Chapter 5: Numerical Differentiation and Integration

5.1 Introduction

Calculus is the mathematics of change. Because engineers and scientists continuously deal with systems and processes that vary over time, calculus is an essential tool in their work. At the heart of calculus lie the related concepts of differentiation and integration.

Differentiation and integration are inversely related processes. For example:

- If a function $y(t)$ represents the position of an object, its derivative gives the velocity.
- Conversely, if the velocity $v(t)$ is known, its integral yields the position.

While many functions can be differentiated or integrated analytically, there are situations where analytical methods fail or become impractical. In such cases, numerical methods become necessary. This unit deals with the numerical approaches to differentiation and integration, particularly when the available function falls into one of the following categories:

1. A simple continuous function such as a polynomial, exponential, or trigonometric function.
2. A complex continuous function that is difficult or impossible to integrate or differentiate analytically.
3. A tabulated function, where values of x and $f(x)$ are provided only at discrete points, as often occurs with experimental or field data.

For the first situation, analytical calculus typically suffices. For the second, analytical solutions may be extremely cumbersome or impossible. In both the second and third cases, approximate numerical methods must be used. Numerical integration (also called numerical quadrature) refers to a family of methods used to approximate the value of a definite integral:

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

Since many functions cannot be integrated analytically, numerical methods such as the **Trapezoidal Rule** and **Simpson's Rules** provide efficient approximations. However, every numerical method introduces **truncation error**, which arises from approximating the integral using polynomial interpolation.

5.2. 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 the choice 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 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.

5.2.1. Derivatives Using Newton's Forward Interpolation Formula

Newton's forward interpolation is given by

$$y = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots + \frac{p(p-1)(p-2)\cdots(p-n+1)}{n!}\Delta^n y_0$$

Where $p = \frac{x - x_0}{h}$ (1)

Differentiating equation (1) with respect to p, we get:

$$\frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!}\Delta^3 y_0 + \cdots$$

And $\frac{dy}{dx} = \frac{dy}{dp}.\frac{dp}{dx} = \frac{1}{h}\frac{dy}{dp}$ (2)

Therefore,

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!}\Delta^3 y_0 + \frac{4p^3 - 18p^2 + 22p - 6}{4!}\Delta^4 y_0 + \cdots\right] \quad (3)$$

At $x = x_0$, $p = 0$, therefore, putting $p = 0$ in (3), we get:

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

Differentiating equation (3) again w.r.t. 'x', we get:

$$\frac{d^2y}{dx^2}=\frac{d}{dp}\left(\frac{dy}{dx}\right)\frac{dp}{dx}=\frac{1}{h}\frac{d}{dp}\left(\frac{dy}{dx}\right)$$

$$=\frac{1}{h^2}\left[\Delta^2 y_0+(p-1)\Delta^3 y_0+\frac{6p^2-18p+11}{12}\Delta^4 y_0+\cdots\right] \tag{5}$$

Putting $p = 0$ in (5), we get:

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

5.2.2. Derivatives Using Newton's Backward Difference Formula

Newton's backward interpolation formula is given by:

$$P_n(x)=y_n+p\nabla y_n+\frac{p(p+1)}{2!}\nabla^2 y_n+\frac{p(p+1)(p+2)}{3!}\nabla^3 y_n+\cdots$$
$$+\frac{p(p+1)(p+2)\cdots(p+n-1)}{n!}\nabla^n y_n$$

Where $p=\dfrac{x-x_n}{h}$ (1)

Differentiating both sides of equation (1) with respect to x, we get:

$$\frac{dy}{dx}=\frac{1}{h}\left[\nabla y_n+\frac{2p+1}{2!}\nabla^2 y_n+\frac{3p^2+6p+2}{3!}\nabla^3 y_n+\frac{4p^3+18p^2+22p+6}{4!}\nabla^4 y_n+\cdots\right] \tag{2}$$

At $x = x_n$, $p = 0$. Therefore putting $p = 0$ in (2), we get:

$$\left[\frac{dy}{dx}\right]_{x=x_n}=\frac{1}{h}\left[\nabla y_n+\frac{1}{2}\nabla^2 y_n+\frac{1}{3}\nabla^3 y_n+\frac{1}{4}\nabla^4 y_n+\cdots\right] \tag{3}$$

Again differentiating both sides of equation (2) w.r.t. x, we get:

$$\frac{d^2y}{dx^2}=\frac{1}{h^2}\left[\nabla^2 y_n+\frac{6p+1}{6}\nabla^3 y_n+\frac{12p^2+36p+22}{24}\nabla^4 y_n+\cdots\right] \tag{4}$$

At $x = x_n$, $p = 0$. Therefore putting $p = 0$ in (4), we get:

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n}=\frac{1}{h^2}\left[\nabla^2 y_n+\nabla^3 y_n+\frac{11}{12}\nabla^4 y_n+\cdots\right] \tag{5}$$

Example 5.1: From the following table, find *i)* $\frac{dy}{dx}$ *at x = 0.1* *ii)* $\frac{dy}{dx}$ *at x = 0.4.*

x	*0.1*	*0.2*	*0.3*	*0.4*
y	*0.9975*	*0.9900*	*0.9776*	*0.9604*

Solution: First we construct the difference table:

X	Y	Δ**y**	Δ^2**y**	Δ^3**y**
0.1	*0.9975*			
		-0.0075		
0.2	*0.9900*		-0.0049	
		-0.0124		0.0001
0.3	*0.9776*		-0.0048	
		-0.0172		
0.4	*0.9604*			

(i) Since the approximation is desired at the beginning of the table, we use Newton's Forward Interpolation Formula.

Here, x_0 = 0.1, h = 0.1 and y_0 = 0.9975. We know that, Newton's forward difference formula gives:

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

$$\left[\frac{dy}{dx}\right]_{x=0.1} = \frac{1}{0.1}\left[-0.0075 - \frac{1}{2}(-0.0049) + \frac{1}{3}(0.0001)\right] = -0.050167$$

(ii) Here we want to find the derivative at x = 0.4, which is at the end of the arguments. Therefore, we apply Newton's backward interpolation formula.

Here, x_0 = 0.1, h = 0.1 and y_n = 0.9604. We know that, Newton's backward difference formula gives:

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \cdots\right]$$

$$\left[\frac{dy}{dx}\right]_{x=0.4} = \frac{1}{0.1}\left[-0.0172 + \frac{1}{2}(-0.0048) + \frac{1}{3}(0.0001)\right] = -0.019567$$

Example 5.2: Using the following table, find

(i) $\frac{dy}{dx}$ at x = 1.1 and ***(ii)*** $\frac{d^2y}{dx^2}$ at x = 1.1.

x	*1.0*	*1.1*	*1.2*	*1.3*	*1.4*	*1.5*	*1.6*
y	*7.989*	*8.403*	*8.781*	*9.129*	*9.451*	*9.750*	*10.031*

Solution: Since the approximation is required around the beginning of the table, we apply Newton's forward difference formula.

The difference table is:

X	y	Δ **y**	Δ^2 **y**	Δ^3 **y**	Δ^4 **y**	Δ^5 **y**	Δ^6 **y**
1.0	*7.989*						
		0.414					
1.1	*8.403*		-0.036				
		0.378		0.006			
1.2	*8.781*		-0.030		-0.002		
		0.348		0.004		0.001	
1.3	*9.129*		-0.026		-0.001		-0.002
		0.322		0.003		-0.001	
1.4	*9.451*		-0.023		-0.002		
		0.299		0.005			
1.5	*9.750*		-0.018				
		0.281					
1.6	*10.031*						

We have,

(i) $$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \frac{1}{5}\Delta^5 y_0 - \frac{1}{6}\Delta^6 y_0 + \cdots\right]$$

Here h = 0.1, and x_0 = 1.1 and taking the appropriate differences, we get:

$$\left[\frac{dy}{dx}\right]_{x=1.1} = \frac{1}{0.1}\left[0.378 - \frac{1}{2}(-0.030) + \frac{1}{3}(0.004) - \frac{1}{4}(-0.001) + \frac{1}{5}(-0.001)\right] = 3.9435$$

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

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.1} = \frac{1}{(0.1)^2}\left[-0.030 - 0.004 + \frac{11}{12}(0.001) - \frac{5}{6}(-0.001)\right] = -0.341$$

Example (Derivatives using **forward differentiation rule** and **Newton's forward difference** formula)

Given the table

x	0	1	2	3
f(x)= 2^x	1	2	4	8

Estimate $f'(0)$ using forward differentiation rule and Newton's forward difference formula

Solution:

Using Forward differentiation rule

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i)}{h} = \frac{f(x_{i+1}) - f(x_i)}{h} = \frac{\Delta y_i}{h}$$

$$f'(0) \approx \frac{f(x_1) - f(x_0)}{h} = \frac{\Delta y_0}{h} = \frac{f(1) - f(0)}{1 - 0} = 1$$

Using Newton's Forward difference formula

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

$$f'(0) \approx 0.8333$$

Exact derivative for $f(x) = 2^x$ is $f'(x) = 2^x ln2$, then $f'(0) = 2^0 * ln(2) \approx 0.6931$

In general, Newton's forward formula is clearly more accurate**.**

5.2.3. Derivatives using Newton's divided differences interpolation formula (for unequally spaced data)

Differentiating term by term, we get

$$f'(x) = f[x_0, x_1] + f[x_0, x_1, x_2](2x - x_0 - x_1) + \cdots$$

and the second derivative will be

$$f''(x) = 2f[x_0, x_1, x_2] + \cdots$$

Evaluating the derivatives at a particular point $x = x_0$, we get

$$f'(x_0) = f[x_0, x_1] + f[x_0, x_1, x_2](x_0 - x_1) + \cdots \quad \text{and} \quad f''(x_0) = 2f[x_0, x_1, x_2] + \cdots$$

Example: For the given unequally spaced data points

x	1	2	4
$f(x) = x^2$	1	4	16

Find $f'(1)$ and compare it with the exact result

Exercise:

The following table gives the distance S (in meter) covered by car in time t (in second).

t	0	2	4	6
S	20	32	76	107

Then determine: a) the ***velocity*** of the car ($\frac{dS}{dt}$) at t = 6sec.

b) the ***acceleration*** of the car ($\frac{d^2S}{dt^2}$) at t = 2 sec.

5.3. 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.
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.

5.3.1. Newton-Cotes Quadrature Formula

Let $y = f(x)$ be a function, where y takes the values $y_0, y_1, y_2, \ldots, y_n$ for $x = x_0, x_1, x_2, \ldots, x_n$. We want to find the value of $I = \int_a^b f(x)dx$.

Let the interval of integration (a, b) be divided into n equal subintervals of width $h = \left(\frac{b-a}{n}\right)$

So that $x_0 = a$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, ..., $x_n = x_0 + nh = b$.

Therefore $I = \int_a^b f(x)dx = \int_{x_0}^{x_0+nh} f(x)dx$ (1)

We can approximate f(x) by Newton's forward interpolation formula which is given by:

$$y = f(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots + \frac{p(p-1)(p-2)\cdots(p-n+1)}{n!}\Delta^n y_0$$

Where $p = \dfrac{x - x_0}{h}$ So $dp = \dfrac{1}{h}dx \Rightarrow dx = hdp$

Therefore equation (1) becomes,

$$I = \int_{x_0}^{x_n} f(x)dx = h\int_0^n \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \right] dp$$

$$= nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \cdots + \text{up to (n+1) terms} \right] \qquad (2)$$

This formula is called Newton cotes- quadrature formula.

5.3.2. The Trapezoidal Rule

The Trapezoidal rule (sometimes referred to simply as the Trapezium rule) is **the simplest practical numerical integration method**. It is based on the principle of finding the **area of a trapezium**. The principle behind the method is to replace the curve $y = f(x)$ by a straight line (linear approximation) as shown in the figure below.

Typically, we approximate the area A under the curve $y = f(x)$ between the ordinates at x_0 and x_1 by $A \cong \frac{h}{2}(y_0 + y_1)$, where $y_0 = f(x_0)$, $y_1 = f(x_1)$ and h is the distance between x_0 and x_1 .

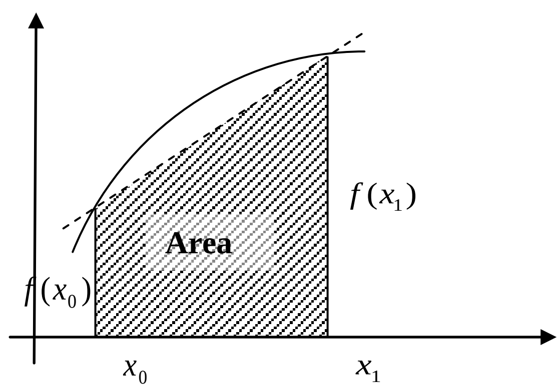

Figure 5.1: Trapezoidal Rule

For the integral $\int_a^b f(x)dx$ the trapezoidal rule can also be applied by subdividing the interval $[a,b]$ into n subintervals $[x_{k-1}, x_k]$, $k = 1,2,3,...,n$, of equal length $h = x_k - x_{k-1}$, with $a = x_0$ and $b = x_n$, followed by applying the trapezoidal rule over each subinterval. The area A under the curve $y = f(x)$ between the ordinates at $a = x_0$ and $b = x_n$ can then be approximated by the **generalized Trapezoidal rule.**

Derivation of The Formula

Putting n =1 in equation (2) and taking the curve $y = f(x)$ through (x_0, y_0) and (x_1, y_1) as a polynomial of degree one so that differences of order higher than one vanish, we get:

$$\int_{x_0}^{x_0+h} f(x)dx = h\left(y_0 + \frac{1}{2}\Delta y_0\right) = \frac{h}{2}\left(2y_0 + (y_1 - y_0)\right) = \frac{h}{2}\left(y_0 + y_1\right).$$

Similarly, for the next sub intervals $(x_0 + h, x_0 + 2h)$, $(x_0 + 2h, x_0 + 3h)$, …, we get:

$$\int_{x_0+h}^{x_0+2h} f(x)dx = \frac{h}{2}\left(y_1 + y_2\right), \quad \int_{x_0+2h}^{x_0+3h} f(x)dx = \frac{h}{2}\left(y_2 + y_3\right), \ \ldots, \quad \int_{x_0+(n-1)h}^{x_0+nh} f(x)dx = \frac{h}{2}\left(y_{n-1} + y_n\right)$$

Adding the above integrals, we get:

$$I = \int_a^b f(x)dx \cong \frac{h}{2}\left(y_0 + y_1\right) + \frac{h}{2}\left(y_1 + y_2\right) + \frac{h}{2}\left(y_2 + y_3\right) + \ldots + \frac{h}{2}\left(y_{n-1} + y_n\right)$$

$$= \frac{h}{2}\left[y_0 + 2\left(y_1 + y_2 + y_3 + \ldots + y_{n-1}\right) + y_n\right]$$

$$= \frac{h}{2}\left[\left(y_0 + y_n\right) + 2\sum_{k=1}^{n-1} y_k\right]$$ which is known as Trapezoidal rule.

5.3.3. The Simpson's Rules

The Simpson's 1/3-Rules

Putting n = 2 in equation (2) and taking the curve through (x_0, y_0),(x_1, y_1) and (x_2, y_2) as a polynomial of degree two so that differences of order higher than two vanish, we get:

$$\int_{x_0}^{x_0+2h} f(x)dx = 2h\left(y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0\right) = \frac{2h}{6}\left[6y_0 + 6(y_1 - y_0) + (y_2 - 2y_1 - y_0)\right] = \frac{h}{3}\left(y_0 + 4y_1 + y_2\right)$$

Similarly, $$\int_{x_0+2h}^{x_0+4h} f(x)dx = \frac{h}{3}\left(y_2 + 4y_3 + y_4\right),$$

$$\int_{x_0+4h}^{x_0+6h} f(x)dx = \frac{h}{3}\left(y_4 + 4y_5 + y_6\right), \ \ldots,$$

$$\int_{x_0+(n-2)h}^{x_0+nh} f(x)dx = \frac{h}{3}\left(y_{n-2} + 4y_{n-1} + y_n\right)$$

Adding the above integrals, we get:

$$I = \int_a^b f(x)dx = \frac{h}{3}\left[y_0 + 4y_1 + y_2\right] + \left[y_2 + 4y_3 + y_4\right] + \ldots + \left[y_{n-2} + 4y_{n-1} + y_n\right]$$

$$= \frac{h}{3}\left[y_0 + 4(y_1 + y_3 + ... + y_{n-1}) + 2(y_2 + y_4 + ... + y_{n-2}) + y_n\right]$$

which is known as Simpson's one-third rule.

Note: To use Simpson's one-third rule, the given interval of integration must be divided into an even number of subintervals.

The Simpson's three-eighth Rules

Putting n = 3 in equation (2) and taking the curve through (x_0, y_0), (x_1, y_1), (x_2, y_2) and (x_3, y_3) as a polynomial of degree three so that differences of order higher than three vanish, we get:

$$\int_{x_0}^{x_0+3h} f(x)dx = 3h\left(y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0 \right)$$

$$= \frac{3h}{8}\left[8y_0 + 12(y_1 - y_0) + 6(y_2 - 2y_1 + y_0) + (y_3 - 3y_2 + 3y_1 - y_0)\right] =$$

$$= \frac{3h}{8}\left(y_0 + 3y_1 + 3y_2 + y_3\right)$$

Similarly, $\int_{x_0+3h}^{x_0+6h} f(x)dx = \frac{3h}{8}\left(y_3 + 3y_4 + 3y_5 + y_6\right)$, …, $\int_{x_0+(n-3)h}^{x_0+nh} f(x)dx = \frac{3h}{8}\left(y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n\right)$

Adding the above integrals, we get:

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{3h}{8}\left[(y_0 + y_n) + 3(y_1 + y_2 + y_4 + y_5 + ... + y_{n-2} + y_{n-1}) + 2(y_3 + y_6 + ... + y_{n-3})\right]$$

which is known as Simpson's three-eighth rule.

Note: To use Simpson's three-eighth rule, the given interval of integration must be divided into sub-intervals whose number n is a multiple of 3.

Example 5.3: Evaluate $\int_0^6 \frac{dx}{1+x^2}$ by using

(i) Trapezoidal Rule

(ii) Simpson's one-third rule

(iii) Simpson's three-eighth rule

Solution: Divide the interval (0, 6) into six parts each of width h = 1.

The value of $f(x) = \frac{1}{1+x^2}$ are given below:

x	0	1	2	3	4	5	6
f(x)	1 y_0	0.5 y_1	0.2 y_2	0.1 y_3	$\frac{1}{17}$ y_4	$\frac{2}{26}$ y_5	$\frac{1}{37}$ y_6

(*i*) By Trapezoidal rule,

$$\int_0^6 \frac{dx}{1+x^2} = \frac{h}{2}\left[(y_0+y_6)+2(y_1+y_2+y_3+y_4+y_5)\right]$$

$$=\frac{1}{2}\left[(1+\frac{1}{37})+2(0.5+0.2+0.1+\frac{1}{17}+\frac{1}{26})\right]=1.410798581$$

(*ii*) By Simpson's one-third rule,

$$\int_0^6 \frac{dx}{1+x^2} = \frac{h}{3}\left[(y_0+y_6)+4(y_1+y_3+y_5)+2(y_2+y_4)\right]$$

$$=\frac{1}{3}\left[(1+\frac{1}{37})+4(0.5+0.1+\frac{1}{26})+2(0.2+\frac{1}{17})\right]=1.366173413$$

(*iii*) By Simpson's three-eighth rule,

$$\int_0^6 \frac{dx}{1+x^2} = \frac{3h}{8}\left[(y_0+y_6)+3(y_1+y_2+y_4+y_5)+2(y_3)\right]$$

$$=\frac{3}{8}\left[(1+\frac{1}{37})+3(0.5+0.2+\frac{1}{17}+\frac{1}{26})+2(0.1+)\right]=1.357080836$$

<u>**Example 5.4**</u>: A river is 80 m wide. The depth y of the river at a distance 'x' from one bank is given by the following table:

x	0	10	20	30	40	50	60	70	80
y	0	4	7	9	12	15	14	8	3

Find the approximate area of cross section of the river using Simpson's one-third rule.

<u>**Solution**</u>: The required area of the cross-section of the river is given by: $A=\int_0^{80} y\,dx$

Here number of sub intervals is 8 and the spacing, h, is 10.

By Simpson's one-third rule, $\int_0^{80} y dx = \frac{h}{3}\left[(y_0 + y_8) + 4(y_1 + y_3 + y_5 + y_7) + 2(y_2 + y_4 + y_6)\right]$

$$= \frac{10}{3}\left[(0+3) + 4(4+9+15+8) + 2(7+12+14)\right] = 710$$

Hence the required area of the cross-section of the river is 710 sq. m.

Note: When the number of subintervals is odd, Simpson's 1/3 rule is applied to the first $\boldsymbol{n-3}$ subintervals and Simpson's 3/8 rule to the last three subintervals.

Example: Approximate $\int_0^5 \frac{1}{1+x^2} dx$, using $h = 1$.

Solution: Not even, we cannot use Simpson's 1/3 alone and Not a multiple of 3, we cannot use Simpson's 3/8 alone

Apply Simpson's 1/3 on the first 2 intervals $[0,2]$,

$$I_{1/3} = \frac{1}{3}\,[1 + 4(0.5) + 0.2] = 1.0667$$

Apply Simpson's 3/8 on the last 3 intervals $[2,5]$

$$I_{3/8} = \frac{3}{8}\,[0.2 + 3(0.1) + 3(0.0588) + 0.0385] = 0.2675$$

Hence, $\int_0^5 \frac{1}{1+x^2} dx \approx 1.0667 + 0.2675 \approx 1.3342$

5.2.4. Error Analysis of Common Numerical Integration Methods

Numerical integration errors arise mainly from:

1. **Truncation Error**
   - ✓ Error due to replacing the function by a polynomial approximant.
   - ✓ Depends on step size h and higher derivatives of $f(x)$.
2. **Round-Off Error**
   - ✓ Due to finite precision in computation.
   - ✓ Usually small compared to truncation error unless n is extremely large.
3. **Step Size**

   The interval $[a, b]$ is divided into n equal subintervals:

   $$h = \frac{b-a}{n}, \qquad x_i = x_0 + ih$$

   Each numerical integration formula uses functional values at these grid points.

Trapezoidal Error

Formula

$$I = \int_a^b f(x)dx = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

Derivation Idea

The rule approximates the curve by straight-line segments.

Error Term (Local)

For one subinterval:

$$E_{loc} = -\frac{h^3}{12} f^{('')}(\xi), \qquad \xi \in [a, b]$$

Error Term (Global)

$$E_T = -\frac{(b-a)h^2}{12} f^{('')}(\xi), \qquad \xi \in [a, b]$$

Hence, the error term for the composite trapezoidal rule is zero if $f\ (x)$ is linear; that is, for a first degree polynomial, the trapezoidal rule gives the exact result.

Simpson's 1/3 Error

It requires even number of subintervals**.**

$$S_n = \int_a^b f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + f(x_n)]$$

Derivation Idea

It approximates the function using a quadratic polynomial on each pair of intervals.

Error Term (Local)

$$E_{local} = -\frac{h^5}{90} f^{(4)}(\xi).$$

Error Term (Global)

$$E_{1/3} = -\frac{(b-a)h^4}{180} f^{(4)}(\xi).$$

Hence, the truncation error bound for Simpson's composite rule is proportional to h^4 whereas the error bound for the composite Trapezoidal rule is proportional to h^2. As a result, Simpson's composite rule is more accurate than the composite trapezoidal rule, provided that the round of error will not cause a problem. Since the error term given above involves the fourth derivative of f, Simpson's composite rule will give the exact results when applied to any polynomial of degree three or less.

Simpson's 3/8 Error

Works when the number of subintervals is a multiple of 3.

$$S_{3/8} = \int_a^b f(x)dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + 2f(x_3) + \cdots + f(x_n)]$$

Error Term (Local)

$$E_{local} = -\frac{3h^5}{80} f^{(4)}(\xi).$$

Error Term (Global)

$$E_{3/8} = -\frac{(b-a)h^4}{80} f^{(4)}(\xi).$$

Simpson's 3/8 rule is 4th order accurate (i.e., the global truncation error is proportional to h^4)

Although the accuracy order matches Simpson's 1/3 rule, Simpson's 3/8 rule has a larger error constant, so it is less accurate for the same step size; hence Simpson's 1/3 is preferred. Simpson's 3/8 rule is mainly used for mixed-panel integration when the number of subintervals is not even.

Comparison of Error Behavior

Method	Global error Term	Order of accuracy
Trapezoidal	$O(h^2)$	2
Simpson's 1/3 Rule	$O(h^4)$	4
Simpson's 3/8 Rule	$O(h^4)$	4

Example 1 (Trapezoidal error bound**):**

Estimate the error bound for the Trapezoidal rule when approximating $\int_0^1 e^x dx$ using 4 subintervals

Solution:

The Trapezoidal rule error formula (for n equal subintervals) is:

$$E_T = -\frac{(b-a)h^2}{12} f^{('')}(\xi), \;\; \xi \in [a,b]$$

Here:

$$\mathrm{a} = 0, \;\; \mathrm{b} = 1, \; \mathrm{n} = 4$$

$$h = \frac{1-0}{4} = 0.25 \qquad f(x) = e^x, \qquad f'^{(x)} = e^x, \qquad f''^{(x)} = e^x.$$

Maximum of $f''(x)$ on [0,1] is $e^1 = e$, Minimum is $e^0 = 1$.

Since, $f'' > 0$, the absolute error bound:

$|E_T| \leq \frac{(b-a)h^2}{12} \max_{0\leq x\leq 1}|f''(x)| \leq \frac{1*(0.25)^2}{12} * e = \frac{\mathbf{0.0625}}{12} * e = 0.005208\dot{3} * e$

$|E_T| \leq 0.005208333 \times 2.718281828 \approx 0.0141570.005208333 \times 2.718281828 \approx 0.014157$

Thus: $|E_T| \leq 0.014160$ (Error bound not actual error.)

Example 2:

A function satisfies $\left|f^{('')}(x)\right| \leq 10$ on $[0, 5]$. What step size h ensures that the Trapezoidal rule has global error less than 0.001?

Solution:

The Trapezoidal rule error formula (for n equal subintervals) is**:** $|E_T| \leq -\frac{(b-a)h^2}{12} \max_{0\leq x\leq 1}|f''(x)|$

Given: $\mathrm{b} - \mathrm{a} = 5$, $M_2 = \max_{0\leq x\leq 1}|f''(x)| = 10$, desired $|E_T| < 0.001$

$$|E_T| \leq \frac{5h^2}{12} \max_{0\leq x\leq 1}|f''(x)| = \frac{5h^2}{12} * 10 < 0.001$$

$$\Rightarrow \frac{5h^2}{12} * 10 < 0.001$$

$$\Rightarrow \frac{50h^2}{12} < 0.001$$

$$\Rightarrow h^2 < \frac{0.001 * 6}{25} = 0.00024$$

$$\Rightarrow h < \sqrt{0.00024} \approx 0.015491$$

So pick h less than that to guarantee the error bound. $h \approx 0.01559$ (so n ≥ 323**)**

Example 3: Using Simpson's 1/3 rule with $n = 4$, approximate $\int_0^2 (1 + x^3)dx$, and compute the theoretical error bound using the fourth derivative.

Solution:

Example 4: Consider the function $f(x) = x^2$ on the interval $[0,1]$. Using the Trapezoidal Rule with $n = 4$ subintervals:

- **a)** Compute the trapezoidal approximation to $\int_0^1 f(x)dx$
- **b)** Find the exact value of the integral.
- **c)** Determine the true error committed by the trapezoidal rule.

d) Estimate the error bound using the trapezoidal error formula.

e) Comment on the accuracy of the approximation and state whether it is an overestimate or underestimate, giving a reason.

Solution:

a) The trapezoidal approximation $\int_0^1 x^2 dx = 0.34375$ which is close to the exact value

b) Exact value $= \int_0^1 x^2 dx = \frac{1}{3} = 0.333 \cdots$

c) True error$= |\ 0.34375 - \frac{1}{3}\ | = 0.01042$, which is small for only 4 subintervals. This shows the trapezoidal rule is reasonably accurate for a smooth function like x^2

d) $|E_T| \leq \frac{1}{96} \approx 0.01042$

e) $f''(x) = 2 > 0$ on $[0,\ 1]$ $\Rightarrow$ function is convex(curves upward), For convex functions, the trapezoid lies above the curve, so the approximation overestimates the true integral.