Numerical Integration

Ch. 21

Lecture Objectives

- To solve various types of engineering problems using numerical integration
- To be able to determine which type of integration technique to use for specific applications – cost benefit

Numerical Integration

- Very common operation in engineering, Examples?
- Functions that are difficult or impossible to analytically integrate can often be numerically integrated
- Discrete data integration (I.e, experimental, maybe unevenly spaced data)
- We will consider two numerical integration techniques:
  - Newton Cotes
  - Gauss Quadrature

Newton Cotes Integration Formula –

- Most common numerical technique
- Replace a complicated function or tabulated data with with an approximate function that we can easily integrate

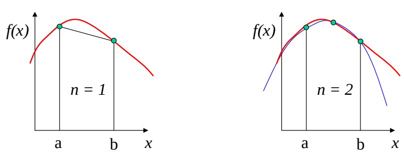
$$I = \int_{x=a}^{x=b} f(x)dx \approx \int_{x=a}^{x=b} f_n(x)dx$$

Nth order polynomial

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

$n = 1$ → straight line
$n = 2$ → parabola

Newton Cotes Integration Formula



Apply piecewise to cover the range $a < x < b$

OPEN & CLOSED forms of Newton-Cotes
•Open form – integration limits extend beyond the range of data (like extrapolation); not usually used for definite integration
•Closed form – data points are located at the beginning and end of integration limits are known → Focus

Newton Cotes Integration Formula – *Trapezoidal Rule*

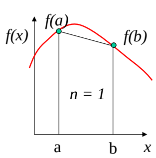
- Use a first order polynomial ($n = 1$, a straight line) to approximate our function $f(x)$

$$I = \int_{x=a}^{x=b} f(x)dx \approx \int_{x=a}^{x=b} f_1(x)dx$$

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b-a}(x-a)$$

$$I = \left[\frac{f(b) - f(a)}{b-a}\frac{x^2}{2} + \frac{bf(a) - af(b)}{b-a}x\right]_a^b$$

$$I = \left[\frac{f(b) - f(a)}{b-a}\frac{(b^2-a^2)}{2} + \frac{bf(a) + af(b)}{b-a}(b-a)\right]_a^b$$



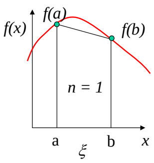
$$I = (b-a)\frac{f(a) + f(b)}{2}$$

Newton Cotes Integration Formula – *Trapezoidal Rule*

- This is in the form width x average height

$$I = \underbrace{(b-a)}_{\text{width}} \underbrace{\frac{f(a)+f(b)}{2}}_{\text{Average height}}$$

- Error for a single application (Truncation Error)

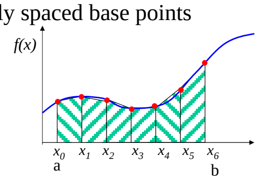


$$E_t = -\frac{1}{12} f''(\xi)(b-a)^3$$

- Exact for a linear function
- functions with 2nd and higher order derivatives will have some error

Trapezoidal Rule – Multiple Applications

- Divide the interval a → b into n segments with n+1 equally spaced base points



h = segment width

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

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

$$I = h\frac{f(x_o)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \cdots + h\frac{f(x_{n-1})+f(x_n)}{2}$$

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

Trapezoidal Rule – Multiple Applications

- Put in the form width x average height

$$I = \underbrace{(b-a)}_{\text{width}} \underbrace{\left[\frac{f(x_o)+2\sum_{i=1}^{n-1} f(x_i)+f(x_n)}{2n}\right]}_{\text{Average height}}$$

- Total Trapezoidal error – sum of individual errors

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

- Approximate E_t by estimating mean 2nd derivative over the entire interval

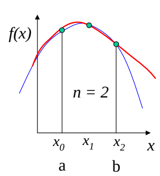
$$\overline{f''} \approx \frac{1}{n}\left(\sum_{i=1}^{n} f''(\xi)\right) \qquad E_a = -\frac{(b-a)^3}{12n^2}\overline{f''}$$

Trapezoidal Rule – Notes

1. For nicely behaved functions a single application of the trapezoid rule will give sufficient accuracy for many engineering purpose
2. For high accuracy (large n), computational effort is higher
3. Round Off Error with large n will limit the accuracy of the trapezoid rule

Simpson's 1/3 Rule -

- Use a higher order polynomial to approximate our function *f(x)* – 2nd order Lagrange polynomial – a unique polynomial that passes through a data points



$$I = \int_{x=x_0}^{x=x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

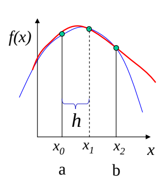
Simpson's 1/3 Rule -

- After integrating & simplifying:

$$I = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2) \right]$$

h = segment width

$$h = \frac{b-a}{2}$$



$$I = \underbrace{(b-a)}_{\text{width}} \underbrace{\left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} \right]}_{\text{Average height}}$$

Simpson's 1/3 Rule –

- Error

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

- Exact for 3rd order polynomials
- Error goes like $(b-a)^5$ compared to 3rd power of trapezoidal rule

Simpson's 1/3 Rule – Multiple Applications

- Requires an <u>Even</u> number of segments

$$I = \underbrace{(b-a)}_{\text{width}} \underbrace{\left[\frac{f(x_o) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{i=2,4,6}^{n} f(x_i) + f(x_n)}{3n} \right]}_{\text{Average height}}$$

n segments
n+1 points

- Error, third order accurate even though we only use 3 points

$$E_a = -\frac{(b-a)^5}{180n^4} \overline{f^{(4)}}$$

Simpson's 3/8 Rule -

- An odd number of segments with an even number of points formula (use a 3rd order polynomial to approximate *f(x))*
- Can be used with Simpson's 1/3 rule to evaluate even or odd number of segment problems.

$$I = \int_{x=a}^{x=b} f(x)dx \approx \int_{x=a}^{x=b} f_3(x)dx$$

$$I = \frac{3}{8}h\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] \qquad h = \frac{b-a}{3}$$

$$I = \underbrace{(b-a)}_{\text{width}} \underbrace{\left[\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_1)}{8} \right]}_{\text{Average height}}$$

Simpson's 3/8 Rule –

- Error

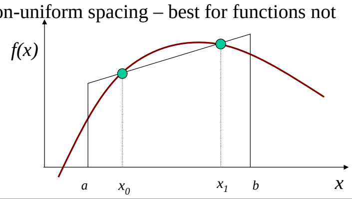
$$E_t = -\frac{(b-a)^5}{6480} f^{(4)}(\xi)$$

- Exact for 3rd order polynomials, slightly more accurate than 1/3 rule
- Simpson's 1/3 rule is preferred since the same accuracy is achieved with few points.

Gauss Quadrature

Newton-Cotes – (ie., trapezoidal rule & Simpson's) the integral was determined by calculating the area under the curve connecting points *a* and *b* (where we evaluate the function at the end points).

Gauss Quadrature – Consider 2 points along a straight line in between *a* and *b* where positive and negative errors balance to reduce total error and give a an improved estimate of the integral. Uses unequal non-uniform spacing – best for functions not tabular data.



Gauss Quadrature – Method of Undetermined Coefficients

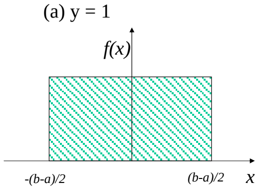
Trapezoidal Rule:

$$I = (b-a)\frac{f(a)+f(b)}{2}$$

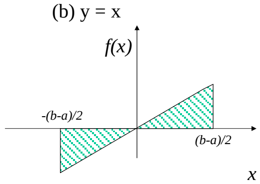
$$I \approx c_0 f(a) + c_1 f(b)$$

Should give exact results if *f(x)* = constant or straight line

(a) y = 1



(b) y = x

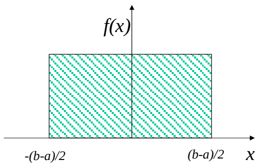


Gauss Quadrature – Method of Undetermined Coefficients

(a) y = 1

Evaluate Exact integral ⟶ $I = \int_{-\frac{b-a}{2}}^{\frac{b-a}{2}} f(x)dx = \int_{-\frac{b-a}{2}}^{\frac{b-a}{2}} 1dx = x\Big|_{-\frac{b-a}{2}}^{\frac{b-a}{2}} = b-a$

Evaluate approximation ⟶ $I = c_0 f(a) + c_1 f(b) = c_0 + c_1$



Set equal to each other:

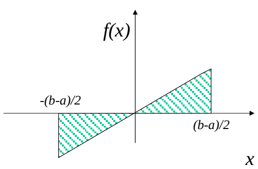
$$b - a = c_0 + c_1$$

Gauss Quadrature – Method of Undetermined Coefficients

(b) y = x

$$I = \int_{-\frac{b-a}{2}}^{\frac{b-a}{2}} f(x)dx = \int_{-\frac{b-a}{2}}^{\frac{b-a}{2}} xdx = \frac{x^2}{2}\Bigg|_{-\frac{b-a}{2}}^{\frac{b-a}{2}} = 0$$

$$I \approx c_0 f(a) + c_1 f(b)$$
$$I \approx c_0\left(-(b-a)/2\right) + c_1\left((b-a)/2\right)$$



$$-c_0\frac{b-a}{2} + c_1\frac{b-a}{2} = 0$$

Gauss Quadrature – Method of Undetermined Coefficients

2 Equations & 2 unknowns solve for c_o and c_1:

$-c_0\frac{b-a}{2} + c_1\frac{b-a}{2} = 0$ ⟶ $c_0 = c_1$

$b - a = c_0 + c_1$ ⟶ $c_0 = c_1 = \frac{b-a}{2}$

Substitute c_o and c_1 back into the original equation:

$$I \approx c_0 f(a) + c_1 f(b)$$

$$I \approx \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$

$$I = (b-a)\frac{f(a) + f(b)}{2}$$

Equivalent to the Trapezoidal Rule!

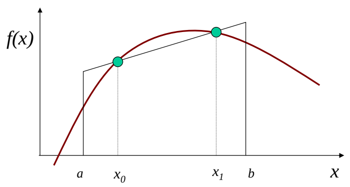
Two Point Gauss Legendre Formula

Extend the method of undetermined coefficients:

$$I \approx c_0 f(x_0) + c_1 f(x_1)$$

c_o & c_1 – unknown constants
$f(x_o)$ & $f(x_1)$ – unknown locations between a & b

We now have 4 unknowns → need 4 equations!



Two Point Gauss Legendre Formula

Need to assume functions again:

$$I \approx c_0 f(x_0) + c_1 f(x_1)$$

(a) $f(x) = 1$
(b) $f(x) = x$
(c) $f(x) = x^2$
(d) $f(x) = x^3$

Parabolic & cubic functions will give us a total of 4 equations

We will get a 2pt linear integration formula formula that will be exact for cubics!

To simplify the math & provide a general formula → select limits of integration to be –1 & 1

Normalized coordinates

Two Point Gauss Legendre Formula

Evaluate the integrals for our 4 equations:

(a) $f(x) = 1$ $\quad c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} 1 dx = 2$

(b) $f(x) = x$ $\quad c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x dx = 0$

(c) $f(x) = x^2$ $\quad c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^2 dx = \frac{2}{3}$

(d) $f(x) = x^3$ $\quad c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^3 dx = 0$

Two Point Gauss Legendre Formula

Rewrite the equations:

$$c_0 + c_1 = 2$$
$$c_0 x_0 + c_1 x_1 = 0$$
$$c_0 x_0^2 + c_1 x_1^2 = \frac{2}{3}$$
$$c_0 x_0^3 + c_1 x_0^3 = 0$$

Solve for co, c1, xo and x1:

$$c_0 = c_1 = 1$$
$$x_0 = -1/\sqrt{3}$$
$$x_1 = 1/\sqrt{3}$$

Two Point Gauss Legendre Formula

2 Point Gauss Legendre Formula (for integration limits –1 to 1:

$$I = f\left(-1/\sqrt{3}\right) + f\left(1/\sqrt{3}\right)$$

3rd order accurate

Need to change variables to translate to other integration limits

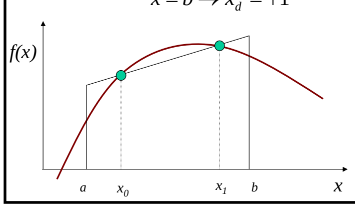
Two Point Gauss Legendre Formula

Changing the limits of integration:

- Introduce a new variable x_d that represents x in our generalized formula (where we use –1 to 1)
- Assume x_d is linearly related to x

$$x = a_0 + a_1 x_d$$
$$x = a \rightarrow x_d = -1$$
$$x = b \rightarrow x_d = +1$$

$$a = a_0 + a_1(-1)$$
$$b = a_0 + a_1(1)$$



$$a_0 = \frac{b+a}{2} \qquad a_1 = \frac{b-a}{2}$$

$$x = a_0 + a_1 x_d$$

Two Point Gauss Legendre Formula

Substitute a_o and a_1 back into our original linear formula

$$x = a_0 + a_1 x_d$$

$$x = \left(\frac{b+a}{2}\right) + \left(\frac{b-a}{2}\right) x_d$$

Differentiate with respect to x_d:

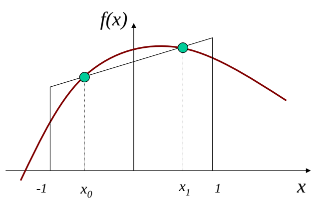
$$dx = \left(\frac{b-a}{2}\right) dx_d$$

Substitute these values of x and dx in the original integral to effectively change the limits of integration without changing the value of the integral.

$$I = \int_a^b f(x)dx \approx \frac{b-a}{2}\left[c_0 f(x_o^{trans}) + c_1 f(x_1^{trans})\right]$$

Gauss-Legendre Quadrature – uses roots of Legendre Polynomials to locate the point at which the integrand is evaluated

$$\int_{-1}^{1} f(x)dx = \sum_{i=0}^{n} c_i f(x_i)$$

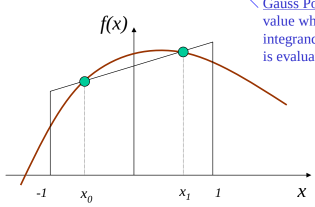


Gauss-Legendre Quadrature – uses roots of Legendre Polynomials to locate the point at which the integrand is evaluated

unknown weighting coefficients

$$\int_{-1}^{1} f(x)dx = \sum_{i=0}^{n} c_i f(x_i)$$

Gauss Points: specific value where the integrand is evaluated



Gauss-Legendre Quadrature – uses roots of Legendre Polynomials to locate the point at which the integrand is evaluated

unknown weighting coefficients

$$\int_{-1}^{1} f(x)dx = \sum_{i=0}^{n} c_i f(x_i)$$

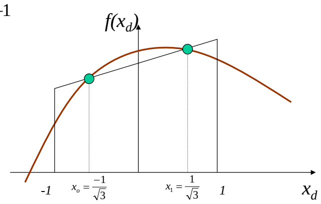
Gauss Points: specific value where the integrand is evaluated

The values of w_i and x_i are chosen so that the formula will be exact up to & including a polynomial of degree (2m-1), where m is the number of points.

Ex: 2 Point → Exact 3rd order polynomial

Gauss-Legendre Quadrature – General form 2 Point Application – from our derivation, we found x_o and x_1 for the integration limits 1 to -1

$$I = \int_{-1}^{1} f(x_d)dx_d \approx c_0 f(x_0) + c_1 f(x_1)$$



$$I \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{-1}{\sqrt{3}}\right)$$

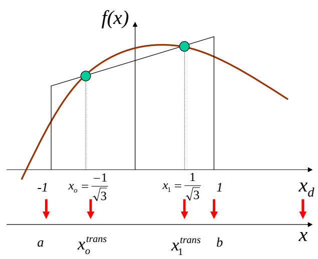
Gauss-Legendre Quadrature – 2 Pt Application – Transformation procedure

$$x = \frac{b+a}{2} + \frac{b-a}{2} x_d$$

$$x_o^{trans} = \frac{b+a}{2} + \frac{b-a}{2}\left(\frac{-1}{\sqrt{3}}\right)$$

$$x_1^{trans} = \frac{b+a}{2} + \frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right)$$

$$dx = \frac{b-a}{2} dx_d$$



$$I = \int_{a}^{b} f(x)dx \approx \frac{b-a}{2}\left[c_0 f(x_o^{trans}) + c_1 f(x_1^{trans})\right]$$

Gauss-Legendre Quadrature – Simple 2 point Example

Integrate the following function from x=0.2 to 0.8:

$$f(x) = 4x^4 + 2x^2 - 1$$

$$I = \int_{.2}^{.8} f(x)dx = \int_{.2}^{.8} 4x^4 + 2x^2 - 1dx$$

$$I = \int_{-1}^{1} f(x_d)dx_d \approx f(-1/\sqrt{3}) + f(1/\sqrt{3})$$

Step 1: Transform limits and Gauss points (x_o & x_1) from general form

$$x_o^{trans} = \frac{b+a}{2} + \frac{b-a}{2}\left(\frac{-1}{\sqrt{3}}\right) = 0.5 + 0.3\left(\frac{-1}{\sqrt{3}}\right) = 0.3267949$$

$$x_1^{trans} = \frac{b+a}{2} + \frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right) = 0.5 + 0.3\left(\frac{1}{\sqrt{3}}\right) = 0.6732050$$

Step 2: perform summation

$$I = \int_a^b f(x)dx \approx \frac{b-a}{2}\left[c_0 f(x_o^{trans}) + c_1 f(x_1^{trans})\right]$$

$$I \approx 0.3\left[(1) f(0.3267949) + (1) f(0.6732050)\right]$$

$$I \approx 0.3\left[4(0.3267949)^4 + 2(0.3267949)^2 - 1 + 4(0.673205)^4 + 20.673205^2 - 1\right]$$

Error Estimate *n*-point Gauss-Legendre Formula

$$E_t = \frac{2^{2n+1}[n!]^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi) \qquad -1 < \xi < 1$$

Where *n* is the number of points in the formula (remember, a n-point formula integrates a polynomial of 2n-1 exactly!)

$f^{(2n)}(\xi)$ is the (2n)th derivative after the change of variable

If the magnitude of the higher order derivatives decrease or only increase slowly with increasing *n*, Gauss formulas are Significantly more accurate than Newton-Cotes formulas.

Matlab Multipoint Example

Built in Matlab integration methods

I=trapz(y)*dx

f=inline('x^2+1')

I=quad(f,0,2)

Integration limits