Numerical Methods of Integration

Submitted By

Richa Sharma

Department of Physics & Astrophysics

University of Delhi

Numerical Integration :

In numerical analysis, **numerical integration** constitutes a broad family of algorithms for calculating the numerical value of a definite integral, and by extension, the term is also sometimes used to describe the numerical solution of differential equations. This article focuses on calculation of definite integrals. Numerical integration over more than one dimension is sometimes described as **cubature**,[1] although the meaning of *quadrature* is understood for higher dimensional integration as well.

The basic problem considered by numerical integration is to compute an approximate solution to a definite integral:

$$\int_a^b f(x)\,dx.$$

If *f(x)* is a smooth well-behaved function, integrated over a small number of dimensions and the limits of integration are bounded, there are many methods of approximating the integral with arbitrary precision.

There are several reasons for carrying out numerical integration. The integrand *f(x)* may be known only at certain points, such as obtained by sampling. Some embedded systems and other computer applications may need numerical integration for this reason.

A formula for the integrand may be known, but it may be difficult or impossible to find an antiderivative which is an elementary function. An example of such an integrand is $f(x) = \exp(-x^2)$, the antiderivative of which (the error function, times a constant) cannot be written in elementary form.

What is integration?

Integration is the process of measuring the area under a function plotted on a graph. Why would we want to integrate a function? Among the most common examples are finding the velocity of a body from an acceleration function, and displacement of a body from a velocity function. Throughout many engineering fields, there are countless applications for integral calculus. Sometimes, the evaluation of expressions involving these integrals can become daunting, if not indeterminate. For this reason, a wide variety of numerical methods has been developed to simplify the integral.

We will discuss the trapezoidal rule of approximating integrals of the form

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

where

$f(x)$ is called the integrand,

$a =$ lower limit of integration

$b =$ upper limit of integration

- The methods that are based on equally spaced data points: these **are Newton-cotes formulas**: the mid-point rule, the trapezoid rule and simpson rule.
- The methods that are based on data points which are not equally spaced:these are Gaussian quadrature formulas.

In numerical analysis, the **Newton–Cotes formulae**, also called the **Newton–Cotes quadrature rules** or simply **Newton–Cotes rules**, are a group of formulae for numerical integration (also called *quadrature*) based on evaluating the integrand at equally-spaced points.

Newton–Cotes formulae can be useful if the value of the integrand at equally-spaced points is given. If it is possible to change the points at which the integrand is evaluated, then other methods such as Gaussian quadratureand Clenshaw–Curtis quadrature are probably more suitable.

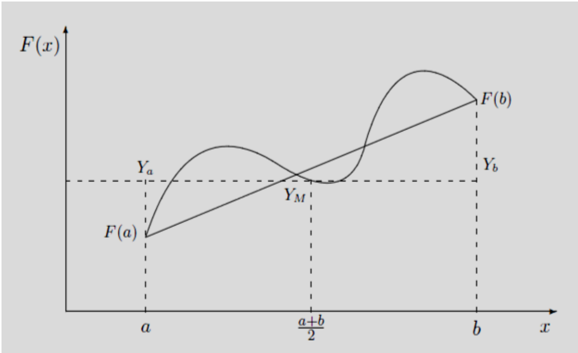
<u>Types of Newton–Cotes formulas</u>

- Mid-Point rule
- Trapezoidal Rule
- Simpson Rule

<u>Mid-point Rule:</u>

compute the area of the rectangle formed by the four points *(a,0),(0,b),(a,f(a+b)/2)) and (b,f(a+b)/2))* such that such that the approximate integral is given by

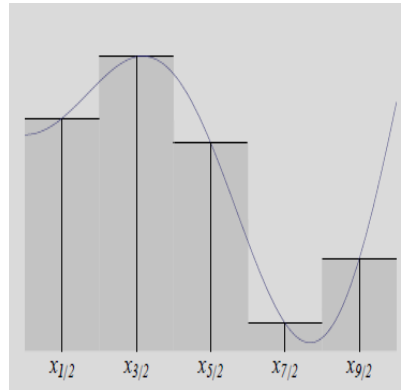
$$\int_a^b F(x)\mathrm{d}x = (b-a)F\left(\frac{a+b}{2}\right)$$



this rule does not make any use of the end points.

Composite Mid-point Rule:

- the interval [a ,b] can be break into smaller intervals and compute the approximation on each sub interval.
- Sub-intervals of size h = $(b-a)/n,$
-
- $$x_i = a + \left(i - \tfrac{1}{2}\right) h \text{ with } i = 1, \ldots, n.$$
-



$$\int_a^b F(x)\mathrm{d}x = h\sum_{i=1}^{n} f(x_i)$$

Error in Mid-point Rule

$$\int_a^b f(x)\,dx - f\left(a_{1/2}\right)(b-a), \quad a_{1/2} = (a+b)/2.$$

expanding both f (x) and f (a_1/2) about the the left endpoint a, and then integrating the taylor expansion

$$\frac{7M}{24}(b-a)^3,$$

$$\text{where } M = \left|f''(x)\right|$$

If we reduce the size of the interval to half its width, the error in the mid-point method will be reduced by a factor of 8.

Trapezoidal Rule :

The trapezoidal rule is based on the Newton-Cotes formula that if one approximates the integrand by an n^{th} order polynomial, then the integral of the function is approximated by the integral of that n^{th} order polynomial. Integrating polynomials is simple.

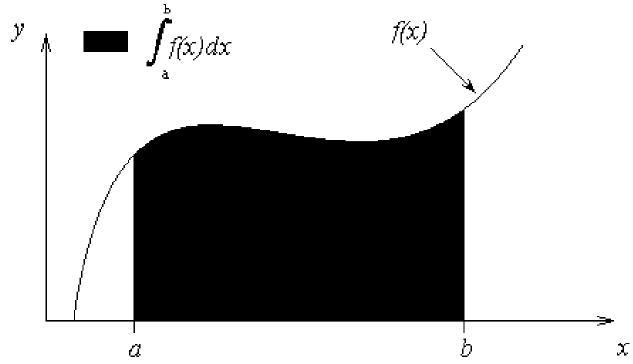


Figure 1 Integration of a function

So if we want to approximate the integral

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

to find the value of the above integral, one assumes

$$f(x) \approx f_n(x)$$

Where,

$$f_n(x) = a_0 + a_1 x + \ldots + a_{n-1}x^{n-1} + a_n x^n .$$

where $f_n(x)$ is a n^{th} order polynomial. The trapezoidal rule assumes $n = 1$, that is, approximating the integral by a linear polynomial (straight line),

$$\int_a^b f(x)dx \approx \int_a^b f_1(x)dx$$

<u>Derivation of the Trapezoidal Rule:</u>

<u>Method 1: Derived from Calculus:</u>

$$\int_a^b f(x)dx \approx \int_a^b f_1(x)dx$$

$$= \int_a^b (a_0 + a_1 x)dx$$

$$= a_0(b-a) + a_1\left(\frac{b^2 - a^2}{2}\right) \quad (1)$$

Now choose, $(a, f(a))$ and $(b, f(b))$ as the two points to approximate $f(x)$ by a straight line from a to b,

$$f(a) = f_1(a) = a_0 + a_1 a$$

$$f(b) = f_1(b) = a_0 + a_1 b$$

Solving the above two equations for a_1 and a_0,

$$a_1 = \frac{f(b) - f(a)}{b-a}$$

$$a_0 = \frac{f(a)b - f(b)a}{b-a}$$

Hence from Equation (1),

$$\int_a^b f(x)dx \approx \frac{f(a)b - f(b)a}{b-a}(b-a) + \frac{f(b)-f(a)}{b-a}\frac{b^2-a^2}{2}$$

$$= (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

Method 2: Derived from Geometry:

The trapezoidal rule can also be derived from geometry. Consider Figure 2. The area under the curve $f_1(x)$ is the area of a trapezoid. The integral

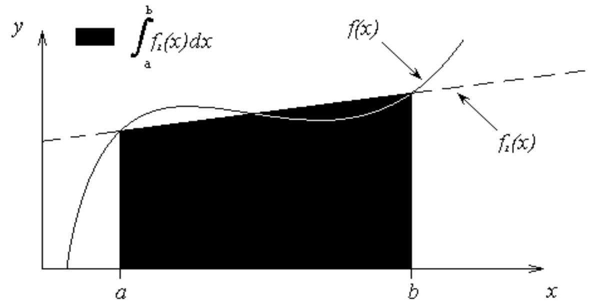


Figure 2 Geometric representation of trapezoidal rule.

$$\int_a^b f(x)dx \approx \text{Area of trapezoid}$$

$$= \frac{1}{2}(\text{Sum of length of parallel sides})*(\text{Perpendicular distance between parallel sides})$$

$$= \frac{1}{2}\left(f(b) + f(a)\right)(b-a)$$

$$= (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

Composite Trapezoidal Rule:

Extending this procedure we now divide the interval of integration $[a,b]$ into n equal segments and then applying the trapezoidal rule over each segment, the sum of the results obtained for each segment is the approximate value of the integral.

Divide $(b-a)$ into n equal segments as shown in Figure 4. Then the width of each segment is

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

The integral I can be broken into h integrals as

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

$$= \int_a^{a+h} f(x)dx + \int_{a+h}^{a+2h} f(x)dx + \ldots + \int_{a+(n-2)h}^{a+(n-1)h} f(x)dx + \int_{a+(n-1)h}^{b} f(x)dx \qquad (2)$$

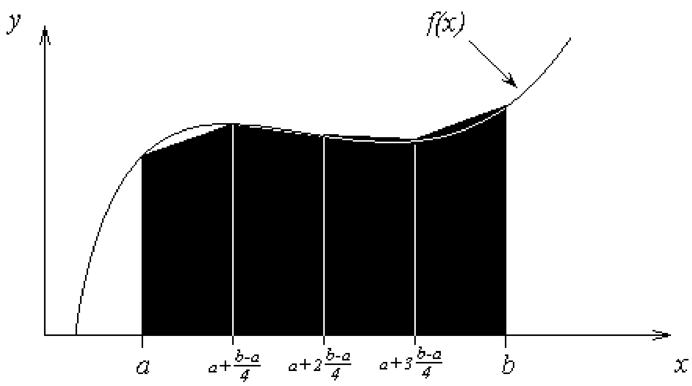


Figure 4 Multiple ($n = 4$) segment trapezoidal rule

Applying trapezoidal rule Equation (2) on each segment gives

$$\int_a^b f(x)dx = [(a+h) - a]\left[\frac{f(a) + f(a+h)}{2}\right]$$

$$+ [(a+2h) - (a+h)]\left[\frac{f(a+h) + f(a+2h)}{2}\right]$$

$$+ \ldots\ldots\ldots\ldots\ldots + [\{a+(n-1)h\} - \{a+(n-2)h\}]\left[\frac{f(a+(n-2)h) + f(a+(n-1)h)}{2}\right]$$

$$+ [b - \{a+(n-1)h\}]\left[\frac{f(a+(n-1)h) + f(b)}{2}\right]$$

$$= h\left[\frac{f(a) + f(a+h)}{2}\right] + h\left[\frac{f(a+h) + f(a+2h)}{2}\right] + \ldots\ldots\ldots\ldots\ldots$$

$$+h\left[\frac{f(a+(n-2)h)+f(a+(n-1)h)}{2}\right]+h\left[\frac{f(a+(n-1)h)+f(b)}{2}\right]$$

$$=h\left[\frac{f(a)+2f(a+h)+2f(a+2h)+\ldots+2f(a+(n-1)h)+f(b)}{2}\right]$$

$$=\frac{h}{2}\left[f(a)+2\left\{\sum_{i=1}^{n-1}f(a+ih)\right\}+f(b)\right]$$

$$=\frac{b-a}{2n}\left[f(a)+2\left\{\sum_{i=1}^{n-1}f(a+ih)\right\}+f(b)\right]$$

Error in Multiple-segment Trapezoidal Rule:

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

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

Where ζ is some point in $[a,b]$.

What is the error then in the multiple-segment trapezoidal rule? It will be simply the sum of the errors from each segment, where the error in each segment is that of the single segment trapezoidal rule. The error in each segment is

$$E_1=-\frac{[(a+h)-a]^3}{12}f''(\zeta_1),\quad a<\zeta_1<a+h$$

$$=-\frac{h^3}{12}f''(\zeta_1)$$

$$E_2=-\frac{[(a+2h)-(a+h)]^3}{12}f''(\zeta_2),\quad a+h<\zeta_2<a+2h$$

$$=-\frac{h^3}{12}f''(\zeta_2)$$

.

.

.

$$E_i = -\frac{\left[(a+ih)-(a+(i-1)h)\right]^3}{12} f''(\zeta_i), \quad a+(i-1)h < \zeta_i < a+ih$$

$$= -\frac{h^3}{12} f''(\zeta_i)$$

.

.

.

$$E_{n-1} = -\frac{\left[\{a+(n-1)h\}-\{a+(n-2)h\}\right]^3}{12} f''(\zeta_{n-1}), \quad a+(n-2)h < \zeta_{n-1} < a+(n-1)h$$

$$= -\frac{h^3}{12} f''(\zeta_{n-1})$$

$$E_n = -\frac{\left[b-\{a+(n-1)h\}\right]^3}{12} f''(\zeta_n), \quad a+(n-1)h < \zeta_n < b$$

$$= -\frac{h^3}{12} f''(\zeta_n)$$

Hence the total error in the multiple-segment trapezoidal rule is

$$E_t = \sum_{i=1}^{n} E_i$$

$$= -\frac{h^3}{12} \sum_{i=1}^{n} f''(\zeta_i)$$

$$= -\frac{(b-a)^3}{12n^3} \sum_{i=1}^{n} f''(\zeta_i)$$

$$= -\frac{(b-a)^3}{12n^2} \frac{\sum_{i=1}^{n} f''(\zeta_i)}{n}$$

The term $\frac{\sum_{i=1}^{n} f''(\zeta_i)}{n}$ is an approximate average value of the second derivative $f''(x), a < x < b$.

Hence

$$E_t = -\frac{(b-a)^3}{12n^2} \frac{\sum_{i=1}^{n} f''(\zeta_i)}{n}$$

- The methods we presented so far were defined over finite domains, but it will be often the case that we will be dealing with problems in which the domain of integration is infinite.
- We will now investigate how we can transform the problem to be able to use standard methods to compute the integrals.

Gauss Quadrature

- Gaussian Quadrature & Optimal Nodes
- Using Legendre Polynomials to Derive Gaussian Quadrature Formulae
- Gaussian Quadrature on Arbitrary Intervals

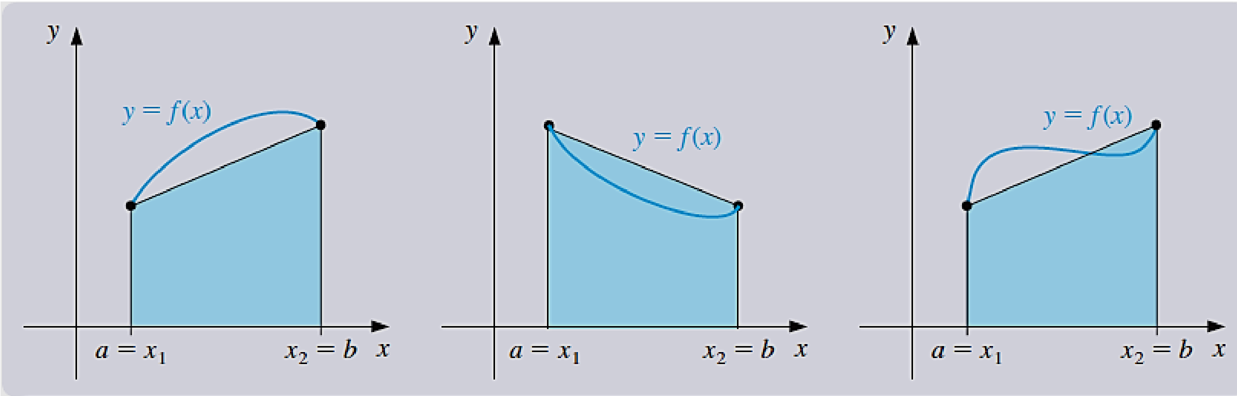
Gaussian Quadrature: Contrast with Newton-Cotes

- The Newton-Cotes formulas were derived by integrating interpolating polynomials.
- The error term in the interpolating polynomial of degree n involves the $(n + 1)$st derivative of the function being approximated, . . .
- so a Newton-Cotes formula is exact when approximating the integral of any polynomial of degree less than or equal to n.
- All the Newton-Cotes formulas use values of the function at equally-spaced points.
- This restriction is convenient when the formulas are combined to form the composite rules which we considered earlier, . . .

But in Gaussian Quadrature

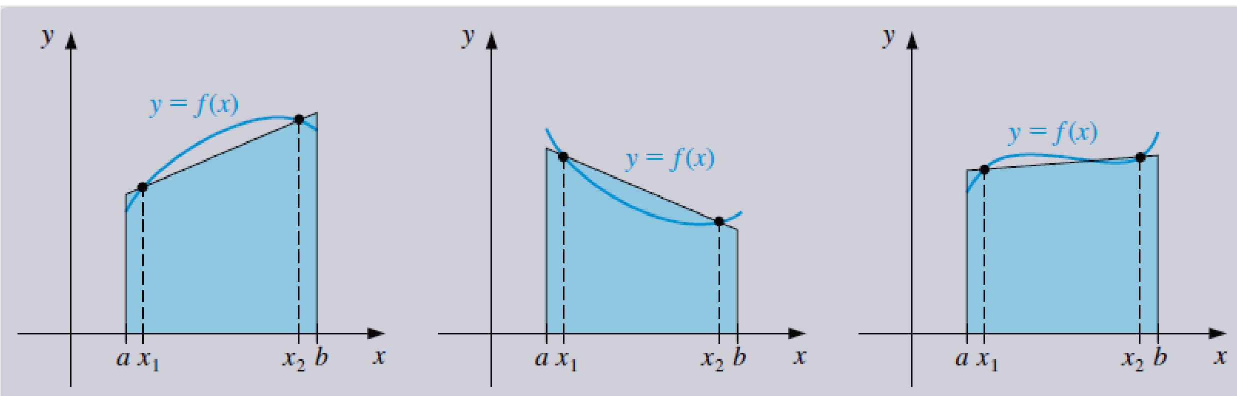
- we may find sets of weights and abscissas that make the formulas exact for integrands that are composed of some real function multiplied by a polynomial
- gives us a huge advantage in calculating integrals numerically.

Consider, for example, the Trapezoidal rule applied to determine the integrals of the functions whose graphs are as shown.



It approximates the integral of the function by integrating the linear function that joins the endpoints of the graph of the function.

But this is not likely the best line for approximating the integral. Lines such as those shown below would likely give much better approximations in most cases.



Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally-spaced, way.

Gaussian Quadrature: Introduction

Choice of Integration Nodes :

- The nodes $x_1, x_2, \ldots, x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, \ldots, c_n$, are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i).$$

- assume that the best choice of these values produces the exact result for the largest class of polynomials, . . .
- The coefficients $c_1, c_2, \ldots, c_n$, in the approximation formula are arbitrary, and the nodes $x_1, x_2, \ldots, x_n$ are restricted only by the fact that they must lie in $[a, b]$, the interval of integration.
- This gives us $2n$ parameters to choose.
- The way that this is done is through viewing the integrand as being composed of some weighting function W(x) multiplied by some polynomial P(x) so that

$$f(x)=W(x)P(x)$$

- Instead of using simple polynomials to interpolate the function, quadrature use the set of polynomials that are orthogonal over the interval with weighting function W(x).
- With this choice of interpolating polynomial, we find that if we evaluate P(x) at the zeroes (x_i) of the interpolating polynomial of desired order, and multiply each evaluation by a weighting factor (w_i)
- we can obtain a result that is exact up to twice the order of the interpolating polynomial!
- Gaussian quadrature method based on the polynomials p_m as follows

Let $x_0, x_1, \ldots, x_n$ be the roots of p_{n+1}.

Let l_i the *ith* Lagrange interpolating polynomial for these roots, i.e. l_i is the unique polynomial of degree $\leq n$. Then

$$\int_a^b f(x)w(x)\,dx \approx \sum_{i=0}^{n} w_i f(x_i)$$

where the weights w_i are given by

$$w_i = \int_a^b \ell_i(x) w(x).$$

Gaussian Quadrature: Illustration ($n = 2$)

Example: Formula when $n = 2$ on $[-1, 1]$

Suppose we want to determine c_1, c_2, x_1, and x_2 so that the integration formula

$$\int_{-1}^{1} f(x)\, dx \approx c_1 f(x_1) + c_2 f(x_2)$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2(2) - 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3,$$

for some collection of constants, a_0, a_1, a_2, and a_3.

Because

$$\begin{aligned} & \int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\, dx \\ = \quad & a_0 \int 1\, dx + a_1 \int x\, dx + a_2 \int x^2\, dx + a_3 \int x^3\, dx \end{aligned}$$

this is equivalent to showing that the formula gives exact results when $f(x)$ is 1, x, x^2, and x^3.

Hence, we need c_1, c_2, x_1, and x_2, so that

$$\begin{aligned} c_1 \cdot 1 + c_2 \cdot 1 &= \int_{-1}^{1} 1 \, dx = 2 \\ c_1 \cdot x_1 + c_2 \cdot x_2 &= \int_{-1}^{1} x \, dx = 0 \\ c_1 \cdot x_1^2 + c_2 \cdot x_2^2 &= \int_{-1}^{1} x^2 \, dx = \frac{2}{3} \\ c_1 \cdot x_1^3 + c_2 \cdot x_2^3 &= \int_{-1}^{1} x^3 \, dx = 0 \end{aligned}$$

A little algebra shows that this system of equations has the unique solution

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3} \quad \text{and} \quad x_2 = \frac{\sqrt{3}}{3},$$

which gives the approximation formula

$$\int_{-1}^{1} f(x) \, dx \approx f\left(\frac{-\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

This formula has degree of precision 3, that is, it produces the exact result for every polynomial of degree 3 or less.

Using Legendre Polynomials to Derive Gaussian Quadrature Formulae:

An Alternative Method of Derivation

- We will consider an approach which generates more easily the nodes and coefficients for formulas that give exact results for higher-degree polynomials.
- This will be achieved using a particular set of orthogonal polynomials (functions with the property that a particular definite integral of the product of any two of them is 0).

- This set is the is the Legendre polynomials, a collection $\{P_0(x), P_1(x), \ldots, P_n(x), \ldots,\}$ with properties:
  (1) For each n, $P_n(x)$ is a monic polynomial of degree n.
  (2) $\int_{-1}^{1} P(x)P_n(x)\,dx = 0$ whenever $P(x)$ is a polynomial of degree less than n.

The first few Legendre Polynomials

$$P_0(x) = 1, \qquad P_1(x) = x, \qquad P_2(x) = x^2 - \frac{1}{3}$$

$$P_3(x) = x^3 - \frac{3}{5}x \qquad \text{and} \qquad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}$$

- The roots of these polynomials are distinct, lie in the interval $(-1, 1)$, have a symmetry with respect to the origin, and, most importantly,
- they are the correct choice for determining the parameters that give us the nodes and coefficients for our quadrature method

The nodes $x_1, x_2, \ldots, x_n$ needed to produce an integral approximation formula that gives exact results for any polynomial of degree less than $2n$ are the roots of the nth-degree Legendre polynomial.

Theorem

Suppose that $x_1, x_2, \ldots, x_n$ are the roots of the nth Legendre polynomial $P_n(x)$ and that for each $i = 1, 2, \ldots, n$, the numbers c_i are defined by

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x)\, dx = \sum_{i=1}^{n} c_i P(x_i)$$

Proof :

- Let us first consider the situation for a polynomial $P(x)$ of degree less than n.
- Re-write $P(x)$ in terms of $(n - 1)$st Lagrange coefficient polynomials with nodes at the roots of the nth Legendre polynomial $Pn(x)$.

Since $P(x)$ is of degree less than n, the nth derivative of $P(x)$ is 0, and this representation of is exact. So

Therefore

$$P(x) = \sum_{i=1}^{n} P(x_i) L_i(x) = \sum_{i=1}^{n} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i)$$

and

$$\int_{-1}^{1} P(x)\, dx = \int_{-1}^{1} \left[\sum_{i=1}^{n} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i) \right] dx$$

$$= \sum_{i=1}^{n} \left[\int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx \right] P(x_i) = \sum_{i=1}^{n} c_i P(x_i)$$

Hence the result is true for polynomials of degree less than n.

- Now consider a polynomial $P(x)$ of degree at least n but less than $2n$.
- Divide $P(x)$ by the nth Legendre polynomial $P_n(x)$.
- This gives two polynomials $Q(x)$ and $R(x)$, each of degree less than n, with
$$P(x) = Q(x) P_n(x) + R(x)$$
- Note that x_i is a root of $P_n(x)$ for each $i = 1, 2, \ldots, n$, so we have
$$P(x_i) = Q(x_i) P_n(x_i) + R(x_i) = R(x_i)$$
- We now invoke the unique power of the Legendre polynomials.

First, the degree of the polynomial $Q(x)$ is less than n, so (by the Legendre orthogonality property),

$$\int_{-1}^{1} Q(x)P_n(x)\, dx = 0$$

Then, since $R(x)$ is a polynomial of degree less than n, the opening argument implies that

$$\int_{-1}^{1} R(x)\, dx = \sum_{i=1}^{n} c_i R(x_i)$$

Putting these facts together verifies that the formula is exact for the polynomial $P(x)$:

$$\begin{aligned}\int_{-1}^{1} P(x)\, dx &= \int_{-1}^{1} [Q(x)P_n(x) + R(x)]\, dx \\ &= \int_{-1}^{1} R(x)\, dx \\ &= \sum_{i=1}^{n} c_i R(x_i) \\ &= \sum_{i=1}^{n} c_i P(x_i)\end{aligned}$$

The constants c_i needed for the quadrature rule can be generated from the equation given in the theorem:

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx$$

but both these constants and the roots of the Legendre polynomials are extensively tabulated.

Gaussian Quadrature on Arbitrary Intervals:

Transform the Interval of Integration from [a,b] to [−1, 1]

An integral $\int_a^b f(x)\,dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables

$$t = \frac{2x - a - b}{b - a} \Longleftrightarrow x = \frac{1}{2}[(b-a)t + a + b]$$

This permits Gaussian quadrature to be applied to any interval $[a, b]$, because

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b-a)t + (b+a)}{2}\right)\frac{(b-a)}{2}\,dt$$

Gauss–Laguerre quadrature :

Gauss–Laguerre quadrature is an extension of Gaussian quadrature method for approximating the value of integrals of the following kind:

$$\int_0^{+\infty} e^{-x} f(x)\,dx.$$

In this case

$$\int_0^{+\infty} e^{-x} f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where x_i is the i-th root of Laguerre polynomial $L_n(x)$ and the weight w_i is given by

$$w_i = \frac{x_i}{(n+1)^2[L_{n+1}(x_i)]^2}.$$

Gauss–Hermite quadrature :

Gauss–Hermite quadrature is also an extension of Gaussian quadrature method for approximating the value of integrals of the following kind:

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx.$$

In this case

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where n is the number of sample points to use for the approximation. The x_i are the roots of the Hermite polynomial $H_n(x)$ ($i = 1,2,...,n$) and the associated weights w_i are given by

$$w_i = \frac{2^{n-1} n! \sqrt{\pi}}{n^2[H_{n-1}(x_i)]^2}.$$