

MODULE 6

NUMERICAL INTEGRATION

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6.1 Introduction

This module discusses the mathematical problem of evaluating a definite integral of the form $\int_a^b f(x)dx$. We point out the special features that distinguish the family of Newton-Cotes methods from other numerical integration methods. We use a geometrical approach to derive the Trapezoidal (Trapezium) rule and Simpson's rule.

The need for numerical integration methods is firmly established by the following two examples.

- (i) The definite integral $\int_0^1 e^{x^2} dx$ is perfectly defined but the anti-derivative of the integrand $f(x) = e^{x^2}$ cannot be expressed using known mathematical functions, and therefore the value of definite integral cannot be evaluated analytically. We are therefore forced by circumstances to resort to using a numerical method.

- (ii) The definite integral $\int_1^2 \frac{dx}{8-x^3}$ can be evaluated analytically. What we need is to find the anti-derivative $F(x)$ of the integrand $f(x) = \frac{1}{8-x^3}$.

After investing a lot of time and efforts one finds the complicated expression

$$F(x) = \frac{\sqrt{3}}{12} \tan^{-1}\left(\frac{x+1}{\sqrt{3}}\right) + \frac{1}{24} \ln\left(\frac{x^2 + 2x + 4}{x^2 - 4x - 4}\right) + C$$

where C is an arbitrary constant of integration. This complicated result makes the evaluation of the definite integral $\int_1^2 \frac{dx}{8-x^3}$ almost impossible to carry out with any meaningful degree of accuracy. Again in this case we are forced to go numerical.

6.2 Objectives

On completion of this module the learner will be able to:

- Give sound mathematical reasons why numerical integration methods are needed
- Write down the general format of all numerical methods
- State the characteristic features of the Newton-Cotes family of numerical integration methods
- Explain why the Trapezium rule and Simpson's rule are Newton-Cotes methods
- Give a geometrical derivation and apply the Trapezium Rule
- Give a geometrical derivation and apply Simpson's rule

6.3 General Format of Numerical Integration Formulas

Numerical methods for approximating the definite integral $\int_a^b f(x)dx$ have the general form

$$\int_a^b f(x)dx \cong \sum_{k=0}^n W_k f(x_k) = W_0 f(x_0) + W_1 f(x_1) + \dots + W_n f(x_n).$$

The coefficients W_k are called **weighting coefficients** and x_k are the abscissas or **nodes** taken from the range $[a,b]$ of integration at which the integrand is to be evaluated.

6.4 Newton-Cotes Formulas

The numerical integration methods known as Newton-Cotes type of methods are derived from the general formula by:

- (i) Requiring that the nodes x_k be chosen at equal distance over the range of integration $[a,b]$ such that $x_k = x_0 + kh$, $k = 0,1,2,\dots,n$, where $x_0 = a$, $x_n = b$ and $h = \frac{b-a}{n}$.
- (ii) Determining the $n+1$ weights W_k in such a way that the resulting formula gives the exact value of the integral for all polynomial functions $f(x) = p_k(x)$, $k = 0,1,2,\dots,n$

The Trapezoidal rule and Simpson's rule fall in this category of methods.

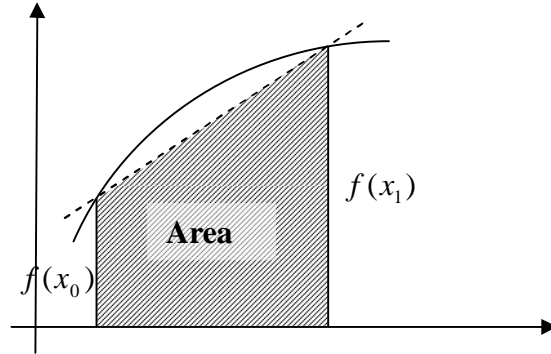
6.5 Derivation and Application of the Trapezium Rule

Leading questions:

- What kind of a geometrical figure is a trapezium?
- What sides of a trapezium determine its area?
- How is the area of a trapezium determined?

The Trapezoidal rule (also referred as Trapezium rule) is **the simplest of all numerical integration method**.

The method 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.



What has been done is to approximate the area A under the curve $y = f(x)$ between the ordinates at x_0 and x_1 by $A \cong \frac{h}{2}(f_0 + f_1)$, where $f_0 = f(x_0)$, $f_1 = f(x_1)$ and h is the distance between x_0 and x_1 .

For the integral $\int_a^b f(x)dx$ the trapezoidal rule can now be applied by subdividing the interval $[a, b]$ into n subintervals

$$[x_0, x_1], [x_1, x_2], [x_2, x_3], \dots, [x_{n-2}, x_{n-1}], [x_{n-1}, x_n]$$

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**

$$\begin{aligned} A = \int_a^b f(x)dx &\cong \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \frac{h}{2}(f_2 + f_3) + \dots + \frac{h}{2}(f_{n-1} + f_n) \\ &\cong \frac{h}{2}[f_0 + 2(f_1 + f_2 + f_3 + \dots + f_{n-1}) + f_n] \\ &\cong \frac{h}{2}\left[(f_0 + f_n) + 2\sum_{k=1}^{n-1} f_k\right] \end{aligned}$$

Observation

In this generalized Trapezoidal Rule, the nodes are chosen to be the equidistant points $x_k = x_0 + (k - 1)h$, $k = 1, 2, 3, \dots, n$ while the weighting coefficients W_k have been determined such that the formula gives exact value of the integral for all linear functions of the form $y = f(x) = ax + b$. These turn out to be:

$$W_0 = W_n = \frac{h}{2}; \quad W_1 = W_2 = W_3 = \dots = W_{n-1} = h.$$

Worked Example

Let us approximate the definite integral $\int_1^2 \frac{dx}{x}$ by the Trapezoidal Rule with $n = 10$

Solution

In this example the integrand is $f(x) = \frac{1}{x}$ and $h = 0.1$

We evaluate the function at the points $x_i = 1 + (i - 1)0.1$, $i = 1, 2, 3, \dots, 10$ and obtain the following table of pairs of values:

Value of the function $f(x) = \frac{1}{x}$

x	$f(x)$	x	$f(x)$
1.0	1.0	1.6	0.625
1.1	0.9091	1.7	0.5882
1.2	0.8333	1.8	0.5556
1.3	0.7692	1.9	0.5263
1.4	0.7143	2.0	0.5
1.5	0.6667		

Application of the generalized trapezoidal rule gives the approximate value $\int_1^2 \frac{dx}{x} \cong \frac{0.1}{2} [1.0 + 2(6.1877) + 0.5] = 0.69377$.

6.6 Derivation and Application of Simpson's Rule

Simpson's Rule is derived with a view to make it give exact values of the definite integral $\int_a^b f(x)dx$ for all quadratic functions $f(x) = ax^2 + bx + c$.

In its simplest form we subdivide the interval $[a,b]$ into two equal subintervals using the points x_0, x_1, x_2 , where $x_0 = a$, $x_2 = b$ and $x_1 = \frac{1}{2}(a+b)$, and replace the curve of the general function $y = f(x)$ over the interval $[x_0, x_2]$ by the quadratic interpolation polynomial

$$y = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f_0 + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f_1 + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f_2$$

$$= \frac{1}{h^2} \left[\frac{1}{2}(x-x_1)(x-x_2)f_0 - (x-x_0)(x-x_2)f_1 + \frac{1}{2}(x-x_0)(x-x_1)f_2 \right]$$

The definite integral $\int_{x_0}^{x_2} f(x)dx$ is then approximated by the integral $\int_{x_0}^{x_2} ydx$.

Without loss of generality, one takes $x_0 = 0$, $x_1 = h$, $x_2 = 2h$ and ultimately

arrives at the formula
$$\int_{x_0}^{x_2} ydx = \frac{h}{3}[f_0 + 4f_1 + f_2]$$

Because the formula uses values at three points (two equal intervals), a generalized Simpson's Rule is only possible when **the number of subintervals is even:**

$$[x_0, x_2], [x_2, x_4], [x_4, x_6], \dots, [x_{2n-2}, x_{2n}].$$

One applies the formula over each subinterval and adds the results to get the **generalized Simpson's Rule formula**

$$\int_a^b f(x)dx = \frac{h}{3}[f_0 + 4f_1 + f_2] + [f_2 + 4f_3 + f_4] + \dots + [f_{2n-2} + 4f_{2n-1} + f_{2n}]$$

$$= \frac{h}{3}[(f_0 + f_{2n}) + 4(f_1 + f_3 + \dots + f_{2n-1}) + 2(f_2 + f_4 + \dots + f_{2n-2})]$$

$$= \frac{h}{3} \left[(f_0 + f_n) + 4 \sum_{k=1}^n f_{2k-1} + 2 \sum_{k=1}^{n-1} f_{2k} \right]$$

Worked Example

Approximate $\int_1^2 \frac{dx}{x}$ using Simpson's rule using an interval of length $h = 0.1$

Solution

This is the same problem solved above using the Trapezoidal Rule. We certainly can apply Simpson's Rule because the number of subintervals is even ($n = 10$). Using the values given in the Table 3.1 one obtains

$$\int_1^2 \frac{dx}{x} \cong \frac{0.1}{3} [1.0 + 4(3.4595) + 2(2.7282) + 0.5] = 0.693147 .$$

Open Questions

- (i) What is the exact value of the integral $\int_1^2 \frac{dx}{x}$?
- (ii) Which of the two numerical methods, **Trapezium rule** and **Simpson's rule**, is more accurate?
- (iii) How does the accuracy of the result obtained using these two numerical methods affected by taking a smaller interval h (increasing the number of subintervals / refining the partitioning of the range of integration)?

6.7 Summary

The learner is now equipped with some powerful and reliable tools for approximating the definite integral of any functions which can easily be evaluated. The trapezium rule is simpler to apply but also less accurate than Simpson's rule for the same interval length. Simpson's rule is more accurate, but at a cost. One has to evaluate the function at more nodal points and the number of subintervals must be even!