftrightarrow\ 1.144 = 1.154 - 0.01 \leq \int_0^1 \sqrt{1+x^2}dx \leq 1.154 + 0.01 = 1.164.$$

Example 6.5. Use the composite trapezoidal rule to find the area under the curve $f(x) = \frac{300x}{1+e^x}$ from $x = 0$ to $x = 10$ with $n = 2$.

Solution: Using $n = 2$, we get: $h = \frac{10-0}{2} = 5$,

$$f(0) = \frac{300 \times 0}{1+e^0} = 0,\ f(5) = \frac{300 \times 5}{1+e^5} = 10.039,\ f(10) = \frac{300 \times 10}{1+e^{10}} = 0.136,$$

$$\begin{aligned}
I &\approx \frac{h}{2}\left[f(a) + 2\left\{\sum_{i=1}^{n-1} f(a+ih)\right\} + f(b)\right] \\
&\frac{5}{2}\left[f(0) + 2\left\{\sum_{i=1}^{2-1} f(0+5)\right\} + f(10)\right] \\
&= \frac{5}{2}\left[f(0) + 2f(5) + f(10)\right] \\
&= \frac{5}{2}\left[0 + 2(10.039) + 0.136\right] = 50.537.
\end{aligned}$$

So what is the true value of this integral?

$$\int_0^{10} \frac{300x}{1+e^x} dx = 246.59.$$

Making the absolute relative true error

$$|\in_t| = \left|\frac{246.59 - 50.535}{246.59}\right| \times 100 = 79.506\%$$

Example 6.6. Use composite trapezoidal rule to find $I = \int_0^2 \frac{1}{\sqrt{x}} dx$ with $n =$.

Solution: We cannot use the trapezoidal rule for this integral, as the value of the integrand at $x = 0$ is infinite. However, it is known that a discontinuity in a curve will not change the area under it. We can assume any value for the function at $x = 0$. The algorithm to define the function so that we can use the multiple-segment trapezoidal rule is given below:

Function $f(x)$
If $x = 0$ Then $f = 0$
If $x \neq 0$ Then $f = x^{-0.5}$
End Function

Basically, we are just assigning the function a value of zero at $x = 0$. Everywhere else, the function is continuous. This means that the true value of our integral will be just that-true. Let's see what happens using the composite trapezoidal rule. Using two segments *i.e.* $n = 2$, we get:

$$h = \frac{2-0}{2} = 1, \; f(0) = 0, \; f(1) = \frac{1}{\sqrt{1}} = 1, \; f(2) = \frac{1}{\sqrt{2}} = 0.70711,$$

$$\begin{aligned} I &\approx \frac{h}{2}\left[f(a) + 2\left\{\sum_{i=1}^{n-1} f(a+ih)\right\} + f(b)\right] \\ &= \frac{1}{2}\left[f(0) + 2\left\{\sum_{i=1}^{2-1} f(0+1)\right\} + f(2)\right] = \frac{1}{2}\left[f(0) + 2f(1) + f(2)\right] \\ &= \frac{1}{2}\left[0 + 2(1) + 0.70711\right] = 1.3536. \end{aligned}$$

So what is the true value of this integral? $\int_0^2 \frac{1}{\sqrt{x}} dx = 2.8284$.
Thus, making the absolute relative true error

$$|\in_t| = \left|\frac{2.8284 - 1.3536}{2.8284}\right| \times 100 = 52.145\%.$$

Table (6.1) *Values obtained using composite trapezoidal rule for* $\int_0^2 \frac{1}{\sqrt{x}} dx.$

n	Approximate Value	E_t	$\lvert\in_t\rvert$
2	1.354	1.474	52.14%
4	1.792	1.036	36.64%
8	2.097	0.731	25.85%
16	2.312	0.516	18.26%
32	2.463	0.365	12.91%
64	2.570	0.258	9.128%
128	2.646	0.182	6.454%
256	2.699	0.129	4.564%
512	2.737	0.091	3.227%
1024	2.764	0.064	2.282%
2048	2.783	0.045	1.613%
4096	2.796	0.032	1.141%

Example 6.7. Compute the composite trapezoidal approximation for $\int_0^2 \sqrt{x} dx$ using a regular partition with $n = 4$. Compare the estimate with the exact value.

Solution: So with n = 4, each subinterval will have length $h = \frac{b-a}{4} = \frac{1}{2}$.
Then $x_0 = 0 =$; $x_1 = x_0 + h = \frac{1}{2}$; $x_2 = x_1 + h = \frac{1}{2} + \frac{1}{2} = 1$; $x_3 = x_2 + h = 1 + \frac{1}{2} = \frac{3}{2}$ and $x_4 = x_3 + h = \frac{3}{2} + \frac{1}{2} = \frac{4}{2} = 2$.

$$
\begin{aligned}
I &= \int_0^2 \sqrt{x}dx \\
&= \frac{h}{2}[f(x_0) + 2f(x_1) + 2f(x_2) + 2f(x_3) + f(x_4)] \\
&= \frac{1}{4}[\sqrt{0} + 2\sqrt{\frac{1}{2}} + 2\sqrt{1} + 2\sqrt{\frac{3}{2}} + \sqrt{2}] \\
&= \frac{1}{4}[0 + \sqrt{2} + 2 + \sqrt{6} + \sqrt{2}] = \frac{1}{4}[2 + 2\sqrt{2} + \sqrt{6} + \sqrt{2}] \approx 1.81948.
\end{aligned}
$$

The exact value of the integral is

$$\int_0^2 \sqrt{x}dx = \frac{2}{3}x^{\frac{3}{2}}\Big|_0^2 = \frac{2}{3}2^{\frac{3}{2}} - \frac{2}{3}0^{\frac{3}{2}} = \frac{2}{3}[2\sqrt{2}] = 1.88562.$$

The approximation underestimates the actual area, the error is

$$1.88562 - 1.81948 = 0.06614$$

and that is

$$\frac{0.06614}{1.88562} \approx 0.035076$$

or 3.51% of the exact value.

Example 6.8. Evaluate the integral $\int_0^{1.2} e^x dx$, taking six intervals by using composite trapezoidal rule.

Solution: Since $a = 0$, $b = 1.2$, $n = 6$, hence $h = \frac{b-a}{n} = \frac{1.2-0}{6} = 0.2$.

x	0	0.2	0.4	0.6	0.8	1.0	1.2
y = f(x)	0	1.221	1.492	1.822	2.226	2.718	3.320
	y0	y1	y2	ys	y4	y5	y6

The trapezoidal rule can be written as

$$
\begin{aligned}
I &= \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + 2y_4 + 2y_5 + y_6] \\
&= \frac{0.2}{2}[0 + 2(1.221 + 1.492 + 1.822 + 2.226 + 2.718) + 3.320] \\
&= 2.328.
\end{aligned}
$$

The exact value is $= \int_0^{1.2} e^x dx = 2.320$.

Example 6.9. Evaluate $\int_0^{12} \frac{1}{1+x^2}dx$ by using composite trapezoidal rule, taking n = 6.

Solution: Since $a = 0$, $b = 12$, $n = 6$, hence $h = \frac{b-a}{n} = \frac{12-0}{6} = 2$.

x	0	2	4	6	8	10	12
y = f(x)	1.00000	0.20000	0.05882	0.02703	0.01538	0.00990	0.00690

The trapezoidal rule can be written as

$$\begin{aligned} I &= \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + 2y_4 + 2y_5 + y_6] \\ &= \frac{2}{2}[1 + 2(0.2 + 0.05882 + 0.02703 + 0.01538 + 0.00990) + 0.00690] \\ &= 1.62916. \end{aligned}$$

The exact value is

$$\int_0^{12} \frac{1}{1+x^2}dx = tan^{-1}(x)\Big|_0^{12} = 1.48766.$$

Example 6.10. Use composite trapezoid rule with $n = 5$ estimate $\int_1^5 \sqrt{1+x^2}dx$.

Solution: For $n = 5$, we have $h = \frac{b-a}{n} = \frac{5-1}{5} = 0.8$.
Computing the values for $y_0, y_1, y_2, y_3, y_4, y_5$.

x	1	1.8	2.6	3.4	4.2	5
$y = \sqrt{1+x^2}$	1.41	2.06	2.78	3.54	4.32	5.10

The trapezoidal rule can be written as

$$\begin{aligned} I &= \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + 2y_4 + y_5] \\ &= \frac{.8}{2}[1.41 + 2(2.06 + 2.78 + 3.54 + 4.32) + 5.10] \\ &= 12.284. \end{aligned}$$

Example 6.11. Use composite trapezoid rule with $n = 4$ estimate $\int_1^6 x^4 dx$.

Solution: For $n = 4$, we have $h = \frac{b-a}{n} = \frac{6-1}{4} = 1.25$.

$$x_0 = 1, \quad x_1 = 2.25, \quad x_2 = 3.5, \quad x_3 = 4.75, \quad x_4 = 6.$$

Computing the values for y_0, y_1, y_2, y_3, y_4.

x	1	2.25	3.5	4.75	6
$y = \sqrt{1+x^2}$	1	25.628	150.06	509.06	1296

The trapezoidal rule can be written as

$$\begin{aligned} I &= \int_1^6 x^4 dx = \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + y_4] \\ &= \frac{1.25}{2}[1 + 2(25.628 + 150.06 + 509.06) + 1296] \\ &= 1662.81. \end{aligned}$$

The exact value is

$$\int_1^6 x^4 dx = \left.\frac{x^5}{5}\right|_1^6 = 1555.$$

Example 6.12. Consider evaluating $\int_0^2 \frac{1}{1+x^2} dx$ using composite trapezoid method. How large should n be chosen in order to ensure that

$$|E_{ctm}| \leq 5 \times 10^{-6}. \tag{6.6}$$

Solution: We begin by calculating the derivatives:

$$f'(x) = \frac{-2x}{(1+x^2)^2}, \quad f''(x) = \frac{-2+6x^2}{(1+x^2)^3}.$$

From a graph of $f''(x)$,

$$\max_{0 \leq x \leq 2} |f''(x)| = 2.$$

Therefore

$$E_{ctm} = -\frac{(b-a)h^2}{12} f''(c), \text{ hence } \left| E_{ctm} \leq \frac{2h^2}{12} \times (2) \right| = \frac{h^2}{3}.$$

To ensure this, we choose h so small that

$$\frac{h^2}{3} \leq 5 \times 10^{-6}.$$

This is equivalent to choosing h and n to satisfy

$$h \leq 0.003873 \implies n = \frac{2}{h} \geq 516.4.$$

Thus $n \geq 517$ will imply (6.6)

Example 6.13. Determine the values of n and h required to approximate $\int_0^2 e^{2x} dx$ within (error$\leq 5 \times 10^{-4}$) using composite trapezoid method.

Solution: We begin by calculating the derivatives:

$$f'(x) = 2e^{2x}, \ \ f''(x) = 4e^{2x}.$$

From a graph of $f''(x)$,

$$\max_{0\leq x\leq 2} \left|f''(x)\right| = 218.3.$$

Therefore

$$E_{ctr} = -\frac{(b-a)h^2}{12}f''(c), \text{ hence } |E_{ctr}| \leq \frac{2h^2}{12} \times (218.3) = \frac{218.3h^2}{6}.$$

To ensure this, we choose h so small that

$$\frac{218.3h^2}{6} \leq 5 \times 10^{-4}.$$

This is equivalent to choosing h and n to satisfy

$$h \leq 0.003707095374473 \implies n = \frac{2}{h} \geq 539.5.$$

Thus $n \geq 540$ will imply the result.

6.4 Simpson's 1/3 Rule

The trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating the polynomial over interval of integration. Simpson's 1/3 rule is an extension of Trapezoidal rule where the integrand is approximated by a second order polynomial.

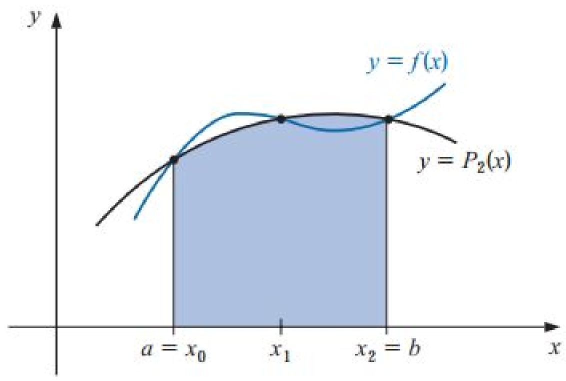


Figure 6.4: *Simpson's 1/3 Integration of a function.*

6.4.1 Derivation of the Simpson 1/3 Rule

In Simpson's 1/3 rule the integrand is approximated by a second order polynomial. To construct a second degree polynomial, we need three points. Let $x_0 = a$, $x_1 = \frac{b+a}{2}$, $x_2 = b$, hence the interval width $h = \frac{b-a}{2}$.

Method 1: Derived from Lagrange Interpolation Polynomial

Since we have three points $(a = x_0, y_0)$, (x_1, y_1) and $(x_2 = b, y_2)$ where $y_i = f(x_i)$ for $i = 0$, 1, 2, we construct Lagrange interpolation polynomial of degree two:

$$\begin{aligned} P_2(x) = &\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1) \\ &+ \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2). \end{aligned}$$

Using (6.1), we obtain:

$$\begin{aligned} I &= \int_{x_0=a}^{x_2=b} f(x)dx \approx \int_{x_0=a}^{x_2=b} P_2(x)dx \\ &= f(x_0)\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx + f(x_1)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}dx \\ &+ f(x_2)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx. \end{aligned} \tag{6.7}$$

Since the points are equally spaced nodes, we have $x_2 - x_1 = x_1 - x_0 = h$, $x_2 - x_0 = 2h$. Hence

$$\begin{aligned} I_1 &= f(x_0)\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx = \frac{f(x_0)}{2h^2}\int_{x_0}^{x_2}(x-x_1)(x-x_2)dx \\ &= \frac{f(x_0)}{2h^2}\left[(x-x_1)\frac{(x-x_2)^2}{2}\Big|_{x_0}^{x_2} - \int_{x_0}^{x_2}\frac{(x-x_2)^2}{2}dx\right] \\ &= \frac{f(x_0)}{2h^2}\left[2h^3 - \frac{(x-x_2)^3}{6}\Big|_{x_0}^{x_2}\right] = \frac{f(x_0)}{2h^2}\left[2h^3 - \frac{8h^3}{6}\right] \\ &= \frac{f(x_0)}{2h^2}\left[\frac{2h^3}{3}\right] = \frac{h}{3}f(x_0). \end{aligned}$$

Similarly;

$$I_2 = f(x_1)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}dx = \frac{4}{3}hf(x_1),$$

and

$$I_3 = f(x_2)\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx = \frac{1}{3}hf(x_2).$$

Substituting the value of I_1, I_2 and I_3 in (6.7), we obtain

$$\begin{aligned} I &= \int_{x_0}^{x_2} f(x)dx = I_1 + I_2 + I_3 \\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \quad \text{where } h = \frac{b-a}{2} \quad \text{(Simpson 1/3 rule)} \\ &= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{b+a}{2}\right) + f(b)\right] + E_{sm}, \end{aligned} \tag{6.8}$$

where $E_{sm} = -\frac{(b-a)^5}{2880}f^{(4)}(\zeta) = -\frac{h^5}{90}f^{(4)}(\zeta),\ \ a < \zeta < b$.

The formula (6.8) which can be viewed as the sum of the areas of three rectangles.

Method 2: Derived from Newton Forward Difference interpolation Polynomial

Since a second degree polynomial contains three constants, it is necessary to know three consecutive function values forming two intervals as shown in Figure 6.4. Substituting $s = 2$ in the Equation (6.4) and taking the curve through the points (x_0, y_0), (x_1, y_1) and (x_2, y_2) as a polynomial of second degree (parabola) so that the differences of order higher than two vanished, we obtain:

$$\begin{aligned} I_1 &= \int_{x_0}^{x_2} f(x)dx = 2h\left[y_0 + 4\Delta y_0 + \frac{1}{6}\Delta^2 y_0\right] \\ &= \frac{h}{3}(y_0 + 4y_1 + y_2) \\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + E_{sm}, \quad \text{(Simpson 1/3 rule)} \end{aligned} \tag{6.9}$$

where $E_{sm} = -\frac{(b-a)^5}{2880} f^{(4)}(\zeta) = -\frac{h^5}{90} f^{(4)}(\zeta), \;\; a < \zeta < b.$

6.5 Composite Simpson 1/3 Rule of Integration

Consider the integral $I = \int_a^b f(x)dx$.
Let us divide the interval (a, b) into n sub intervals of width h so that:

$$x_0 = a, \;\; x_1 = x_0 + h, \;\; x_2 = x_1 + h = x_0 + 2h, \ldots, x_n = x_{n-1} + h = x_0 + nh = b,$$

where $h = \frac{b-a}{n}$; n even natural number.
Now using (6.8), we obtain

$$\begin{aligned} I &= \int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx \\ &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \ldots + \int_{x_{n-2}}^{x_n} f(x)dx \\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + \frac{h}{3}[f(x_2) + 4f(x_3) + f(x_4)] + \ldots \\ &+ \frac{h}{3}[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)] \\ &= \frac{h}{3}[f(x_0) + 4(f(x_1) + f(x_3) + \ldots + f(x_{n-1})) \\ &+ 2(f(x_2) + f(x_4) + \ldots + f(x_{n-2})) + f(x_n)] \\ &= \frac{h}{3}[O_1 + 4O_2 + 2O_3], \end{aligned} \tag{6.10}$$

where $O_1 = f(x_0) + f(x_n)$ (sum of end ordinates), $O_2 = f(x_1) + f(x_3) + \ldots + f(x_{n-1})$ (sum of odd ordinates), $O_3 = f(x_2) + f(x_4) + \ldots + f(x_{n-2})$ (sum of even ordinates). Equation (6.10) is known as Composite Simpson's 1/3 rule. Also can be written as follows:

$$\int_a^b f(x)dx \cong \frac{b-a}{3n}\left[f(t_0) + 4 \sum_{\substack{i=1 \\ i=odd}}^{n-1} f(t_i) + 2 \sum_{\substack{i=2 \\ i=even}}^{n-2} f(t_i) + f(t_n) \right].$$

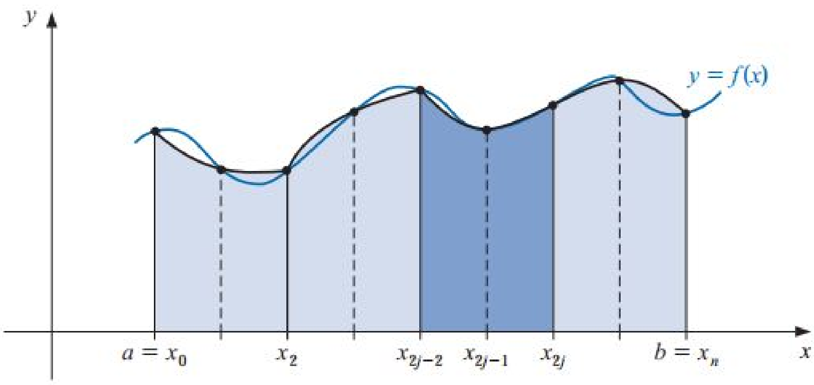


Figure 6.5: *Composite Simpson 1/3 method.*

6.5.1 Error in Composite Simpson's 1/3 Rule

The true error in a single application of Simpson's 1/3 rule is given by

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\zeta), \;\; a < \zeta < b.$$

In composite Simpson's 1/3 rule, the error is the sum of the errors in each application of Simpson's 1/3 rule. The error in the n segments Simpson's 1/3 rule is given by:

$$
\begin{aligned}
E_1 &= -\frac{(x_2-x_0)^5}{2880} f^{(4)}(\zeta_1) = -\frac{h^5}{90} f^{(4)}(\zeta_1), \quad x_0 < \zeta_1 < x_2. \\
E_2 &= -\frac{(x_4-x_2)^5}{2880} f^{(4)}(\zeta_2) = -\frac{h^5}{90} f^{(4)}(\zeta_2), \quad x_2 < \zeta_2 < x_4. \\
&\vdots \\
E_i &= -\frac{(x_{2i}-x_{2(i-1)})^5}{2880} f^{(4)}(\zeta_i) = -\frac{h^5}{90} f^{(4)}(\zeta_i), \quad x_{2(i-1)} < \zeta_i < x_{2i}. \\
&\vdots \\
E_{\frac{n}{2}-1} &= -\frac{(x_{n-2}-x_{n-4})^5}{2880} f^{(4)}(\zeta_{\frac{n}{2}-1}) \\
&= -\frac{h^5}{90} f^{(4)}(\zeta_{\frac{n}{2}-1}), \quad x_{n-4} < \zeta_{\frac{n}{2}-1} < x_{n-2}.
\end{aligned}
$$

and

$$
E_{\frac{n}{2}} = -\frac{(x_n-x_{n-2})^5}{2880} f^{(4)}\left(\zeta_{\frac{n}{2}}\right) = -\frac{h^5}{90} f^{(4)}\left(\zeta_{\frac{n}{2}}\right), x_{n-2} < \zeta_{\frac{n}{2}} < x_n.
$$

Hence, the total error in the composite Simpson's 1/3 rule is

$$
E_{sm} = \sum_{i=1}^{\frac{n}{2}} E_i = -\frac{h^5}{90} \sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i),
$$

where $x_{2i-2} < \zeta < x_{2j}; j = 1, 2 \ldots, \frac{n}{2}$.
If $f \in C^4[a,b]$, the Extreme Value Theorem [If $f \in C[a,b]$, then c_1, $c_2 \in [a,b]$ exist with $f(c_1) \le f(x) \le f(c_2)$, for all $x \in [a,b]$. In addition, if f is differentiable on (a,b), then the numbers c_1 and c_2 occur either at the endpoints of $[a,b]$ or where f' is zero.] implies that $f^{(4)}$ assumes its maximum and minimum in $[a,b]$. Since

$$
\min_{x\in[a,b]} f^{(4)}(x) \le f^{(4)}(\zeta_j) \le \max_{x\in[a,b]} f^{(4)}(x),
$$

we have

$$
\frac{n}{2} \min_{x\in[a,b]} f^{(4)}(x) \le \sum_{j=1}^{\frac{n}{2}} f^{(4)}(\zeta_j) \le \frac{n}{2} \max_{x\in[a,b]} f^{(4)}(x)
$$

and

$$
\min_{x\in[a,b]} f^{(4)}(x) \le \frac{2}{n} \sum_{j=1}^{\frac{n}{2}} f^{(4)}(\zeta_j) \le \max_{x\in[a,b]} f^{(4)}(x),
$$

By the Intermediate Value Theorem [If $f \in C[a,b]$ and K is any number between $f(a)$ and $f(b)$, then there exists a number c in (a,b) for which $f(c) = K$.], there is a $\zeta \in (a,b)$ such that

$$
f^{(4)}(\zeta) = \frac{2}{n} \sum_{j=1}^{\frac{n}{2}} f^{(4)}(\zeta_j).
$$

Thus

$$E_{sm} = -\frac{h^5}{90}\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i) = -\frac{h^5 n}{180} f^{(4)}(\zeta),$$

or, since $h = \frac{b-a}{n}$,

$$E_{sm} = -\frac{(b-a)}{180} h^4 f^{(4)}(\zeta).$$

Example 6.14. Use Simpson's 1/3 rule to integrate $f(x) = 0.2 + 25x + 3x^2 + 8x^3$ from $a = 0$ to $b = 2$.

Solution: let $f(0) = 0.2$, $f(1) = 36.2$ and $f(2) = 126.2$, $h = \frac{b-a}{2} = \frac{2-0}{2} = 1$.

$$\begin{aligned} I &= \frac{h}{3}[f(0) + 4f(1) + f(2)] \\ &= \frac{1}{3}[0.2 + 4(36.2) + 126.2] = 90.4 \end{aligned}$$

The exact integral is

$$I = \int_0^2 f(x)\,dx = \left.(0.2\,x + 12.5\,x^2 + x^3 + 2x^4)\right]_0^2 = 90.4.$$

Example 6.15. Use Simpson's 1/3 rule to integrate $f(x) = 0.2 + 25x + 3x^2 + 2x^4$ from $a = 0$ to $b = 2$.

Solution: Let $f(0) = 0.2$, $f(1) = 30.2$ $f(2) = 94.2$ and $h = \frac{b-a}{2} = \frac{2-0}{2} = 1$.

$$\begin{aligned} I &= \frac{h}{3}[f(0) + 4f(1) + f(2)] \\ &= \frac{1}{3}[0.2 + 4(30.2) + 94.2] = 71.73 \end{aligned}$$

The exact integral is:

$$I = \int_0^2 f(x)\,dx = \left.(0.2\,x + 12.5\,x^2 + x^3 + 0.4x^5)\right]_0^2 = 71.2.$$

The relative error is:

$$|\in_t| = \left|\frac{71.2 - 71.73}{71.2}\right| \times 100\,\% = 0.7\,\%.$$

Example 6.16. Evaluate $\int_0^6 \frac{1}{1+x^2}dx$ by using (i) Trapezoid rule, (ii) Simpson 1/3 rule, (iii) Composite trapezoid rule with $n = 6$, (iv) Composite Simpson method with $n = 6$.

Solution: Here $f(x) = \frac{1}{1+x^2}$.
(i) $f(a) = f(0) = 1$, ff$(b) = f(6) = \frac{1}{37}$ and $h = b - a = 6$. Hence

$$\begin{aligned} \int_0^6 \frac{1}{1+x^2}dx &= \frac{h}{2}[f(a) + f(b)] \\ &= \frac{6}{2}[1 + \frac{1}{37}] = \frac{114}{37} = 3.08108. \end{aligned}$$

(ii) Let $h = \frac{b-a}{2} = \frac{6-0}{2} = 3$, hence $x_0 = a = 0$, $x_1 = x_0 + h = 3$ and $x_2 = x_1 + h = 6 = b$. $f(x_0) = f(0) = 1$, $f(x_1) = f(3) = \frac{1}{10}$ and $f(x_2) = f(6) = \frac{1}{37}$. Hence

$$\begin{aligned}\int_0^6 \frac{1}{1+x^2}dx &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \\ &= \frac{3}{3}[1 + 4(\frac{1}{10}) + \frac{1}{37}] = \frac{185+74+5}{185} = \frac{264}{185} = 1.427027.\end{aligned}$$

For (iii) and (iv) $h = \frac{b-a}{n} = \frac{6-0}{6} = 1$. and we form the follwing table:

x	0	1	2	3	4	5	6
$f(x)$	1	0.5	0.2	0.1	0.0588	0.0385	0.0270

(iii)

$$\begin{aligned}\int_0^6 \frac{1}{1+x^2}dx &= \frac{h}{2}[f(x_0) + 2(f(x_1) + f(x_2) + f(x_3) + f(x_4) + f(x_5)) + f(x_6)] \\ &= \frac{1}{2}[1 + 2((0.5 + 0.2 + 0.1 + 0.0588 + 0.0385) + 0.0270] = 1.4108.\end{aligned}$$

(iv)

$$\begin{aligned}\int_0^6 \frac{1}{1+x^2}dx &= \frac{h}{3}[f(x_0) + 2(f(x_1) + f(x_3) + f(x_5)) + 2(f(x_2) + f(x_4)) + f(x_6)] \\ &= \frac{1}{3}[1 + 4(0.5 + 0.1 + 0.0385) + 2(0.2 + 0.0588) + 0.0270] = 1.3662.\end{aligned}$$

Example 6.17. Approximate the integral $\int_0^\pi \sin(x)\,dx$ using composite Simpson rule for $n = 4$ and $n = 8$.

Solution: As $n = 4$, $h = \frac{b-a}{n} = \frac{\pi}{4}$,

$$\begin{aligned}\int_0^\pi \sin(x)\,dx &\approx \tfrac{\pi}{3\cdot 4}\left[\sin(0) + 4\sin\left(\tfrac{\pi}{4}\right) + 2\sin\left(\tfrac{2\pi}{4}\right) + 4\sin\left(\tfrac{3\pi}{4}\right) + \sin(\pi)\right] \\ &= \tfrac{\pi}{12}\left[4\sqrt{2} + 2\right] \\ &\approx 2.005\end{aligned}$$

As $n = 8$, $FH = \frac{\pi}{8}$,

$$\begin{aligned}\int_0^\pi \sin(x)\,dx &\approx \tfrac{\pi}{3\cdot 8}\left[\sin(0) + 4\sin\left(\tfrac{\pi}{8}\right) + 2\sin\left(\tfrac{2\pi}{8}\right) + \cdots + 4\sin\left(\tfrac{7\pi}{8}\right) + \sin(\pi)\right] \\ &= \tfrac{\pi}{24}\left[2 + 2\sqrt{2} + 8\sin\left(\tfrac{\pi}{8}\right) + 8\sin\left(\tfrac{3\pi}{8}\right)\right] \\ &\approx 2.0003\end{aligned}$$

The question to ask: how accurate the above approximations are?
while the error for the Simpson's rule is denoted as

$$\begin{aligned}E_{sm} = \int_a^b f(x)dx - \frac{h}{3}&\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots\right. \\ &\left. + 4f(x_{n-1}) + f(x_n)\right].\end{aligned}$$

The accuracy of the Simpson's rule: $\left|f^{(4)}(x)\right| \leq M$ for $x \in [a,b]$. Then,

$$|E_{sm}| \leq M \cdot \frac{(b-a)^5}{180n^4}.$$

The above results can be used to obtain the required number of partitions, n.

Example 6.18. Compute the composite Simpson approximation for $\int_0^2 \sqrt{x}dx$ using a regular partition with $n = 4$. Compare the estimate with the exact value.

Solution: So with n = 4, each subinterval will have length $h = \frac{b-a}{4} = \frac{1}{2}$.
Then $x_0 = 0 =$; $x_1 = x_0 + h = \frac{1}{2}$; $x_2 = x_1 + h = \frac{1}{2} + \frac{1}{2} = 1$; $x_3 = x_2 + h = 1 + \frac{1}{2} = \frac{3}{2}$ and $x_4 = x_3 + h = \frac{3}{2} + \frac{1}{2} = \frac{4}{2} = 2$.

$$\begin{aligned}
I &= \int_0^2 \sqrt{x}dx \\
&= \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)] \\
&= \frac{1}{6}[\sqrt{0} + 4\sqrt{\frac{1}{2}} + 2\sqrt{1} + 4\sqrt{\frac{3}{2}} + \sqrt{2}] \\
&= \frac{1}{6}[0 + 2\sqrt{2} + 4 + 2\sqrt{6} + \sqrt{2}] \approx 1.856936.
\end{aligned}$$

The exact value of the integral is

$$\int_0^2 \sqrt{x}dx = \frac{2}{3}x^{\frac{3}{2}}\Big|_0^2 == 1.88562.$$

The approximation underestimates the actual area, the error is is

$$\frac{1.88562}{1.8569367} \approx 0.0286833$$

and that is

$$0.0286833 - 1.88562 = 0.01521$$

or 1.52% of the exact value.

Example 6.19. Determine a value of n so that the composite Simpson's rule will approximate the value of $\int_0^1 \cos\left(x^2\right) dx$ with an error that is less than 0.001.

Solutions:

$$f(x) = \cos\left(x^2\right) \;\Leftrightarrow\; f^{(4)}(x) = 4\left[\left(4x^3 - 3\right)\cos\left(x^2\right) + 12x^2 \sin\left(x^2\right)\right].$$

As $x = 1$, $f^{(4)}(x)$ attains its maximum over $[0,1]$, i.e.,

$$\left|f^{(4)}(x)\right| \leq 4\left[\cos(1) + 12\sin(1)\right] \approx 42.6 \leq 43,\; x \in [0,1].$$

Let $M = 43$.

$$|E_{sm}| \leq M \cdot \frac{(b-a)^5}{180n^4} = 43 \cdot \frac{(1-0)^5}{180n^4} = \frac{43}{180n^4}.$$

As

$$\frac{43}{180n^4} \leq 0.01 \;\Leftrightarrow\; n^4 \geq \frac{4300}{180} = 23.88 \Leftrightarrow\; n \geq 2.2 \;\Rightarrow\; n = 4.$$

Example 6.20. Use composite trapezoid rule and composite Simpson method, estimate the integral $\int_0^2 (x^3 + x)dx$ with $n = 4$ steps.

Solution: Let $f(x) = x^3 + x$. For $a = 0$, $b = 2$ and $n = 4$, we have $h = \frac{b-a}{n} = \frac{2-0}{4} = 0.5$.

$$x_0 = 0,\; x_1 = 0.5,\; x_2 = 1,\; x_3 = 1.5,\; x_4 = 2.$$

Computing the values for $y_i = f(x_i)$; i =0, 1, 2, 3, 4, we have:

$$y_0 = 0,\; y_1 = 0.625,\; y_2 = 2,\; y_3 = 4.875,\; y_4 = 10.$$

Now plug the values into the rule, we get
By Composite trapezoid Rule:

$$\begin{aligned} I = \int_0^2 (x^3 + x)dx &= \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + y_4] \\ &= \frac{0.5}{2}[0 + 2(0.625 + 2 + 4.875) + 10] = 6.26. \end{aligned}$$

The exact value is

$$\int_0^2 (x^3 + x)dx = (\frac{x^4}{4} + \frac{x^2}{2})\Big|_0^2 = \frac{16}{4}\frac{4}{2} = 6.$$

By composite Simpson Rule:

$$\begin{aligned} I = \int_0^2 (x^3 + x)dx &= \frac{h}{3}[y_0 + 4y_1 + 2y_2 + 4y_3 + y_4] \\ &= \frac{0.5}{3}[0 + 4(0.625) + 2(2) + 4(4.875) + 10] = \frac{1}{6}[0 + 2.5 + 4 + 19.5 + 10] = 6. \end{aligned}$$

Example 6.21. Use composite trapezoid rule and composite Simpson method with $n = 4$ estimate $\int_1^3 (2x - 1)dx$.

Solution: Let $f(x) = 2x - 1$. For $a = 1$, $b = 3$ and $n = 4$, we have $h = \frac{b-a}{n} = \frac{3-1}{4} = 0.5$.

$$x_0 = 1,\; x_1 = 1.5,\; x_2 = 2,\; x_3 = 2.5,\; x_4 = 3.$$

Computing the values for $y_i = f(x_i)$; i =0, 1, 2, 3, 4, we have:

$$y_0 = 1,\; y_1 = 2,\; y_2 = 3,\; y_3 = 4,\; y_4 = 5.$$

Now plug the values into the rule, we get
By Composite trapezoid Rule:

$$I = \int_1^3 (2x-1)dx = \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + y_4]$$
$$= \frac{0.5}{2}[1 + 2(2+3+4) + 5] = 6.$$

The exact value is

$$\int_1^3 (2x-1)dx = \left.(x^2 - x)\right|_1^3 = (9-3) - (1-1) = 6.$$

By composite Simpson Rule:

$$I = \int_1^3 (2x-1)dx = \frac{h}{3}[y_0 + 4y_1 + 2y_2 + 4y_3 + y_4]$$
$$= \frac{0.5}{3}[1 + 4(2) + 2(3) + 4(4) + 5] = \frac{1}{6}[1 + 8 + 6 + 16 + 5] = 6.$$

Example 6.22. Use composite trapezoid rule and composite Simpson method, estimate the integral $\int_0^\pi \sin(x)dx$ with $n = 4$ steps.

Solution: Let $f(x) = \sin(x)$. For $a = 0$, $b = \pi$ and $n = 4$, we have $h = \frac{b-a}{n} = \frac{\pi - 0}{4} = \frac{\pi}{4}$.

$$x_0 = 0,\ x_1 = \frac{\pi}{4},\ x_2 = \frac{\pi}{2},\ x_3 = \frac{3\pi}{4},\ x_4 = \pi.$$

Computing the values for $y_i = f(x_i)$; i =0, 1, 2, 3, 4, we have:

$$y_0 = 0,\ y_1 = \frac{1}{\sqrt{2}},\ y_2 = 1,\ y_3 = \frac{1}{\sqrt{2}},\ y_4 = 0.$$

Now plug the values into the rule, we get
By Composite trapezoid Rule:

$$I = \int_0^\pi \sin(x)dx = \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + y_4]$$
$$= \frac{\frac{\pi}{4}}{2}\left[0 + 2\left(\frac{1}{\sqrt{2}} + 1 + \frac{1}{\sqrt{2}}\right) + 0\right]$$
$$= \frac{\pi}{8}\left[\frac{1}{\sqrt{2}} + 2 + \frac{2}{\sqrt{2}}\right] \approx 1.896118898.$$

The exact value is

$$\int_0^{pi} \sin(x) = -\cos(x)|_0^\pi = 2.$$

By composite Simpson Rule:

$$I = \int_0^\pi \sin(x)dx = \frac{h}{3}[y_0 + 4y_1 + 2y_2 + 4y_3 + y_4]$$
$$= \frac{\frac{\pi}{4}}{3}\left[0 + 4\left(\frac{1}{\sqrt{2}}\right) + 2(1) + 4\left(\frac{1}{\sqrt{2}}\right) + 0\right] = \frac{\pi}{12}\left[\frac{4}{\sqrt{2}} + 2 + \frac{4}{\sqrt{2}}\right] = 2.004559755.$$

Example 6.23. Consider evaluating $\int_0^2 \frac{1}{1+x^2}dx$ using composite Simpson method. How large should n be chosen in order to ensure that

$$|E_{csm}| \leq 5 \times 10^{-6}. \tag{6.11}$$

Solution: We begin by calculating the derivatives:

$f'(x) = \frac{-2x}{(1+x^2)^2}$, $f''(x) = \frac{-2+6x^2}{(1+x^2)^3}$, $f'''(x) = \frac{-24x^3+24x}{(1+x^2)^4}$,

and $f^{(iv)} = \frac{120x^4-240x^2+24}{(1+x^2)^5}$.

From a graph of $f^{(iv)}(x)$,

$$\max_{0\leq x\leq 2}\left|f^{(iv)}(x)\right| = 24.$$

Therefore

$E_{tr} = -\frac{(b-a)h^4}{180}f^{(iv)}(c)$, hence $|E_{csm}| \leq \frac{2h^4}{180} \times (24) = \frac{4h^4}{15}$.

To ensure this, we choose h so small that

$$\frac{4h^4}{15} \leq 5 \times 10^{-6}.$$

This is equivalent to choosing h and n to satisfy

$$h \leq 0.0658 \implies n = \frac{3}{h} \geq 45.59.$$

Thus $n \geq 48$ will imply (6.11)

Example 6.24. Determine the values of n and h required to approximate $\int_0^2 e^{2x}dx$ within (error$\leq 5 \times 10^{-4}$) using composite Simpson method.

Solution: We begin by calculating the derivatives:

$f'(x) = 2e^{2x}$, $f''(x) = 4e^{2x}$, $f'''(x) = 8e^{2x}$.

and $f^{(iv)}(x) = 16e^{2x}$.

From a graph of $f^{(iv)}(x)$,

$$\max_{0\leq x\leq 2}\left|f^{(iv)}(x)\right| = 873.5704.$$

Therefore

$E_{csm} = -\frac{(b-a)h^4}{180}f^{(iv)}(c))$, hence $|E_{csm}| \leq \frac{2h^4}{180} \times (873.5704) = \frac{873.5704h^4}{90}$.

To ensure this, we choose h so small that

$$\frac{873.5704h^4}{90} \leq 5 \times 10^{-4}.$$

This is equivalent to choosing h and n to satisfy

$$h \leq 0.084718576714079 \implies n = \frac{3}{h} \geq 35.4.$$

Thus $n \geq 36$ will imply the result.

6.6 EXERCISE

1. Evaluate $\int_0^1 e^{-x^2} dx$, dividing the range into 4 equal part, Using:
   i. Trapezoidal Rule, ii. Simpson's Rule 1/3.

2. Use the Simpson's rule 1/3 to approximate $\int_1^5 \frac{x}{\sqrt{x+1}} dx$ with $n = 8$.

3. Determine the step size h required in order for the Simpson's Rule 1/3 to approximate the integral $\int_0^8 x \, \sin(x) \, dx$, with an error of at most 10^{-4}.

4. Find the error bound for $\int_{-0.5}^{0.5} x \; \ln(x+2) dx$, approximate by the Simpson's rule 1/3.

5. Evaluate $\int_0^{0.5} \frac{x}{\cos(x)} dx$ with $n = 4$, use Simpson's rule 1/3.

6. Evaluate the integral $\int_0^2 x^2 \, e^{-x^2} dx$, and $h = 0.25$ by using
   i. Trapezoidal rule, ii. Simpson's (1/3) Rule.