

MODULE 4: NUMERICAL INTEGRATION

UNIT 1 INTRODUCTION TO NUMERICAL INTEGRATION

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1.0 INTRODUCTION

In numerical analysis, integration seems to be easier than differentiation, which is the reverse in Calculus. Hence the cases where most integrals have no representation in terms of elementary function will only require the use of approximation functions. This is done by the process of numerical integration.

The importance of numerical integration is clearly seen when we consider how frequently derivatives are involved in the formulation of problems in applied analysis. It is well observed that polynomial approximation serves as the basis for a variety of integral formulas, hence the need to have studied some polynomial approximation techniques.

2.0 OBJECTIVE

At the end of this Unit, you should be able to:

- explain what numerical integration is all about ;
- differentiate between analytical approach and numerical approach to integration; and
- be able to list various known methods for numerical quadrature.

3.0 QUADRATURE

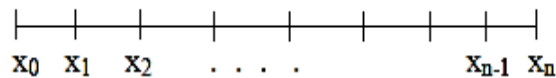
In the study elementary calculus especially integration, there are various techniques involved to evaluate different kind of integrals. Some integral are cumbersome that sometimes are left in form of another integral in a sense. There are several other ones that need the help of special functions or reduction of order before they can be evaluated. This is one reason why numerical integration comes to play a role in the evaluation of such integrals.

The main procedure of numerical integration is to divide the range of interval of integration into some equal intervals and obtain the integral of the first strip of the interval. Upon the first result, other strips are generalized. The other strips after the first are to correct the accuracy of the first, thereby quadrating the strips one after the other. Hence, Numerical integration is commonly referred to as Numerical quadrature and their formulas are called quadrature formulas. It is worth noting that results or formulas derived in this way are also termed as rules rather than methods. Thus, we talk of Trapezoidal rule, Simpson's rules, Newton-Cotes rules, etc. The main idea is, if $P(x)$ is an approximation to $y(x)$ then

$$\int_a^b P(x) dx \approx \int_a^b y(x) dx \quad (3.1)$$

That is the integral of $P(x)$ can be approximated by some numerical schemes which consider some points within the limits of integration. These points are node points or collocating points which are subdivided into by equal spacing on the x -axis.

Thus if the range or limits of integration which is $[a, b]$ are actually points $[x_0, x_n]$, then the interval $[x_0, x_n]$ can be subdivided into equal interval as shown below



Now between any successive interval, is what is called the step length denoted by h , so that

$$h = x_1 - x_0 = x_2 - x_1 = x_3 - x_2 = \dots = x_n - x_{n-1}$$

$$\Rightarrow x_n = x_0 + nh$$

3.1 Quadrature Formulas

There are standard rules in numerical analysis that can be used to estimate the above integral. Among such rules or formulas are:

- (i.) Trapezoidal rule,
- (ii.) Simpson's $\frac{1}{3}$ -rule,
- (iii.) Simpson's $\frac{3}{8}$ -rule,
- (iv.) Newton – Cotes formulas

The Trapezoidal rule is given by

$$\int_{x_0}^{x_n} P(x) dx = \frac{1}{2} h(y_0 + 2y_1 + 2y_2 + \dots + 2y_{n-1} + y_n)$$

The Simpson's $\frac{1}{3}$ -rule is given by

$$\int_{x_0}^{x_n} P(x) dx = \frac{1}{3} h(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \dots + 2y_{n-2} + 4y_{n-1} + y_n)$$

While the Simpson's $\frac{3}{8}$ -rule is given by

$$\int_{x_0}^{x_n} P(x) dx = \frac{3}{8} h (y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \dots + 3y_{n-2} + 3y_{n-1} + y_n)$$

The Newton – Cotes formulas depend on the value of n starting from n = 4 ,6, . . .

The derivations of these formulas are very essential to the learning of Numerical integration. While they are interesting in the learning of the topic, it also helps in the understanding of the workings of these formulae rather than trying to memorize them. Thus attempt will be made to give the required techniques of their derivations and the learner will complete the rest.

3.2 Newton Gregory Formula

The most acceptable way of deriving all these rules listed above is by using the **Newton forward formula** or **Newton backward formula**. However we shall restrict our learning to using the Newton Forward formula for deriving the integration formula in this course. Geometrically the Trapezoidal rule which sometimes is simply called the trapezium formula can be derived by approximating a curve by a straight line, thereby getting a trapezium.

The Newton Gregory Forward formula is given by

$$\begin{aligned} P_k(x) &= y_0 + {}^k C_1 \Delta y_0 + {}^k C_2 \Delta^2 y_0 + {}^k C_3 \Delta^3 y_0 + \dots + {}^k C_n \Delta^n y_0 \\ &= y_0 + k \Delta y_0 + \frac{k(k-1)}{2!} \Delta^2 y_0 + \frac{k(k-1)(k-2)}{3!} \Delta^3 y_0 + \dots + \frac{k(k-1)(k-2)\dots(k-n)}{n!} \Delta^n y_0 \end{aligned} \quad (3.2)$$

Integrating this formula of degree n between x₀ and x_n gives several useful quadrature formulas. Where Δ is a forward difference operator defined as Δy_k = y_{k+1} - y_k

This formula (3.2) is very useful in the derivation of all numerical integration schemes.

The accuracy of these quadrature formulas differs when applied to a definite integral. The smaller the stripe **h** is, the better the accuracy. It must be mentioned here that numerical integration deals with only definite integrals. In other words, indefinite integrals are best

handled by analytical means. However in practice, most practical problems involve definite integrals and so numerical integration is very relevant in physical and day to day problems. Each of these formulas will be discussed in subsequent Units.

4.0 CONCLUSION

The use of quadrature formulas are of high importance to this study. We have introduced all the relevant formulas which we shall later use to evaluate some definite integrals.

5.0 SUMMARY

In this Unit you have learnt that

- (i) *quadrature* is a numerical analysis terminology that refers to numerical integration
- (ii) there are three standard numerical integration formulas viz: Trapezoidal rule, Simpson's rules and Newton – Cotes formulas
- (ii) Newton Gregory formula is the basis for the derivation of these quadrature formulas.

6.0 TUTOR MARKED ASSIGNMENT

Use geometrical approach to derive the trapezoidal rule.

7.0 FURTHER READING AND OTHER RESOURCES

Francis Scheid. (1989) *Schaum's Outlines Numerical Analysis 2nd ed.* McGraw-Hill New York.

Kandassamy P., Thilagarathy K., & Gunevathi K. (1997): Numerical Methods, S. Chand & Co Ltd, New Delhi, India

Leadermann Walter (1981) (Ed.): Handbook of Applicable Mathematics, Vol 3, Numerical Analysis, John Wiley, N. Y.

UNIT 2 TRAPEZOIDAL RULE

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- 3.0 Derivation by Geometrical Approach
 - 3.1 Derivation by Newton's Formula
 - 3.2 Truncation Error
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1.0 INTRODUCTION

Integration is known to be a method of finding area under a curve. In particular, the curve may be bounded by two points on the x-axis. If this be the case, it might interest one to subdivide this area under a curve into small stripes of similar or equal width on the x-axis. As it was mentioned in the last unit we shall attempt to derive these formulas before illustrating their computation by examples.

2.0 OBJECTIVE

At the end of this lesson, you should be able to

- derive Trapezoidal rule geometrically;
- use Newton Gregory formula to derive the Trapezoidal rule;
- implement Trapezoidal rule to evaluate a definite integral; and
- estimate the error of a trapezoidal rule.

3.0 DERIVATION BY GEOMETRICAL APPROACH

Trapezoidal rule, partitions a function $f(x)$ into n equally spaced points on x-axis, leading to various arguments (x_i, x_{i+1}) . In order to derive the trapezoidal rule, the first approach shall be by geometrical means. Consider a function $f(x)$ within the interval $[x_0, x_n]$ as shown in figure 1

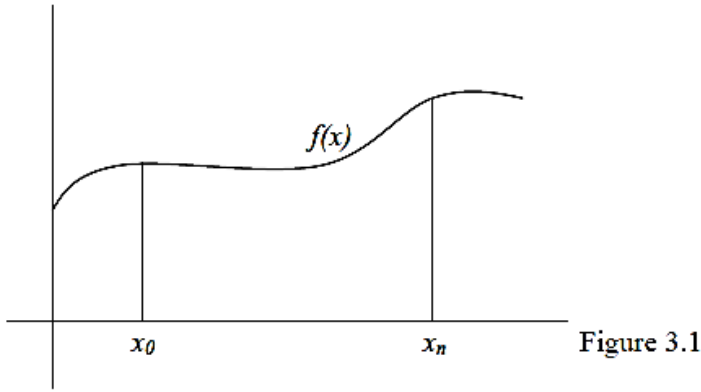


Figure 3.1

The interval is subdivided into n equally spaced intervals with node points $x_0, x_1, x_2, \dots, x_n$.

For any two immediate points x_0, x_1 the diagram below (Figure 2) describes the phenomenon

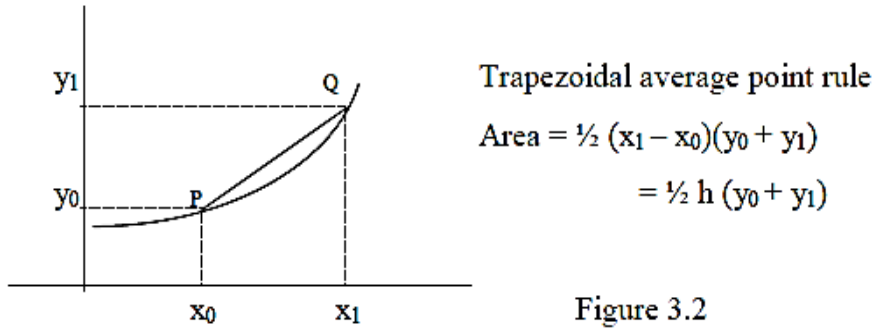


Figure 3.2

The points P, Q are assumed to be very close to each other; thereby it is approximated to be a straight line. Hence, the region x_0PQx_1 is a trapezium with parallel sides x_0P and x_1Q , making $(x_1 - x_0)$ as the width or height.

Thus for the whole region under the curve $f(x)$ bounded by the x-axis between $[x_0, x_n]$, the whole region is subdivided into small strips of small intervals

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

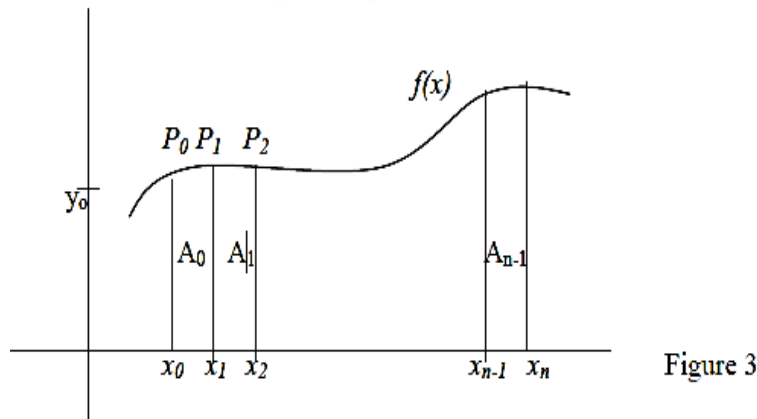


Figure 3

The first strip is assumed to be a trapezium where the point P₀P₁ is taken to be approximately a straight line. This region A₀ is a trapezium x₀P₀P₁x₁ with parallel sides x₀P₀ and x₁P₁ and the height is x₀x₁. Since Area has same meaning as Integration from elementary calculus, then the area of this trapezium A₀ is

$$A_0 = \frac{1}{2} [x_0P_0 + x_1P_1] \times (x_1 - x_0).$$

But x₀P₀ will corresponds to y₀ on y-axis, while x₁P₁ corresponds to y₁, by geometry, hence

$$A_0 = \frac{1}{2} (y_0 + y_1) \times (x_1 - x_0)$$

Let the equally spaced interval be h , then $h = x_i + 1 - x_i$

$$A_0 = \frac{1}{2} h(y_0 + y_1)$$

Similarly in the trapezium A₁, the sides are x₁P₁P₂x₂ and the area of this trapezium is

$$A_1 = \frac{1}{2} (y_1 + y_2) \times (x_2 - x_1)$$

which also gives

$$A_1 = \frac{1}{2} h (y_1 + y_2)$$

Continuing in this way, we obtain all the n areas A₀, A₁, . . . , A_{n-1} and we the sum them up to cover the whole are under the curve and within the required interval $[x_0, x_n]$. Thus we shall have the whole area as

Equation (3.2) is the Trapezium rule and it is the geometrical way of deriving this formula.

3.1 Derivation by Newton's Formula

To derive the same formula by numerical integration, we shall make use of the Newton Forward formula given by

$$\begin{aligned} P_k(x) &= y_0 + {}^kC_1 \Delta y_0 + {}^kC_2 \Delta^2 y_0 + {}^kC_3 \Delta^3 y_0 + \dots + {}^kC_n \Delta^n y_0 \\ &= y_0 + k \Delta y_0 + \frac{k(k-1)}{2!} \Delta^2 y_0 + \frac{k(k-1)(k-2)}{3!} \Delta^3 y_0 + \dots + \frac{k(k-1)(k-2)\dots(k-n)}{n!} \Delta^n y_0 \end{aligned} \quad (3.2)$$

To do this, if we truncate equation (3.2) after 2 terms, we get

$$P_k(x) = y_0 + {}^kC_1 \Delta y_0 = y_0 + k \Delta y_0$$

then we shall integrate this between x₀ and x₁, since n = 1, to get

$$\int_{x_0}^{x_1} P(x) dx = \int_{x_0}^{x_1} (y_0 + k \Delta y_0) dx \quad (3.3)$$

We need to change the variable in the integral from x to k in order to evaluate the integral.

But we established earlier that $x_n = x_0 + nh$

For any arbitrary variable x , we shall write $x = x_0 + kh$, $\Rightarrow dx = h dk$

Thus to take care of the limits of integration,

when $x = x_0$, then $k = 0$, and when $x = x_1$, $x_1 = x_0 + kh \Rightarrow k = 1$

Hence, equation (3.3) becomes

$$\begin{aligned} \int_{x_0}^{x_1} P(x) dx &= h \int_0^1 (y_0 + k\Delta y_0) dk, \\ &= h \left(k y_0 + \frac{1}{2} k^2 \Delta y_0 \right) \Big|_0^1 \\ &= h \left(y_0 + \frac{1}{2} \Delta y_0 \right) \\ \Rightarrow \int_{x_0}^{x_1} P(x) dx &= \frac{1}{2} h (2y_0 + y_1 - y_0) = \frac{1}{2} h (y_0 + y_1) \end{aligned} \quad (3.4)$$

We need to change the variable in the integral from x to k in order to evaluate the integral. But we established earlier that $x_n = x_0 + n_h$

This is similar to the result obtained geometrically by trapezium area A_o . This result (3.4) is termed as *one-phase of the Trapezoidal rule*.

By quadrature technique, we can repeat the same for interval $[x_1, x_2]$ by shifting the point from $[x_0, x_1]$ to $[x_1, x_2]$. That is, 1 replaces 0, while 2 replaces 1 in equation (3.4)

Thus,

$$\int_{x_1}^{x_2} P(x) dx = \frac{1}{2} h (y_1 + y_2)$$

This is called quadrating the points from one interval to a similar interval of equal length. Continuing for interval $[x_0, x_1]$, $[x_1, x_2]$, $[x_2, x_3]$, \dots , $[x_{n-1}, x_n]$, we obtain

$$\begin{aligned} \int_{x_0}^{x_n} P(x) dx &= \int_{x_0}^{x_1} P(x) dx + \int_{x_1}^{x_2} P(x) dx + \int_{x_2}^{x_3} P(x) dx + \dots + \int_{x_{n-1}}^{x_n} P(x) dx \\ &= \frac{1}{2} h (y_0 + y_1) + \frac{1}{2} h (y_1 + y_2) + \frac{1}{2} h (y_2 + y_3) + \dots + \frac{1}{2} h (y_{n-1} + y_n) \\ \Rightarrow \int_{x_0}^{x_n} P(x) dx &= \frac{1}{2} h (y_0 + 2y_1 + 2y_2 + \dots + 2y_{n-1} + y_n) \end{aligned} \quad (3.5)$$

This gives the same formula as obtained in (3.1) and it is often called the *Trapezoidal rule*.

3.3 Truncation Error

It must be observed that this formula is merely an approximation and the error committed is due to the truncation in the Newton's formula. Hence, we can estimate the Truncation Error (TE) of this formula. We define the error as the difference between the exact $y(x)$ and the approximated values $P(x)$. Thus, we write

$$E = \int_{x_0}^{x_n} y(x) dx - \int_{x_0}^{x_n} P(x) dx = \int_{x_0}^{x_n} [y(x) - P(x)] dx$$

$$\text{where } y(x) - P(x) = \frac{\prod_{i=1}^n (x - x_i)}{(n+1)!} y^{(n+1)}(\xi)$$

Then for $n = 1$ we can estimate the TE for the trapezoidal rule as follows:

$$y(x) - P(x) = \frac{(x - x_0)(x - x_1)}{2!} y^{(2)}(\xi)$$

Hence,

$$\begin{aligned} E &= \int_{x_0}^{x_1} \frac{(x - x_0)(x - x_1)}{2!} y^{(2)}(\xi) dx = \left(\frac{x^3}{6} - \frac{x_1 x^2}{4} - \frac{x_0 x^2}{4} - \frac{x_0 x_1 x}{2} \right) y^{(2)}(\xi) \Big|_{x_0}^{x_1} \\ &= \left(\frac{h^3}{6} - \frac{x_1 h^2}{4} - \frac{x_0 h^2}{4} - \frac{x_0 x_1 h}{2} \right) y^{(2)}(\xi) \\ &= \left(\frac{h^3}{6} - \frac{h^3}{4} \right) y^{(2)}(\xi) = -\frac{h^3}{12} y^{(2)}(\xi) \end{aligned}$$

which is the error committed within the first strip $[x_0, x_1]$

Now applying it on the whole range of trapezoidal rule:

$$\int_{x_0}^{x_n} P(x) dx = \frac{1}{2} h(y_0 + y_1) + \frac{1}{2} h(y_1 + y_2) + \dots + \frac{1}{2} h(y_{n-1} + y_n)$$

The error thus become

$$\begin{aligned} E &= -\frac{h^3}{12} y^{(2)}(x_0) - \frac{h^3}{12} y^{(2)}(x_1) + \dots + \frac{-h^3}{12} y^{(2)}(x_{n-1}) \\ &= -\frac{h^3}{12} [y_0^{(2)} + y_1^{(2)} + \dots + y_{n-1}^{(2)}] \end{aligned}$$

Let the derivative be bounded by $m < y^{(2)} < M$. The sum is between nm and nM . This sum will be written as $ny''(\xi)$ for $x_0 < \xi < x_n$

But $nh = x_n - x_0$

$$E = -\frac{h^3}{12}ny^{(2)}(\xi)$$

Thus,
$$E = -\frac{h^2}{12}(x_n - x_o)y^{(2)}(\xi)$$

which is the error committed when using trapezoidal rule to estimate an integral.

3.3 Numerical Example

Example 1

By using the Trapezoidal rule integrate \sqrt{x} between argument 1.00 and 1.30 for the data below

x	1.0	1.05	1.10	1.15	1.20	1.25	1.30
\sqrt{x}	1.00	1.0247	1.04881	1.07238	1.09544	1.11803	1.14017

Obtain the actual error and estimate the truncation error

Solution:

From the table of values given above, we observe that $n = 6$, and $y = \sqrt{x}$, so we read from the second row of the table that $y_0 = 1.00$ and so on up to $y_6 = 1.14017$; the step length $h = 0.05$ (since $h = 1.05 - 1 = 1.10 - 1.05 = 0.05$).

The Trapezoidal rule is given by equation (3.5) as

$$\int_{x_0}^{x_n} P(x) dx = \frac{1}{2}h(y_0 + 2y_1 + 2y_2 + \dots + 2y_{n-1} + y_n)$$

Thus with $n = 6$, we have

$$\int_{x_0}^{x_6} P(x) dx = \frac{1}{2}h(y_0 + 2y_1 + 2y_2 + 2y_3 + 2y_4 + 2y_5 + y_6)$$

Substituting the values from the table we have

$$\int_{1.00}^{1.30} \sqrt{x} dx = \frac{1}{2}(0.05) \left\{ 1 + 2(1.02470) + 2(1.04881) + 2(1.07238) \right. \\ \left. + 2(1.09544) + 2(1.11803) + 1.14017 \right\} \\ = 0.32147$$

The actual integral can be obtained analytically as

$$\int_{1.00}^{1.30} \sqrt{x} \, dx = \frac{2}{3} x^{3/2} \Big|_1^{1.3} = 0.321486$$

Hence the actual error is $E = 0.321485 - 0.32147 = 0.000015 = 1.5 \times 10^{-5}$

The Truncation Error of the Trapezoidal rule is

$$-\frac{(x_n - x_0)}{12} h^2 y^{(2)}(\xi) = -\frac{(0.30)}{12} (0.05)^2 \left(\frac{-x^{-3/2}}{4} \right) \\ = 0.000016$$

maximum error is obtained when $x = \xi = 1.00$

Example 2

Evaluate $\int_0^{\pi/3} \sin x \, dx$ with $h = \frac{\pi}{12}$, correct to 5 decimal places using Trapezoidal rule

Solution

Let $y = \sin x$, then we construct the table of values with a step length of $h = \frac{\pi}{12}$ as given below

	x_0	x_1	x_2	x_3	x_4
x	0	$\frac{\pi}{12}$	$\frac{\pi}{6}$	$\frac{\pi}{4}$	$\frac{\pi}{3}$
$y = \sin x$	0.00	0.25882	0.50000	0.70711	0.86603
y	y_0	y_1	y_2	y_3	y_4

$$\int_{x_0}^{x_4} P(x) \, dx = \frac{1}{2} h (y_0 + 2y_1 + 2y_2 + 2y_3 + y_4)$$

$$\int_0^{\pi/3} \sin x \, dx = \frac{1}{2} \left(\frac{\pi}{12} \right) [0 + 2(0.25882) + 2(0.5) + 2(0.70711) + 0.86603] \\ = 0.4971426 \cong 0.49714 \quad (\text{correct to 5 decimal places})$$

Analytically,

$$\int_0^{\pi/3} \sin x \, dx = -\cos x \Big|_0^{\pi/3} = -\cos \frac{\pi}{3} + \cos 0 = 0.5$$

Hence the absolute error is $E = 0.5 - 0.49714 = 0.00286 = 2.86 \times 10^{-3}$

4.0 CONCLUSION

The lesson has clearly shown that we need not know how to integrate a function before we can get an approximate value for such integral within a limiting boundary. We have also shown that the error committed can be compared with the actual value. This error is improved if the step length h is probably reduced.

5.1 SUMMARY

In this Unit you have learnt

- (i) how to derive the trapezoidal rule both in geometrical way and using the Newton Gregory formula
- (ii) how to implement the trapezoidal rule to evaluate definite integrals
- (iii) that the error can be estimated by comparing with the analytical solution
- (iv) that the truncation error of the rule can be estimated

6.0 TUTOR MARKED ASSIGNMENT

Evaluate $\int_2^5 \frac{2}{x+1} dx$ with $h = \frac{1}{2}$, correct to 5 decimal places using Trapezoidal rule

7.1 FURTHER READING AND OTHER RESOURCES

Conte S. D. and Boor de Carl *Elementary Numerical Analysis an Algorithmic Approach* 2nd ed. McGraw-Hill Tokyo.

Francis Scheid. (1989) *Schaum's Outlines Numerical Analysis* 2nd ed. McGraw-Hill New York.

Okunuga, S. A., & Akanbi M, A., (2004). *Computational Mathematics, First Course*, WIM Pub. Lagos, Nigeria.

UNIT 3: SIMPSON'S RULES

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- 2.0 Objective
- 3.0 Derivation of Simpson's $\frac{1}{3}$ – Rule,
 - 3.1 Error Estimate of the Simpson's $\frac{1}{3}$ – Rule
 - 3.2 Numerical Example
 - 3.3 Result by computer output
- 4.0 Conclusion
- 5.0 Summary
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1.0 INTRODUCTION

There are two popular Simpson's rules. One is called the Simpson's $\frac{1}{3}$ – rule while the other is the Simpson's $\frac{3}{8}$ – rule. The Simpson's rules are similarly useful in approximating definite integrals. We shall discuss the Simpson's $\frac{1}{3}$ – rule in this Unit. Simpson's $\frac{1}{3}$ – rule is a technique that uses 2 steps at a time to estimate the integral of $P(x)$ as against single step used by Trapezoidal rule. So, the interval $[x_0, x_n]$ is taken in two by two steps as $[x_0, x_2], [x_2, x_4], [x_4, x_6], \dots, [x_{n-2}, x_n]$. This idea will help us to derive a scheme that would be suitable for integration of various functions.

2.0 OBJECTIVE

At the end of this unit you should be able to

- derive the Simpson's $\frac{1}{3}$ – rule;
- distinguish between Simpson's rule and Trapezoidal rule;
- identify where Simpson's rule is applicable in terms of number of node points; and
- solve problems using the Simpson's $\frac{1}{3}$ rule.

3.0 DERIVATION OF SIMPSON'S $\frac{1}{3}$ - RULE

In order to develop a formula based on Simpson's rule, we shall consider the integration of Newton Forward Formula (NFF) given in Unit 1 of this Module. Recall the NFF, we have

$$\begin{aligned}
P_k(x) &= y_0 + {}^k C_1 \Delta y_0 + {}^k C_2 \Delta^2 y_0 + {}^k C_3 \Delta^3 y_0 + \dots + {}^k C_n \Delta^n y_0 \\
&= y_0 + k \Delta y_0 + \frac{k(k-1)}{2!} \Delta^2 y_0 + \frac{k(k-1)(k-2)}{3!} \Delta^3 y_0 + \dots + \frac{k(k-1)(k-2)\dots(k-n)}{n!} \Delta^n y_0
\end{aligned} \tag{3.1}$$

If we integrate within the interval $[x_0, x_2]$ and truncating after the third term, we shall obtain

$$\int_{x_0}^{x_2} P(x) dx = \int_{x_0}^{x_2} \left(y_0 + k \Delta y_0 + \frac{k(k-1)}{2} \Delta^2 y_0 \right) dx \tag{3.2}$$

The integration has to be limited to x_2 as $n = 2$ and this suggest the truncation also at Δ^2 .

Using the same technique employed earlier in Unit 2, to change the variable to k , we shall write

$$x = x_0 + kh, \Rightarrow dx = h dk$$

Thus to take care of the limits of integration, we examine x_0 and x_2 , so that

When $x = x_0$, then $k = 0$, and when $x = x_2$, $x_2 = x_0 + kh \Rightarrow k = 2$

Hence, the integral (3.2) becomes

$$\begin{aligned}
\int_{x_0}^{x_2} P(x) dx &= h \int_0^2 \left(y_0 + k \Delta y_0 + \frac{k(k-1)}{2} \Delta^2 y_0 \right) dk \\
&= h \left(k y_0 + \frac{1}{2} k^2 \Delta y_0 + \left(\frac{k^3}{6} - \frac{k^2}{4} \right) \Delta^2 y_0 \right) \Bigg|_0^2 \\
&= h \left(2 y_0 + 2 \Delta y_0 + \frac{1}{3} \Delta^2 y_0 \right) \\
&= h \left[2y_0 + 2(y_1 - y_0) + \frac{1}{3} (y_2 - 2y_1 + y_0) \right] \\
&= \frac{1}{3} h [y_0 + 4y_1 + y_2] \tag{3.3}
\end{aligned}$$

which is a part or **one phase** of the Simpson's $\frac{1}{3}$ - rule.

By quadrature, we can shift to the next two steps, that is, $[x_2, x_4]$ to get the next integral as:

$$\int_{x_2}^{x_4} P(x) dx = \frac{1}{3} h (y_2 + 4y_3 + y_4)$$

Continuing this interval up to (x_{n-2}, x_n) and summing up all the phases, we have

$$\begin{aligned} \int_{x_0}^{x_n} P(x) dx &= \int_{x_0}^{x_2} P(x) dx + \int_{x_2}^{x_4} P(x) dx + \dots + \int_{x_{n-2}}^{x_n} P(x) dx \\ \int_{x_0}^{x_n} P(x) dx &= \frac{1}{3} h (y_0 + 4y_1 + y_2) + \frac{1}{3} h (y_2 + 4y_3 + y_4) + \dots + \frac{1}{3} h (y_{n-2} + 4y_{n-1} + y_n) \\ \int_{x_0}^{x_n} P(x) dx &= \frac{1}{3} h (y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \dots + 2y_{n-2} + 4y_{n-1} + y_n) \end{aligned} \quad (3.4)$$

Equation (3.4) is known as **the Simpson's $\frac{1}{3}$ – rule**. It must be noted that due to the nature of this formula, the formula will only be valid, if n is an **even integer**. That is, there must exist odd number of ordinates or collocating points within $[x_0, x_n]$. Note that the formula has alternate coefficients of 4 and 2 starting with 4 and then followed by 2 and ending the second to the last term as 4 with exception of the first and the last term that have coefficient of 1.

3.1 Error Estimate of The Simpson's $\frac{1}{3}$ –Rule

The error committed while deriving the Simpson's $\frac{1}{3}$ –rule is the error of truncation after the third term at Δ^2 . For this reason the truncation error can be estimated likewise as it was done for the trapezoidal Rule. Thus, if $n = 2$, the error committed on Simpson's $\frac{1}{3}$ –rule, which is the Truncation error is given by

$$E = -\frac{(b-a)}{180} h^4 y^{(4)}(\xi) \quad (3.5)$$

The reader is advised to verify this claim.

3.2 Determination of Step Length

Sometimes we may be given problems without specifying the step length h . However if the number of ordinates are given, which is the same as our n then we can determine the step length. To calculate the step length, the required formula is given by

$$h = \frac{b-a}{m-1}$$

where m is the number of ordinates given, a and b are the boundary of the integral. For example given the integral $\int_2^5 P(x) dx$ and we are required to use 7 ordinates, then we

recognize $m = 7$, $a = 2$ and $b = 5$, hence the step length h is obtained as

$$h = \frac{5 - 2}{7 - 1} = 0.5$$

Hence our $x_0 = 2$ then add 0.5 to subsequent x_i until you get to $b = 5$. The last value must be the seventh ordinate which is x_6 . Thus we shall have $x_0 = 2$, $x_1 = 2.5$, $x_2 = 3$, $x_3 = 3.5$, $x_4 = 4$, $x_5 = 4.5$, $x_6 = 5$

3.3 Numerical Example

Example 1

Integrate $y = \sqrt{x}$ within the limits 1.00 and 1.30 using the Simpson's $\frac{1}{3}$ - rule with 7 ordinates and working with 5 decimal places. Hence estimate the error of this method.

Solution:

We first observe that this is the same question as the previous one in Trapezoidal rule. However in this case the table of values is not given hence we are to generate the table of values by computing the corresponding values of y for a given value of x . Furthermore we are to use 7 ordinates means that we need y_0, y_1, \dots, y_6 , that is $n = 6$ (even), hence Simpson rule is applicable. Also since we are told to use 7 ordinates, we are required to determine the step length h . To do this, the given values are

$a = 1.00$, $b = 1.30$ and $m = 7$ thus,
the step length is calculated as

$$h = \frac{b - a}{m - 1} = \frac{1.30 - 1.00}{7 - 1}$$

We then generate the table of values using calculator to find \sqrt{x} for various values of x on the table.

	x_0	x_1	x_2	x_3	x_4	x_5	x_6
x	1.0	1.05	1.10	1.15	1.20	1.25	1.30
$y = \sqrt{x}$	1.00	1.0247	1.04881	1.07238	1.09544	1.11803	1.14017
y	y_0	y_1	y_2	y_3	y_4	y_5	y_6

Hence the table of values is similar to the example given in Unit 2 for this same question. By equation (3.4) the Simpson's $\frac{1}{3}$ - rule is

$$\int_{x_0}^{x_n} P(x)dx = \frac{1}{3}h(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \dots + 2y_{n-2} + 4y_{n-1} + y_n)$$

$$\int_1^{1.3} \sqrt{x} dx = \frac{1}{3}h(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + .4y_5 + y_6)$$

Thus we evaluate the integral by simply substituting from our table above as

$$\int_{1.00}^{1.30} \sqrt{x} dx = \frac{1}{3}(0.05) \left\{ 1 + 4(1.02470) + 2(1.04881) + 4(1.07238) \right. \\ \left. + 2(1.09544) + 4(1.11803) + 1.14017 \right\}$$

$$= 0.32149$$

The analytical result of this integral is 0.321485, correct to 6 decimal places. However correct to 5 decimal places will be 0.32149. It seems the error is zero. However if we had computed up to 6 places of decimal the error will be pronounced.

All the same we can still estimate the error as $0.32149 - 0.321485 = 5 \times 10^{-6}$. This seems to be more accurate than the result given by the Trapezoidal rule in the last Unit.

The Truncation error stated above for Simpson's $\frac{1}{3}$ – rule is:

$$E = -\frac{(b-a)}{180} h^4 y^{(4)}(\xi)$$

Hence to estimate the Truncation Error with this problem we write

$$E = -\frac{(0.3)}{180} (0.05)^4 y^{(4)}(\xi) = -\frac{(0.3)}{180} (0.05)^4 \left(-\frac{15}{16} x^{-7/2}\right)$$

$$= 9.0 \times 10^{-9}$$

Definitely, the Simpson's $\frac{1}{3}$ – rule is more accurate than the Trapezoidal rule.

3.3 Result by Computer Output

The above problem is coded in basic language and the result is easily obtained on a digital computer as given below:

The learner is encouraged to try to code this also as given below and run the program to verify the result below. The program is written and coded to solve the example above using the Trapezoidal rule, Simpson's 1/3 rule and the Simpson's 3/8 rule. The program and the output are given next:

```

CLS
OPEN "SIMP1b.BAS" FOR OUTPUT AS #1
M = 10

REDIM X(M + 2), YS(M + 2), YT(M + 2), AY(M + 2), EY(M + 2)
DEF FNF (X) = SQR(X)

DEF FNE (X) = (2 / 3) * X ^ (3 / 2)

X(0) = 1: H = .05

PRINT #1, TAB(11); "I"; TAB(31); "X(I)"; TAB(51); "Y(I)";

FOR N = 6 TO M
SUMTR = 0: SUMSP1 = 0: SUMSP3
= 0 FOR I = 1 TO N + 1
J = I - 1: Y(J) = FNF(X(J))
  'IF N <= 8 OR N = M THEN
  PRINT #1, TAB(10); J; TAB(30); X(J); TAB(50); Y(J);
  X(I) = X(J) + H:

  'IMPLEMENTATION OF THE
  RULES IF J = 0 OR J = N THEN
  TR = Y(J): SP1 = Y(J)
  ELSEIF J MOD 2 = 0 THEN SP1 = 2 * Y(J): TR = 2 * Y(J) ELSEIF J
  MOD 2 = 1 THEN SP1 = 4 * Y(J): TR = 2 * Y(J)
  END IF

  IF J = 0 OR J = N THEN

  SP3 = Y(J)
  ELSEIF J MOD 3 = 1 OR J MOD 3 = 2 THEN
  SP3 = 3 * Y(J)
  ELSEIF J MOD 3 = 0 THEN SP3 = 2 * Y(J)
  END IF

  SUMTR = SUMTR + TR: SUMSP1 = SUMSP1 + SP1: SUMSP3 = SUMSP3 + SP3
IF J = N THEN EX = FNE(X(J)) - FNE(X(0))
NEXT I

'PRINT #1, TAB(1); " I"; TAB(15); "X(I)";
'PRINT #1, TAB(30); "YT(I)"; TAB(45); "YS(I)"; TAB(60); "ET(I)"; TAB(75); ES(I)

INTTR = H * SUMTR / 2: ERTR = ABS(INTTR - EX)
INTSP1 = H * SUMSP1 / 3: ERSP1 = ABS(INTSP1 - EX)
INTSP3 = 3 * H * SUMSP3 / 8: ERSP3 = ABS(INTSP3 - EX)

```

```

PRINT #1, TAB(5); "TRAPEZOIDAL"; TAB(35); "SIMPSON 1/3"; TAB(55); "SIMPSON 3/8" PRINT
#1, TAB(5); INTTR; TAB(35); INTSP1; TAB(55); INTSP3
PRINT #1, TAB(1); "EX"; TAB(5); EX; TAB(35); EX; TAB(55); EX
PRINT #1, TAB(1); "ER"; TAB(5); ERTR; TAB(35); ERSP1; TAB(55); ERSP3

```

NEXT N

END

The result obtained after the program is imputed and ran is given next:

I	X(I)	Y(I)
0	1	1
1	1.05	1.024695
2	1.1	1.048809
3	1.15	1.07238
4	1.2	1.095445
5	1.25	1.118034
6	1.3	1.140175

	TRAPEZOIDAL	SIMPSON 1/3	SIMPSON 3/8
	.3214726	.3214853	.3214853
EX	.321485	.321485	.321485
ER	1.248717E-05	2.980232E-07	2.682209E-07

I	X(I)	Y(I)
0	1	1
1	1.05	1.024695
2	1.1	1.048809
3	1.15	1.07238
4	1.2	1.095445
5	1.25	1.118034
6	1.3	1.140175
7	1.35	1.161895

	TRAPEZOIDAL	SIMPSON 1/3	SIMPSON 3/8
	.3790243	.3598532	.3646492
EX	.3790384	.3790384	.3790384
ER	1.40667E-05	1.918522E-02	1.438922E-02

0	1	1
1	1.05	1.024695
2	1.1	1.048809
3	1.15	1.07238
4	1.2	1.095445
5	1.25	1.118034
6	1.3	1.140175
7	1.35	1.161895
8	1.4	1.183216

TRAPEZOIDAL	SIMPSON 1/3	SIMPSON 3/8
.4376521	.4376682	.4304055
EX .4376678	.4376678	.4376678
ER 1.567602	3.874302E-07	7.26226E-03

0	1	1
1	1.05	1.024695
2	1.1	1.048809
3	1.15	1.07238
4	1.2	1.095445
5	1.25	1.118034
6	1.3	1.140175
7	1.35	1.161895
8	1.4	1.183216
9	1.45	1.204159

TRAPEZOIDAL	SIMPSON 1/3	SIMPSON 3/8
.4973365	.4774578	.4973541
EX .4973536	.4973536	.4973536
ER 1.713634E-05	1.989585E-02	4.768372E-07

0	1	1
1	1.05	1.024695
2	1.1	1.048809
3	1.15	1.07238
4	1.2	1.095445
5	1.25	1.118034
6	1.3	1.140175
7	1.35	1.161895
8	1.4	1.183216
9	1.45	1.204159
10	1.5	1.224745

	TRAPEZOIDAL	SIMPSON 1/3	SIMPSON 3/8
	.5580591	.5580781	.542896
EX	.5580776	.5580776	.5580776
ER	1.853704E-05	4.172325E-07	.0151816

Source: Computational Mathematics by Okunuga & Akanbi

Example 2

Evaluate $\int_1^3 \frac{1}{x+1} dx$ using the Simpson's one-third rule with $h = \frac{1}{4}$, working with four floating point arithmetic

x	1	1.25	1.5	1.75	2	2.25	2.5	2.75	3.0
y	0.5	0.4444	0.4000	0.3636	0.3333	0.3077	0.2857	0.2666	0.25
	y ₀	y ₁	y ₂	y ₃	y ₄	y ₅	y ₆	y ₇	y ₈

We observe that $n=8$, which is even. Hence the Simpson's 1/3 rule is applicable. The appropriate formula again from equation (3.4) is written as

$$\int_1^3 \frac{1}{x+1} dx = \frac{1}{3}h(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + 4y_5 + 2y_6 + 4y_7 + y_8)$$

$$\int_1^3 \frac{1}{x+1} dx = \frac{1}{3} \times (0.25) \times \left[0.5 + 4(0.4444) + 2(0.4) + 4(0.3636) + 2(0.3333) \right. \\ \left. + 4(0.3077) + 2(0.2857) + 4(0.2666) + 0.25 \right] \\ = 0.6931$$

Analytical solution is $\int_1^3 \frac{1}{x+1} dx = \ln(x+1) \Big|_1^3 = \ln 4 - \ln 2 = 0.693147 \cong 0.6931$

The two results agreed. So up to 4 decimal places the numerical result is as accurate as the exact solution.

4.0 CONCLUSION

From the above discussion with two examples well discussed, it can be deduce that the Simpson 1/3 rule will only be applicable when n is even. The Simpson's 1/3 rule is equally seen to be well accurate with very small error when compared to the analytical solution obtained from direct integration. The learner is encouraged to resolve all the example given so far and do the calculation to ascertain the values given in this study.

5.0 SUMMARY

In this Unit you have learnt

- (i) how to derive the Simpson's $\frac{1}{3}$ - rule using the Newton Forward formula
- (ii) how to implement the Simpson's $\frac{1}{3}$ - rule to evaluate definite integrals
- (iii) that the number of ordinates must be odd before the rule can be applicable,
- (iv) that the error can be estimated by comparing with the analytical solution
- (v) that the truncation error of the rule can be equally estimated

6.0 TUTOR MARKED ASSIGNMENT

1. Evaluate $\int_2^5 \frac{2}{x-1} dx$ with $h = \frac{1}{2}$, correct to 5 decimal places using Simpson's $\frac{1}{3}$ - rule
2. Integrate $\left(x + \frac{1}{x}\right)^2$ between 3 and 7 using Simpson's $\frac{1}{3}$ - rule with 9 ordinates

7.0 FURTHER READING AND OTHER RESOURCES

Atkinson K. E. (1978): An Introduction to Numerical Analysis, 2nd Edition, John Wiley & Sons, N. Y

Conte S. D. and Boor de Carl *Elementary Numerical Analysis an Algorithmic Approach* 2nd ed. McGraw-Hill Tokyo.

Francis Scheid. (1989) *Schaum's Outlines Numerical Analysis* 2nd ed. McGraw-Hill New York.

Kandassamy P., Thilagarathy K., & Gunevathi K. (1997): Numerical Methods, S. Chand & Co Ltd, New Delhi, India

Okunuga, S. A., and Akanbi M, A., (2004). Computational Mathematics, First Course, WIM Pub. Lagos, Nigeria.

UNIT 4 NEWTON-COTES FORMULAS

CONTENTS

- 1.0 Introduction
- 2.0 Objective
- 3.0 Simpson $\frac{3}{8}$ Rule
 - 3.1 The Form of Newton Cotes Formula
- 4.0 Conclusion
- 5.0 Summary
- 6.0 Tutor Marked Assignment
- 7.0 Further Reading and other Resources

1.0 INTRODUCTION

Apart from Trapezoidal rule and Simpson $\frac{1}{3}$ rule, we also have the Simpson $\frac{3}{8}$ rule. Beyond this we have other formulas based on the same Newton Forward Formula (NFF) with higher n . For example we recall that Trapezoidal rule use interval $[x_0, x_1]$, Simpson $\frac{1}{3}$ rule use $[x_0, x_2]$, and Simpson $\frac{3}{8}$ rule will use $[x_0, x_3]$ to obtain a one-phase of its formula. The formulas that use $[x_0, x_n]$, where n is greater than 3, are called Newton-Cotes formula. Invariably, Newton–Cotes formula generalizes all the rules including the ones earlier discussed. We shall in this unit consider the remaining formulas for approximating definite integrals.

2.0 OBJECTIVE

At the end of this unit you should be able to

- derive the Simpson $\frac{3}{8}$ rule;
- distinguish between the Newton – Cotes formulas;
- differentiate between Simpson’s rule and Trapezoidal rule;
- recognize where Simpson rule is applicable in terms of number of node points; and
- solve problems using the Simpson’s $\frac{1}{3}$ rule.

3.0 SIMPSON $\frac{3}{8}$ RULE

The Simpson $\frac{3}{8}$ formula follows from the Simpson $\frac{1}{3}$ rule. The complete derivation will not be given in this unit, but a sketch of it. However the technique is virtually the same as the ones earlier proved, since the derivation is from the same Newton Forward Formula. The learner is advised to verify some of the formulas stated in this Unit.

Suppose the Newton Forward Formula (NFF) is truncated after the fourth term or after the third forward difference (that is for $n = 3$) and integration is carried out within $[x_0, x_3]$, we can write

$$\int_{x_0}^{x_3} P(x) dx = \int_{x_0}^{x_3} \left(y_0 + k\Delta y_0 + \frac{k(k-1)}{2} \Delta^2 y_0 + \frac{k(k-1)(k-2)}{3!} \Delta^3 y_0 \right) dx \quad (3.1)$$

Changing the variables from x to k and integrating, we shall obtain

$$\int_{x_0}^{x_3} P(x) dx = \frac{3}{8} h (y_0 + 3y_1 + 3y_2 + y_3) \quad (3.2)$$

This is known as a one-phase of the Simpson $\frac{3}{8}$ – rule.

When quadrature principle is applied, we obtain the Simpson $\frac{3}{8}$ – rule finally as

$$\int_{x_0}^{x_n} P(x) dx = \frac{3}{8} h (y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \dots + 3y_{n-2} + 3y_{n-1} + y_n) \quad (3.3)$$

The coefficients are also systematic. The inner coefficients are 3, 3, 2, while the first and last term have 1 as the coefficient. The number of ordinates can only be 4, 7, 10, and so on. When we have 4 ordinates we have the formula

$$\int_{x_0}^{x_3} P(x) dx = \frac{3}{8} h (y_0 + 3y_1 + 3y_2 + y_3) \quad (3.4)$$

For 7 ordinates we have

$$\int_{x_0}^{x_6} P(x) dx = \frac{3}{8} h (y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + y_6) \quad (3.5)$$

And for 10 ordinates we have

$$\int_{x_0}^{x_9} P(x) dx = \frac{3}{8} h (y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + 3y_7 + 3y_8 + y_9) \quad (3.6)$$

The implementation is exactly the same as we have demonstrated with Simpson $\frac{3}{8}$ rule.

3.1 The Form of Newton Cotes Formula

Now as n increases, the number of terms to be included in the NFF will equally increase and the set of formulas that will be obtained are termed as Newton-Cotes (N-C) formula.

We can generally represent the integration value of the NFF within a general interval $[x_0, x_n]$ as

$$\int_{x_0}^{x_n} P(x) dx = Ch (c_0 y_0 + c_1 y_1 + \dots + c_n y_n) \quad (3.7)$$

Equation (3.7) provides only one phase of the formula and by quadrature; we can generalize to obtain any of these formulae.

Thus, the table of values of coefficients $c_r, r = 0, 1, 2, \dots, n$ in equation (3.7) is given below:

Rule	n	F	c ₀	c ₁	c ₂	c ₃	c ₄	c ₅	c ₆
Trapezoidal	1	1/2	1	1					
Simpson 1/3	2	1/3	1	4	1				
Simpson 3/8	3	3/8	1	3	3	1			
N-C of n = 4	4	2/45	7	32	13	32	7		
N-C of n = 6	6	1/140	41	216	27	272	27	216	41

F in the table represents the factor of the formula, while $c_r, r = 0, 1, 2, \dots, n$ are the coefficients

Equation (3.7) provides a general quadrature formula due to Newton and Cotes and it embraces all class of formulas, which follows the NFF in a given interval. Hence, such quadrature formulas that have the form of equation (3.7) are called Newton-Cotes formula.

For example Newton Cotes formula for $n = 4$ from the above table can be written for 5 ordinates as

$$\int_{x_0}^{x_4} P(x) dx = \frac{2}{45} h (7y_0 + 32y_1 + 13y_2 + 32y_3 + 7y_4) \quad (3.8)$$

Each of the Newton Cotes formula is completely written or obtained by implementing quadrature technique on one-phase of the scheme. For example equation (3.4) is one phase of the Simpson 3/8 rule. By quadrature equation (3.5) gives 2 phase of the scheme and so on. Equation (3.8) is also one-phase of the Newton Cotes formula ($n = 4$) and by quadrature technique we can get the two-phase as

$$\int_{x_0}^{x_4} P(x) dx = \frac{2}{45} h (7y_0 + 32y_1 + 13y_2 + 32y_3 + 14y_4 + 32y_5 + 13y_6 + 32y_7 + 7y_8)$$

Similar procedure is applicable to other Newton-Cotes formula.

Self Assessment Test

Write from the table the next possible Newton-Cotes formula for $n = 4$

4.0 CONCLUSION

We have seen that there are several other formulas that can be used for approximate integration. The simplest of them is the Trapezoidal rule without any restriction on the number of ordinates. The other formulas or rules however have some restriction on the number of ordinates that must be prescribed before each of them could be used.

5.0 SUMMARY

Remember that in this Unit you have learnt

- (i) how to derive the Simpson's 3/8- rule using the Newton Forward formula
- (ii) the structure of the Newton-Cotes formulas
- (iii) that the implementation of any of the Newton Cotes formulas is similar to Simpson's $\frac{1}{3}$ - rule for evaluating definite integrals
- (iv) that the number of ordinates is important before a particular rule can be applied,
- (v) that the formulas are obtained by quadraturing the one-phase of the formula.

6.0 TUTOR MARKED ASSIGNMENT

1. Evaluate $\int_2^5 \frac{2}{x-1} dx$ with $h = \frac{1}{2}$, correct to 5 decimal places using Simpson 3/8- rule. Compare

your result with the analytical solution

2. Integrate $\sqrt{x+1}$ between 3 and 7, correct to 5 decimal places, using
 - (i) Simpson's 3/8- rule with 7 ordinates
 - (ii) Newton Cotes formula ($n=4$) with 9 ordinates

Compare your result with the analytical solution and deduce which of the two is more accurate

- 3 Evaluate $\int_1^5 \log_e x dx$ correct to 6 decimal places with 9 ordinates

- Use
- (i) Trapezoidal rule
 - (ii) Simpson 1/3-rule
 - (iii) Newton Cotes formula ($n=4$)

For evaluation. Obtain the actual error, which of these is most accurate?

- Simpson's 3/8- rule with 7 ordinates
- Newton Cotes formula ($n=4$) with 9 ordinates

7.0 FURTHER READING AND OTHER RESOURCES

Atkinson K. E. (1978): *An Introduction to Numerical Analysis*, 2nd Edition, John Wiley & Sons, N. Y

Conte S. D. & Boor de Carl *Elementary Numerical Analysis an Algorithmic Approach* 2nd ed. McGraw-Hill Tokyo.

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