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Numerical Analysis I

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March 8, 2021

Chapter 6

Numerical Differentiation and Integration

6.1 INTRODUCTION

The differentiation and integration are losely linked processes which are actually inversely related. For example, if the given function $y(t)$ represents an objects position as a function of time, its differentiation provides its velocity,

$$v(t) = \frac{d}{dt}y(t)$$

On the other hand, if we are provided with velocity $v(t)$ as a function of time, its integration denotes its position.

$$y(t) = \int_0^t v(t)\,dt$$

There are so many methods available to find the derivative and definite integration of a function. But when we have a complicated function or a function given in tabular form, they we use numerical methods. In the present chapter, we shall be concerned with the problem of numerical differentiation and integration.

6.2 NUMERICAL DIFFERENTIATION

The method of obtaining the derivatives of a function using a numerical technique is known as numerical differentiation. There are essentially two situations where numerical differentiation is required.
They are:

1. The function values are known but the function is unknown, such functions are called tabulated function.

2. The function to be differentiated is complicated and, therefore, it is difficult to differentiate.

The choice of the formula is the same as discussed for interpolation if the derivative at a point near the beginning of a set of values given by a table is required then we use Newton's forward interpolation formula, and if the same is required at a point near the end of the set of given tabular values, then we use Newton's backward interpolation formula. The central difference formula (Bessel's and Stirling's) used to calculate value for points near the middle of the set of given tabular values. If the values of x are not equally spaced, we use Newton's divided difference interpolation formula or Lagrange's interpolation formula to get the required value of the derivative.

6.2.1 Derivatives Using Newton's Forward Interpolation Formula

Consider the data $(x_i, f(x_i))$ given at equispaced points $x_i = x_0 + ih, i = 0, 1, 2, \ldots, n$ where h is the step length. The Newton's forward Interpolation formula is given by

$$\begin{aligned} y &= y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots + \frac{u(u-1)\cdots(u-(n-1))}{n!}\Delta^n y_0 \\ &= y_0 + u\Delta y_0 + \frac{u^2-u}{2!}\Delta^2 y_0 + \frac{u^3-3u^2+2u}{3!}\Delta^3 y_0 + \frac{u^4-6u^3+11u^2-6u}{4!}\Delta^4 y_0 \\ &\quad + \frac{u^5-10u^4+35u^3-50u^2+24u}{5!}\Delta^5 y_0 + \cdots \end{aligned} \tag{6.1}$$

where $u = \frac{x-x_0}{h}$
Differentiating equation (6.1) with respect to x, we get

$$\begin{aligned} \frac{dy}{dx} &= \frac{dy}{du}\frac{du}{dx} = \frac{1}{h}\frac{dy}{du} \\ \frac{dy}{dx} &= \frac{1}{h}\Bigg[\Delta y_0 + \frac{2u-1}{2!}\Delta^2 y_0 + \frac{3u^2-6u+2}{3!}\Delta^3 y_0 + \frac{4u^3-18u^2+22u-6}{4!}\Delta^4 y_0 \\ &\quad + \frac{5u^4-40u^3+105u^2-100u+24}{5!}\Delta^5 y_0 + \cdots\Bigg] \end{aligned} \tag{6.2}$$

Again differentiating equation (6.2) with respect to x, we get

$$\begin{aligned} \frac{d^2y}{dx^2} &= \frac{d}{du}\left(\frac{dy}{dx}\right)\frac{du}{dx} = \frac{1}{h} \times \frac{d}{du}\left(\frac{dy}{dx}\right) \\ &= \frac{1}{h^2}\Bigg[\Delta^2 y_0 + \frac{6u-6}{3!}\Delta^3 y_0 + \frac{12u^2-36u+22}{4!}\Delta^4 y_0 \\ &\quad + \frac{20u^3-120u^2+210u-100}{5!}\Delta^5 y_0 + \cdots\Bigg] \end{aligned} \tag{6.3}$$

and so on.
Equations (6.2) & (6.3) give the approximate derivatives of $f(x)$ at arbitrary point $x = x_0 + uh$.
When $x = x_0, u = 0$, Eqs.(6.2) and (6.3) becomes

$$\left[\frac{dy}{dx}\right]_{x=x_0} = f'(x_0) = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right] \tag{6.4}$$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = f''(x_0) = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \cdots\right] \tag{6.5}$$

and so on.

Example 6.1. *Find the value of* $\frac{dy}{dx}$ *and* $\frac{d^2y}{dx^2}$ *at* $x = 0.1$ *from the following table:*

x	0.1	0.2	0.3	0.4
y	0.9975	0.9900	0.9776	0.9604

Solution: The forward difference table is

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
0.1	0.9975			
		$\boxed{-0.0075}$		
0.2	0.9900		$\boxed{-0.0049}$	
		-0.0124		$\boxed{0.0001}$
0.3	0.9776		-0.0048	
		-0.0172		
0.4	0.9604			

We have $h = 0.1, x_0 = 0.1,$ and $u = \frac{x-x_0}{h}$. For $x = 0.1$, we get $u = 0$.
Therefore,

$$\begin{aligned}\left[\frac{dy}{dx}\right]_{x=x_0} &= \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0\right] \\ &= \frac{1}{0.1}\left[-0.0075 - \frac{1}{2}(-0.0049) + \frac{1}{3}(0.0001)\right] = -0.050167.\end{aligned}$$

Example 6.2. *The table given below reveals the velocity 'v'of a body during the time 't 'specified. Find its acceleration at* $t = 1.1$.

t :	*1.0*	*1.1*	*1.2*	*1.3*	*1.4*
v :	*43.1*	*47.7*	*52.1*	*56.4*	*60.8*

Solution: The difference table is:

t	v	Δv	$\Delta^2 v$	$\Delta^3 v$	$\Delta^4 v$
1.0	43.1				
		4.6			
1.1	47.7		-0.2		
		$\boxed{4.4}$		0.1	
1.2	52.1		$\boxed{-0.1}$		0.1
		4.3		$\boxed{0.2}$	
1.3	56.4		0.1		
		4.4			
1.4	60.8				

Let $t_0 = 1.1,\ y_0 = 47.7$ and $h = 0.1$
Acceleration at $t = 1.1$ is given by

$$\begin{aligned}\left[\frac{dv}{dt}\right]_{t=t_0} &= \frac{1}{h}\left[\Delta v_0 - \frac{1}{2}\Delta^2 v_0 + \frac{1}{3}\Delta^3 v_0\right] \\ &= \frac{1}{0.1}\left[4.4 - \frac{1}{2}(-0.1) + \frac{1}{3}(0.2)\right] \\ &= 45.1667.\end{aligned}$$

Hence the required acceleration is 45.1667.

Example 6.3. *Find $f'(1.1)$ and $f''(1.1)$ from the following table:*

x	*1.0*	*1.2*	*1.4*	*1.6*	*1.8*	*2.0*
$f(x)$	*0*	*0.1*	*0.5*	*1.25*	*2.4*	*3.9*

Solution: We first construct the forward difference table as shown below

x	y	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$	$\Delta^5 f(x)$
1.0	1					
		0.1				
1.2	0.1		0.3			
		0.4		0.05		
1.4	0.5		0.35		0	
		0.75		0.05		0
1.6	1.25		0.40		0	
		1.15		0.05		
1.8	2.40		0.45			
		1.5				
2.0	3.9					

Since $x = 1.1$ is a non-tabulated point near the beginning of the table, we take $x_0 = 1.0$ and compute $u = \frac{x-x_0}{h} = \frac{1.1-1.0}{0.2} = 0.5$.

Hence,
$$\begin{aligned}
f'(x) &= \frac{1}{h}\left[\Delta f(x_0) + \frac{2u-1}{2!}\Delta^2 f(x_0) + \frac{3u^2-6u+2}{3!}\Delta^3 f(x_0)\right]\\
f'(1.1) &= \frac{1}{0.2}\left[0.1 + 0 + \frac{3(0.5)^2 - 6(0.5) + 2}{6}(0.05)\right]\\
&= 0.4895\\
f''(x) &= \frac{1}{h^2}\left[\Delta^2 f(x_0) + \frac{6u-6}{3!}\Delta^3 f(x_0)\right]\\
f''(1.1) &= \frac{1}{(0.2)^2}\left[0.3 + \frac{6(0.5)-6}{6}(0.05)\right]\\
&= 6.875.
\end{aligned}$$

6.2.2 Derivatives Using Newton's Backward Interpolation Formula

Consider the data $(x_i, f(x_i))$ given at equispaced points $x_i = x_0 + ih$, where h is the step length. The Newton's backward interpolation formula is given by

$$\begin{aligned}
y &= y_n + u\nabla y_n + \frac{u(u+1)}{2!}\nabla^2 y_n + \frac{u(u+1)(u+2)}{3!}\nabla^3 y_n + \cdots + \frac{u(u+1)\cdots(u+(n-1))}{n!}\nabla^n y_0\\
&= y_n + u\nabla y_n + \frac{u^2+u}{2!}\nabla^2 y_n + \frac{u^3+3u^2+2u}{3!}\nabla^3 y_n + \frac{u^4+6u^3+11u^2+6u}{4!}\nabla^4 y_n\\
&\quad + \frac{u^5-10u^4+35u^3-50u^2+24u}{5!}\nabla^5 y_n + \cdots \qquad (6.6)
\end{aligned}$$

where $u = \frac{x-x_n}{h}$
Differentiating equation (6.6) with respect to x, we get

$$\frac{dy}{dx} = \frac{1}{h}\Big[\nabla y_n + \frac{2u+1}{2!}\nabla^2 y_n + \frac{3u^2+6u+2}{3!}\nabla^3 y_n + \frac{4u^3+18u^2+22u+6}{4!}\nabla^4 y_n + \frac{5u^4+40u^3+105u^2+100u+24}{5!}\nabla^5 y_0 + \cdots\Big] \quad (6.7)$$

Again differentiating equation (6.7) with respect to x, we get

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\Big[\nabla^2 y_n + \frac{6u+6}{3!}\nabla^3 y_n + \frac{12u^2+36u+22}{4!}\nabla^4 y_n + \frac{20u^3+120u^2+210u+100}{5!}\nabla^5 y_0 + \cdots\Big] \quad (6.8)$$

and so on.
Equations (6.7) and (6.8) can be used to determine the approximate differentiation of first, second, etc. order at any point x, where $x = x_n + uh$.

If $x = x_n$, then $u = 0$.

Equations (6.7) and (6.8) become

$$f'(x_n) = \frac{1}{h}\Big[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \cdots\Big] \quad (6.9)$$

$$f''(x_n) = \frac{1}{h^2}\Big[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{4}\nabla^5 y_n + \cdots\Big] \quad (6.10)$$

Example 6.4. *Find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ of $y = e^x + 1$ at $x = 2.5$ from the following table:*

x	*1.0*	*1.5*	*2.0*	*2.5*
y	*3.7183*	*5.4817*	*8.3891*	*13.1825*

Solution: The backward difference table is given below.

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$
1.0	3.7183			
		1.7634		
1.5	5.4817		1.1440	
		2.9074		0.7420
2.0	8.3891		1.8860	
		4.7934		
2.5	13.1825			

We have $h = 0.5, x_n = 2.5$, and $u = \frac{x-x_n}{h}$. For $x = 2.5$, we get $u = 0$.

From the formula

$$\begin{aligned}
\left[\frac{dy}{dx}\right]_{x=x_n} &= \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n\right] \\
&= \frac{1}{0.5}\left[4.7934 + \frac{1}{2}(1.8860) + \frac{1}{3}(0.7420)\right] \\
&= 11.9675. \\
\left[\frac{d^2y}{dx^2}\right]_{x=x_n} &= \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n\right] \\
&= \frac{1}{(0.25)^2}\left[1.8660 + 0.7420\right] \\
&= 10.5120.
\end{aligned}$$

Example 6.5. *From the following table, find the values of* $\frac{dy}{dx}$ *and* $\frac{d^2y}{dx^2}$ *at* $x = 2.03$.

x	1.96	1.98	2.00	2.02	2.04
y	0.7825	0.7739	0.7651	0.7563	0.7473

Solution: The backward difference table is

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
1.96	0.7825				
		-0.0086			
1.98	0.7739		-0.0002		
		-0.0088		0.0002	
2.00	0.7651		0		-0.0004
		-0.0088		-0.0002	
2.02	0.7563		-0.0002		
		-0.0090			
2.04	0.7473				

Here, $x_n = 2.04, h = 0.02$ and $u = \frac{x-x_n}{h}$. For $x = 2.03$, we get $u = -0.5$
Therefore,

$$\begin{aligned}
y'(x) &= \frac{1}{h}\left[\nabla y_n + \frac{2u+1}{2!}\nabla^2 y_n + \frac{3u^2+6u+2}{3!}\nabla^3 y_n + \frac{4u^3+18u^2+22u+6}{4!}\nabla^4 y_n\right] \\
y'(2.03) &= \frac{1}{0.02}\Bigg[-0.0090 + 0 + \frac{3(-0.5)^2+6(-0.5)+2}{6}(-0.0002) \\
&\qquad + \frac{4(-0.5)^3+18(-0.5)^2+22(-0.5)+6}{24}(-0.0004)\Bigg] \\
&= -0.44875 \\
y''(x) &= \frac{1}{h^2}\left[\nabla^2 y_n + \frac{6u+6}{3!}\nabla^3 y_n + \frac{12u^2+36u+22}{4!}\nabla^4 y_n\right] \\
y''(2.03) &= \frac{1}{(0.02)^2}\left[-0.0002 + (-0.5+1)(-0.0002) + \frac{12(-0.5)^2+36(-0.5)+22}{24}(-0.0004)\right] \\
&= -1.05
\end{aligned}$$

Example 6.6. *The distance covered by an athlete for the 50 meter race is given in the following table:*

$Time(sec)$	0	1	2	3	4	5	6
$Distance(meter)$	0	2.5	8.5	15.5	24.5	36.5	50

Determine the speed of the athlete at $t = 5$ $sec.$, *correct to two decimals.*

Solution: Here we are to find derivative at $t = 5$ which is near the end of the table, hence we shall use the formula obtained from Newton's backward difference formula. The backward difference table is as follows:

t	s	∇s	$\nabla^2 s$	$\nabla^3 s$	$\nabla^4 s$	$\nabla^5 s$	$\nabla^6 s$
0	0						
		2.5					
1	2.5		3.5				
		6		-2.5			
2	8.5		1		3.5		
		7		1		$\boxed{-3.5}$	
3	15.5		2		$\boxed{0}$		1
		9		$\boxed{1}$		-2.5	
4	24.5		$\boxed{3}$		-2.5		
		$\boxed{12}$		-1.5			
5	36.5		1.5				
		13.5					
6	50						

The speed of the athlete at $t = 5$ sec is given by

$$\begin{aligned}
\left(\frac{ds}{dt}\right)_{t=5} &= \frac{1}{h}\left[\nabla s_5 + \frac{1}{2}\nabla^2 s_5 + \frac{1}{3}\nabla^3 s_5 + \frac{1}{4}\nabla^4 s_5 + \frac{1}{5}\nabla^5 s_5\right] \\
&= \frac{1}{1}\left[12 + \frac{1}{2}(3) + \frac{1}{3}(1) + \frac{1}{4}(0) + \frac{1}{5}(-3.5)\right] \\
&= 13.1333 \text{ meter/sec.}
\end{aligned}$$

6.2.3 Derivatives Using Stirling's Interpolation Formula

If we want to determine the values of the derivatives of the function near the middle of the given set of arguments. We may apply any central difference formula. Therefore using Stirling's formula, we get

$$\begin{aligned}
f(x) = y_0 + \frac{u}{1!}\left[\frac{\Delta y_0 + \Delta y_{-1}}{2}\right] + \frac{u^2}{2!}\Delta^2 y_{-1} + \frac{u^3-u}{3!}\left[\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right] \\
+ \frac{u^4-u^2}{4!}\Delta^4 y_{-2} + \frac{u^5-5u^3+4u}{5!}\left[\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2}\right] + \cdots \qquad (6.11)
\end{aligned}$$

Where $u = \frac{x-x_0}{h}$
When Equation (6.11) is differentiated with respect to x successively, we obtain

$$\begin{aligned} f'(x) &= \frac{1}{h}\left[\frac{\Delta y_0 + \Delta y_{-1}}{2} + u\Delta^2 y_{-1} + \frac{3u^2-1}{6}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right)\right. \\ &\quad \left. + \frac{2u^3-u}{12}\Delta^4 y_{-2} + \frac{5u^4-15u^2+4}{120}\left(\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2}\right) + \cdots\right] \end{aligned} \tag{6.12}$$

and

$$\begin{aligned} f''(x) &= \frac{1}{h^2}\left[\Delta^2 y_{-1} + u\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{6u^2-1}{12}\Delta^4 y_{-2}\right. \\ &\quad \left. + \frac{2u^3-3u}{12}\left(\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2}\right) + \cdots\right] \end{aligned} \tag{6.13}$$

At $x = x_0, u = 0$ and Equation (6.12) and (6.13) become

$$\begin{aligned} f'(x_0) &= \frac{1}{h}\left[\frac{\Delta y_0 + \Delta y_{-1}}{2} - \frac{1}{6}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{1}{30}\left(\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2}\right) + \cdots\right] \\ f''(x_0) &= \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \frac{1}{90}\Delta^6 y_{-3} + \cdots\right] \end{aligned}$$

Example 6.7. *Find $f'(0.6)$ and $f''(0.6)$ from the following table:*

x	0.4	0.5	0.6	0.7	0.8
$f(x)$	1.5836	1.7974	2.0442	2.3275	2.6510

Solution: Here, the derivatives are required at the central point $x = 0.6$, so we use Stirling's formula. The difference table is:

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$
$x_{-2} = 0.4$	1.5836				
		0.2138			
$x_{-1} = 0.5$	1.7974		0.0330		
		0.2468		0.0035	
$x_0 = 0.6$	2.0442		0.0365		0.0002
		0.2833		0.0037	
$x_1 = 0.7$	2.3275		0.0402		
		0.3235			
$x_2 = 0.8$	2.6510				

Her we have $x_0 = 0.6, x = 0.6, h = 0.1, u = \frac{x-x_0}{h} = \frac{0.6-0.6}{0.1} = 0$
By using Stirling's formula for derivatives, we get

$$\begin{aligned} \left[\frac{dy}{dx}\right]_{x=x_0} &= \frac{1}{h}\left[\frac{\Delta y_0 + \Delta y_{-1}}{2} - \frac{1}{6}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right)\right] \\ \left[\frac{dy}{dx}\right]_{x=0.6} &= \frac{1}{0.1}\left[\frac{0.2468 + 0.2833}{2} + 0 - \frac{1}{6}\left(\frac{0.0035 + 0.0037}{2}\right) + 0\right] \\ &= 10(0.26505 - 0.0006) \end{aligned}$$

$$\begin{aligned} f'(0.6) &= 2.6445. \\ \left[\frac{d^2y}{dx^2}\right]_{x=x_0} &= \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2}\right] \\ &= \frac{1}{(0.1)^2}\left[0.0365 + 0 - \frac{1}{12}(0.0002)\right] \\ &= 100(0.0365 - 0.000016) \\ f''(0.6) &= 3.6484. \end{aligned}$$

Example 6.8. *Compute the values of $f'(3.1)$ and $f''(3.1)$ using the following table.*

x	1	2	3	4	5
$f(x)$	0	1.4	3.3	5.6	8.1

Solution: The central difference table is

x	$y=f(x)$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
$x_{-2}=1$	0				
		1.4			
$x_{-1}=2$	1.4		0.5		
		1.9		-0.1	
$x_0=3$	3.3		0.4		-0.1
		2.3		-0.2	
$x_1=4$	5.6		0.2		
		2.5			
$x_2=5$	8.1				

Let $x_0 = 3, h = 1, u = \frac{3.1-3}{1} = 0.1$

$$\begin{aligned} f'(x) &= \frac{1}{h}\left[\frac{\Delta y_0 + \Delta y_{-1}}{2} + u\Delta^2 y_{-1} + \frac{3u^2-1}{6}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{2u^3-u}{12}\Delta^4 y_{-2}\right] \\ f'(1.6) &= \frac{1}{1}\left[\frac{1.9+2.3}{2} + (0.1)(0.4) + \frac{3(0.1)^2-1}{6}\left(\frac{-0.1-.2}{2}\right) + \frac{2(0.1)^3-0.1}{12}(-0.1)\right] \\ &= 2.1 + 0.04 + 0.02425 + 0.00082 \\ &= 2.16507 \\ f''(x) &= \frac{1}{h^2}\left[\Delta^2 y_{-1} + u\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{6u^2-1}{12}\Delta^4 y_{-2}\right] \\ &= \frac{1}{1^2}\left[0.4 + 0.1\left(\frac{-0.1-0.2}{2}\right) + \frac{6(0.1)^2-1}{12}(-0.1)\right] \\ &= 0.4 - 0.015 + 0.00783 \\ &= 0.39283. \end{aligned}$$

6.2.4 Derivatives Using Newton's Divided Difference Formula

The divided difference interpolation polynomial fitting the data $(x_i, f(x_i)), i = 0, 1, 2, \ldots, n$ is given by

$$\begin{aligned} y = f(x) = y_0 + (x - x_0)f[x_0, x_1] + (x - x_0)(x - x_1)f[x_0, x_1, x_2] + \\ \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})f[x_0, x_1, x_2, \ldots, x_n] \end{aligned} \tag{6.14}$$

Differentiating Equation (6.14) with respect to x, we get

$$\begin{aligned} f'(x) = f[x_0, x_1] + [(x - x_0) + (x - x_1)]f[x_0, x_1, x_2] + [(x - x_1)(x - x_2) + (x - x_0)(x - x_2) \\ + (x - x_0)(x - x_1)]f[x_0, x_1, x_2, x_3] + [(x - x_1)(x - x_2)(x - x_3) + (x - x_0)(x - x_2)(x - x_3) \\ + (x - x_0)(x - x_1)(x - x_3) + (x - x_0)(x - x_1)(x - x_2)]f[x_0, x_1, x_2, x_3, x_4] + \cdots \end{aligned} \tag{6.15}$$

If the derivative $f'(x)$ is required at any particular point $x = x^*$, then we substitute $x = x^*$ in (6.15). If the data is equispaced, then the formula is simplified.
Differentiating Equation (6.15) again, we obtain

$$\begin{aligned} f''(x) = 2f[x_0, x_1, x_2] + 2[(x - x_0) + (x - x_1) + (x - x_2)]f[x_0, x_1, x_2, x_3] \\ + 2[(x - x_0)(x - x_1) + (x - x_0)(x - x_2) + (x - x_0)(x - x_3) + (x - x_1)(x - x_2) \\ + (x - x_1)(x - x_3) + (x - x_2)(x - x_3)]f[x_0, x_1, x_2, x_3, x_4] + \cdots \end{aligned} \tag{6.16}$$

If the second derivative $f''(x)$ is required at any point $x = x^\star$, then we substitute $x = x^\star$ in (6.16). Again, if the data is equispaced, then the formula is simplified.

However, we can also determine the Newton's divided differences interpolation polynomial and differentiate it to obtain $f'(x)$ and $f''(x)$.
Example 6.9. Find the first and second derivatives at $x = 1.6$, for the function represented by the following tabular data:

x	*1.0*	*1.5*	*2.0*	*3.0*
$f(x)$	*0.0*	*0.40547*	*0.69315*	*1.09861*

Solution: The data is not equispaced. We use the divided difference formulas to find the derivatives. We have the following difference table:

x	$f(x)$	First d.d	Second d.d	Third d.d
1.0	0.0000			
		0.81094		
1.5	0.40547		- 0.235580	
		0.57536		0.061157
2.0	0.69315		- 0.113267	
		0.40546		
3.0	1.09861			

Substituting $x = 1.6$ in the formula

$$\begin{aligned} f'(x) &= f[x_0, x_1] + [(x - x_0) + (x - x_1)]f[x_0, x_1, x_2] + [(x - x_1)(x - x_2) \\ &\quad + (x - x_0)(x - x_2) + (x - x_0)(x - x_1)]f[x_0, x_1, x_2, x_3] \\ \text{we obtain } f'(1.6) &= 0.81094 + [(1.6 - 1.0) + (1.6 - 1.5)](-0.23558) + [(1.6 - 1.5)(1.6 - 2.0) \\ &\quad + (1.6 - 1.0)(1.6 - 2.0) + (1.6 - 1.0)(1.6 - 1.5)](0.061157) \\ &= 0.81094 + 0.7(-0.23558) - 0.22(0.061157) = 0.63258. \end{aligned}$$

Substituting $x = 1.6$ in the formula

$$\begin{aligned} f''(x) &= 2f[x_0, x_1, x_2] + 2[(x - x_0) + (x - x_1) + (x - x_2)]f[x_0, x_1, x_2, x_3] \\ \text{we obtain } f''(1.6) &= 2(-0.23558) + 2[(1.6 - 1.0) + (1.6 - 1.5) + (1.6 - 2.0)](0.061157) \\ &= -0.47116 + 0.03669 = -0.43447. \end{aligned}$$

Remark 6.1. *Often, in applications, we require the maximum and/ or minimum of a function given as a tabulated data. We may obtain the interpolation polynomial, differentiate it and set it equal to zero to find the stationary points. Alternatively, we can use the numerical differentiation formula for finding the first derivative, set it equal to zero to find the stationary points. The numerical values obtained for the second derivatives at these stationary points decides whether there is a maximum or a minimum at these points.*

Example 6.10. *Find x for which y is maximum and find this value of y*

x	*1.2*	*1.3*	*1.4*	*1.5*	*1.6*
y	*0.9320*	*0.9636*	*0.9855*	*0.9975*	*0.9996*

Solution: The Difference table is as follows:

x	y	Δ	Δ^2	Δ^3	Δ^4
1.2	0.9320				
		0.0316			
1.3	0.9636		-0.0097		
		0.0219		-0.0002	
1.4	0.9855		-0.0099		0.0002
		0.120		0	
1.5	0.9975		-0.0099		
		0.0021			
1.6	0.9996				

Let $y_0 = 0.9320$ and $x_0 = 1.2$

By Newton's forward difference formula

$$
\begin{aligned}
y &= y_0 + u\Delta y_0 + \frac{u(u-1)}{2}\Delta^2 y_0 + \ldots \\
&= 0.9320 + 0.031u + \frac{u(u-1)}{2}(-0.0097) \qquad \text{(Neglecting higher differences)} \\
\frac{dy}{du} &= 0.0316 + \left(\frac{2u-1}{2}\right)(-0.0097)
\end{aligned}
$$

At a maximum,

$$
\begin{aligned}
& \frac{dy}{du} = 0 \\
\Rightarrow \quad & 0.0316 = \left(u - \frac{1}{2}\right)(0.0097) \quad \Rightarrow u = 3.76 \\
\therefore \quad & x = x_0 + uh = 1.2 + (0.1)(3.76) = 1.576
\end{aligned}
$$

To find y_{max}, we use backward difference formula,

$$
\begin{aligned}
& x = x_n + uh \\
\Rightarrow \quad & 1.576 = 1.6 + (0.1)u \Rightarrow u = -0.24 \\
& y(1.576) = y_n + u\nabla y_n + \frac{u(u+1)}{2!}\nabla^2 y_n + \frac{u(u+1)(u+2)}{3!}\nabla^3 y_n \\
& = 0.9996 - (0.24 \times 00021) + \frac{(-0.24)(1-0.24)}{2}(-0.0099) \\
& \frac{dy}{du} = 0.9999988 = 0.9999\text{nearly}
\end{aligned}
$$

$\therefore$ Maximum $y = 0.9999$. (Approximately)

PROBLEM SET 6.1

1. From the following table find the value of $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at the point $x = 1.0$.

x	1	1.1	1.2	1.3	1.4	1.5
y	5.4680	5.6665	5.9264	6.2551	6.6601	7.1488

[**Ans.** 1.7020, 5.4040]

2. From the following table of values of x and y, obtain $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ for $x = 1.2, 2.2$ and 1.6

x	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y	2.7183	3.3201	4.0552	4.9530	6.0496	7.3891	9.0250

[**Ans.** $y'(1.2) = 3.3205, y''(1.2) = 3.318; y'(2.2) = 9.0228, y''(2.2) = 8.992; y'(1.6) = 4.953, y''(1.6) = 4.9525$]

3. A rod is rotating in a plane. The following table gives the angle θ(radians) through which the rod has turned for various values of the time t (seconds).

t	0	0.2	0.4	0.6	0.8	1.0	1.2
θ	0	0.12	0.49	1.12	2.02	3.20	4.67

Calculate the angular velocity and acceleration of the rod when $t = 0.6$ sec.

[**Ans.** (i) 3.82 radians/sec. (ii) 6.75 radians/sec^2]

4. From the table below, for what value of x, y is minimum? Also find this value of y.

x	3	4	5	6	7	8
y	0.25	0.240	0.259	0.262	0.250	0.224

[**Ans.** 5.6875, 0.2628]

6.3 NUMERICAL INTEGRATION

Like numerical differentiation, we need to seek the help of numerical integration techniques in the following situations:

1. Functions do not possess closed from solutions. Example:
   $f(x) = C \int_0^x e^{-t^2}\, dt.$

2. Closed form solutions exist but these solutions are complex and difficult to use for calculations.

3. Data for variables are available in the form of a table, but no mathematical relationship between them is known as is often the case with experimental data.

6.4 NEWTON-COTES CLOSED QUADRATURE FORMULA

The general form of the problem of numerical integration may be stated as follows:

Given a set of data points $(x_i, y_i), i = 0, 1, 2, \ldots, n$ of a function $y = f(x)$, where $f(x)$ is not explicitly known. Here, we are required to evaluate the definite integral

$$I = \int_a^b y\, dx \tag{6.17}$$

Here, we replace $y = f(x)$ by an interpolating polynomial $\phi(x)$ in order to obtain an approximate value of the definite integral of Equation (6.17).

In what follows, we derive a general formula for numerical integration by using Newton's forward difference formula. Here, we assume the interval (a, b) is divided into n-equal subintervals such that

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

$a = x_0 < x_1 < x_2 < \cdots < x_n = b$

with $x_n = x_0 + nh$

where $h =$ the internal size

$n =$ the number of subintervals

a and $b =$ the limits of integration with $b > a$.

Hence, the integral in Equation (6.17) can be written as

$I = \int_{x_0}^{x_n} y\, dx$

Using Newton's forward interpolation formula, we have

$$I = \int_{x_0}^{x_n} \left[y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \frac{u(u-1)(u-2)(u-3)}{4!}\Delta^4 y_0 + \cdots \right] dx$$

where $x = x_0 + uh$

$$I = h \int_0^n \left[y_0 + u\Delta y_0 + \frac{u^2-u}{2!}\Delta^2 y_0 + \frac{u^3-3u^2+2u}{3!}\Delta^3 y_0 + \frac{u^4-6u^3+11u^2-6u}{4!}\Delta^4 y_0 + \cdots \right] du$$

Hence, after simplification, we get

$$
\begin{aligned}
I = \int_{x_0}^{x_n} y\,dx = nh\Big[& y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 \\
& + \frac{1}{24}\left(\frac{n^4}{5} - \frac{3n^3}{2} + \frac{11n^2}{3} - 3n\right)\Delta^4 y_0 + \frac{1}{120}\left(\frac{n^5}{6} - 2n^4 + \frac{35n^3}{4} - \frac{50n^2}{3} + 12n\right)\Delta^5 y_0 \\
& + \frac{1}{720}\left(\frac{n^6}{7} - \frac{5n^5}{2} + 17n^4 - \frac{225n^3}{4} + \frac{274n^2}{3} - 60n\right)\Delta^6 y_0 + \cdots\Big]
\end{aligned}
\tag{6.18}
$$

The formula given by Equation (6.18) is known as *Newton-Cotes closed quadrature formula.* From the general formula ((6.18)), we can derive or deduce different integration formulae by substituting $n = 1, 2, 3, \ldots$, etc.

6.5 TRAPEZOIDAL RULE

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.

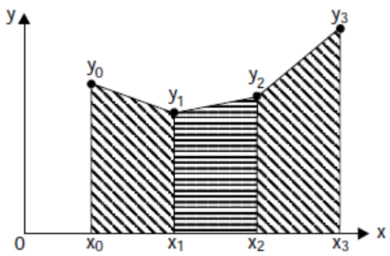

Figure 6.1

Each subinterval with the line approximation for the function forms a trapezoid as shown in Figure 6.1. The area of each trapezoid is computed by multiplying the interval size h by the average value of the function value in that subinterval. After the individual trapezoidal areas are obtained, they are all added to obtain the overall approximation to the integral.

Substituting $n = 1$ in Equation (6.18) and considering the curve $y = f(x)$ through the points (x_0, y_0) and (x_1, y_1) as a straight line (a polynomial of first degree so that the differences of order higher than first become zero), we get

$$
I_1 = \int_{x_0}^{x_1} y\,dx = h\left[y_0 + \frac{1}{2}\Delta y_0\right] = \frac{h}{2}\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}(y_0 + y_1) \tag{6.19}
$$

Similarly, we have

$$
\begin{aligned}
I_2 &= \int_{x_1}^{x_2} y\,dx = \frac{h}{2}(y_1 + y_2) \\
I_3 &= \int_{x_2}^{x_3} y\,dx = \frac{h}{2}(y_2 + y_3)
\end{aligned}
$$

and so on. (see Fig.6.2)

In general, we have

$$I_n = \int_{x_{n-1}}^{x_n} y\,dx = \frac{h}{2}(y_{n-1} + y_n) \tag{6.20}$$

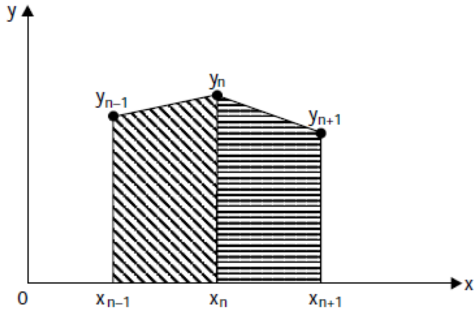

Figure 6.2

Adding all the integrals (Eq.(6.19), Eq.(6.20)) and using the interval additive property of the definite integrals, we obtain

$$I = \sum_{i=1}^{n} I_i = \int_{x_0}^{x_n} y\,dx = \frac{h}{2}\big[y_0 + 2(y_1 + y_2 + y_3 + \cdots + y_{n-1}) + y_n\big] \tag{6.21}$$

Equation (6.21) is known as the *trapezoidal rule*.

Summarising, the trapezoidal rule signifies that the curve $y = f(x)$ is replaced by n-straight lines joining the points $(x_n, y_n), i = 0, 1, 2, 3, \ldots, n$. The area bounded by the curve $y = f(x)$, the ordinates $x = x_0, x = x_n$ and the x-axis is then approximately equivalent to the sum of the areas of the n-trapezoids so obtained.

6.5.1 Error Estimate in Trapezoidal Rule

Let $y = f(x)$ be a continuous function with continuous derivatives in the interval $[x_0, x_n]$. Expanding y in a Taylor's series around $x = x_0$, we get

$$\begin{aligned}\int_{x_0}^{x_1} y\,dx &= \int_{x_0}^{x_1} \left[y_0 + (x - x_0)y_0' + \frac{(x-x_0)^2}{2!}y_0'' + \cdots\right] dx \\ &= hy_0 + \frac{h^2}{2}y_0' + \frac{h^3}{6}y_0'' + \frac{h^4}{24}y_0''' + \cdots \end{aligned} \tag{6.22}$$

Likewise,

$$\begin{aligned}\frac{h}{2}(y_0 + y_1) &= \frac{h}{2}(y_0 + y(x_0 + h)) = \frac{h}{2}\left[y_0 + y_0 + hy_0' + \frac{h^2}{2}y_0'' + \cdots\right] \\ &= hy_0 + \frac{h^2}{2}y_0' + \frac{h^3}{4}y_0'' + \frac{h^4}{12}y_0''' + \cdots \end{aligned} \tag{6.23}$$

Hence, the error e_1 in (x_0, x_1) is obtained from Eqs. (6.22) and (6.23) as

$$e_1 = \int_{x_0}^{x_1} y\,dx - \frac{h}{2}(y_0 + y_1) = \frac{-1}{12}h^3 y_0'' + \cdots$$

In a similar way, we can write

$$e_2 = \int_{x_1}^{x_2} y\, dx - \frac{h}{2}(y_1 + y_2) = \frac{-1}{12}h^3 y_1'' + \cdots$$
$$e_3 = \frac{-1}{12}h^3 y_2'' + \cdots$$
$$e_4 = \frac{-1}{12}h^3 y_3'' + \cdots \tag{6.24}$$

and so on.
In general, we can write

$$e_n = \frac{-1}{12}h^3 y_{n-1}'' + \cdots$$

Hence, the total error E in the interval (x_0, x_n) can be written as

$$E = \sum_{n=1}^{n} e_n = \frac{-h^3}{12}\left[y_0'' + y_1'' + y_2'' + \cdots + y_{n-1}''\right] \tag{6.25}$$

If $y''(\bar{x})$ is the largest value of the n quantities in the right hand side of Eq.(6.25), then we have

$$E = \frac{-1}{12}h^3 n y''(\bar{x}) = -\frac{b-a}{12}h^2 y''(\bar{x}) \tag{6.26}$$

Now, since $h = \frac{b-a}{n}$, the total error in the evaluation of the integral of Eq.(6.17) by the trapezoidal rule is of the order of h^2.

Example 6.11. *Evaluate the integral $\int_0^{1.2} e^x\, dx$, taking six intervals by using trapezoidal rule up to three significant figures.*

Solution: Let $h = \frac{b-a}{n} = \frac{1.2-0}{6} = 0.2$ and $f(x) = e^x$, then the values of y are given for the arguments which are obtained by dividing the interval $(0, 1.2)$ into 6 equal parts given below:

x	0	0.2	0.4	0.6	0.8	1.0	1.2
$y = f(x)$	1 y_0	1.221 y_1	1.492 y_2	1.822 y_3	2.226 y_4	2.718 y_5	3.320 y_6

The trapezoidal rule can be written as

$$\begin{aligned} I &= \frac{h}{2}\left[(y_0 + y_6) + 2(y_1 + y_2 + y_3 + y_4 + y_5)\right] \\ I &= \frac{0.2}{2}\left[(1 + 3.320) + 2(1.221 + 1.492 + 1.822 + 2.226 + 2.718)\right] \\ I &= 2.3278 \approx 2.328 \end{aligned}$$

The exact value is
$\int_0^{1.2} e^x\, dx = e^x\Big|_0^{1.2} = 2.320.$

Example 6.12. *Evaluate $\int_0^{12} \frac{1}{1+x^2}\, dx$ by using trapezoidal rule, taking $n = 6$, correct to five* *significant figures.*

Solution: Dividing the interval $(0, 12)$ into 6 equal parts, each of width $h = \frac{b-a}{n} = \frac{12-0}{6} = 2$.
The values of $f(x) = \frac{1}{1+x^2}$ at each points of sub-divisions are given by

x	0	2	4	6	8	10	12
$y = f(x)$	1	0.2	0.05882	0.02703	0.01538	0.00990	0.00690
	y_0	y_1	y_2	y_3	y_4	y_5	y_6

The trapezoidal rule can be written as

$$
\begin{aligned}
I &= \frac{h}{2}\left[(y_0 + y_6) + 2(y_1 + y_2 + y_3 + y_4 + y_5)\right] \\
I &= \frac{2}{2}\left[(1 + 0.00690) + 2(0.2 + 0.05882 + 0.02703 + 0.01538 + 0.00990)\right] \\
I &= 1.62916
\end{aligned}
$$

The exact value is
$\int_0^{12} \frac{1}{1+x^2}\, dx = tan^{-1}x\Big|_0^{12} = 1.48766.$

Exercise 6.1. *Evaluate* $\int_2^6 \log_x^{10}\, dx$ *by using trapezoidal rule, taking* $n = 8$*, correct to four decimal places.*

Solution: Dividing the interval $(2, 6)$ into 8 equal parts, each of width $h = \frac{6-2}{8} = 0.5$.
The values of $f(x) = \log_{10}^{x}$ are given below:

x	2	2.5	3.0	3.5	4.0	4.5	5.0	5.5	6.0
$f(x)$	0.3010	0.3979	0.4771	0.5440	0.6020	0.6532	0.6989	0.7403	0.7781
	y_0	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

The trapezoidal rule is

$$
\begin{aligned}
I &= \frac{h}{2}\left[(y_0 + y_8) + 2(y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7)\right] \\
I &= \frac{0.5}{2}\left[(0.3010 + 0.7781) + 2(0.3979 + 0.4771 + 0.5440 + 0.6020 + 0.6532 + 0.6989 + 0.7403)\right] \\
I &= 2.32666
\end{aligned}
$$

The exact value is given by
$\int_2^6 \log_x^{10}\, dx = [x \log x - x]_2^6 = 6.06685$