NUMERICAL INTEGRATION (NUMERICAL QUADRATURE)

Dr. Gabriel Obed Fosu

Department of Mathematics
Kwame Nkrumah University of Science and Technology
Google Scholar: https://scholar.google.com/citations?user=ZJfCMyQAAAAJ&hl=en&oi=ao
ResearchGate ID: https://www.researchgate.net/profile/Gabriel_Fosu2

Lecture Outline

1. Trapezium Rule
2. Simpson's 1/3 Rule
3. Simpson's 3/8 Rule
4. Romberg Method
5. Integration Rules Based on Non-uniform Mesh Spacing

Integration Rules Based on Uniform Mesh Spacing

1. Generally, integration problems deals with finding an approximate value of the integral
$$I = \int_a^b w(x) f(x) dx \tag{1}$$
where $w(x) > 0$ the weight function lies in the open interval (a, b), and I a definite integral.
2. I reduces to an indefinite integral when the limits of integration are not specified.
3. When $w(x) = 1$ and x_k's are equidistant with $x_0 = a,\ x_n = b,\ h = \dfrac{b-a}{N}$, where N is the number of subdivision, then the integral (1) reduces to
$$I = \int_{x_0}^{x_n} f(x) dx \tag{2}$$
4. This integral (2) defines the area under the curve above the $x-$axis within the interval $[x_0,\ x_n]$.

Integration Rules Based on Uniform Mesh Spacing

The following integration techniques will be employed in finding the value of this area.

1. Trapezium Method
2. Simpson's Method
3. Romberg Method

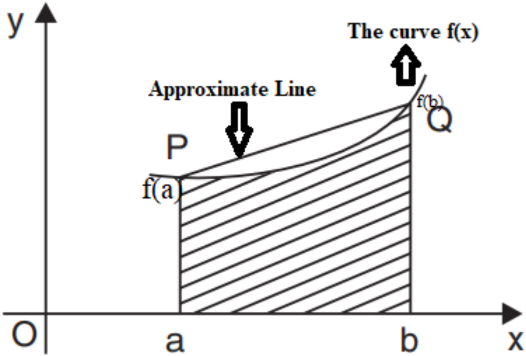
Note

These methods are called Newton–Cotes formulas, or the Newton–Cotes quadrature rules or simply Newton–Cotes rules.

These techniques are all based on evaluating the integrand at equally spaced points. They are named after Isaac Newton and Roger Cotes.

Simple Trapezium Rule

This is also called the trapezoidal method. Let the curve $y = f(x),\ a \le x \le b$ be approximated by the line joining the points $P(a, f(a))$ and $Q(b, f(b))$ on the curve as illustrated below



Simple Trapezium Rule

Then the trapezium method uses the area under the approximate line to obtain the formula

$$I = \frac{1}{2}h\left[f(a) + f(b)\right] \tag{3}$$

$$= \frac{1}{2}(b-a)\left[f(a) + f(b)\right]; \qquad N = 1 \tag{4}$$

Note

The trapezium rule of integration integrates exactly polynomials of degree ≤ 1

Example

Approximate the following integrals using the simple trapezium rule

1. $\int_3^5 2x^2 dx$
2. $\int_0^{\pi/4} \sin(x) dx$

Hence determine the absolute error (AE)

Solution

1. Given $\int_3^5 2x^2 dx$, then $a = 3$ and $b = 5$. The functional values are

$f(a) = f(3) = 2(3)^2 = 18$

$f(b) = f(5) = 2(5)^2 = 50$

Therefore

$$I = \frac{1}{2}(b-a)\left[f(a)+f(b)\right] \tag{5}$$
$$= \frac{1}{2}(5-3)[18+50] \tag{6}$$
$$= 68 \tag{7}$$

For absolute error, the exact solution is required

Exact solution

$$\int_3^5 2x^2\,dx = \left.\frac{2x^3}{3}\right|_3^5 = 65.33 \tag{8}$$

$$AE = |ES - AS| = |65.33 - 68| = 2.66$$

2. Given $\int_0^{\pi/4} \sin(x)dx$, then $a = 0$ and $b = \frac{\pi}{4}$. The functional values are
$f(a) = f(0) = \sin(0) = 0$
$f(b) = f(\pi/4) = \sin(\pi/4) = 0.707$. Therefore

$$\begin{aligned} I &= \frac{1}{2}(b-a)\left[f(a)+f(b)\right] && (9)\\ &= \frac{1}{2}(\pi/4-0)[0+0.707] && (10)\\ &= \frac{\pi}{8}(0.707) && (11)\\ &= 15.9075 && (12) \end{aligned}$$

Exact solution

$$\int_0^{\pi/4} \sin(x)dx = -\cos(x)\Big|_0^{\pi/4} = -\cos(\pi/4)+\cos(0) = 0.293 \quad (13)$$

$$AE = |ES - AS| = |0.293 - 15.9075| = 15.614$$

Composite Trapezium Rule

Here, the idea is to split the interval $(a,\ b)$ into a sequence of N smaller sub-interval with width $h = \dfrac{b-a}{N}$. These yields the composite trapezium formula

$$\int_a^b f(x)\,dx = \frac{h}{2}\left\{f(x_0) + 2\left[f(x_1) + f(x_2) + \cdots + f(x_{N-1})\right] + f(x_N)\right\} \tag{14}$$

Note

The nodal points are given by

$$a = x_0,\ x_1 = x_0 + h,\ x_2 = x_0 + 2h, \cdots, x_N = x_0 + Nh = b \tag{15}$$

Example

Find the approximate solution for the following using the composite trapezium rule with 4 equal sub-intervals.

1. $\displaystyle\int_3^5 2x^2 \; dx$
2. $\displaystyle\int_0^2 \ln(x) \; dx$

Solution

For 4 sub-intervals $\implies h = \dfrac{b-a}{N} = \dfrac{5-3}{4} = 0.5$.

Therefore the x points are

$$x_0 = 3, \quad x_1 = 3.5, \quad x_2 = 4, \quad x_3 = 4.5, \quad x_4 = 5$$

The functional value are

$$f(x_0) = f(3) = 18 \tag{16}$$

$$f(x_1) = f(3.5) = 24.5 \tag{17}$$

$$f(x_2) = f(4) = 32 \tag{18}$$

$$f(x_3) = f(4.5) = 40.5 \tag{19}$$

$$f(x_4) = f(5) = 50 \tag{20}$$

Substituting into the formula

$$\int_a^b f(x)dx = \frac{h}{2}\left\{f(x_0) + 2\left[f(x_1) + f(x_2) + \cdots + f(x_{N-1})\right] + f(x_N)\right\} \tag{21}$$

$$\int_3^5 2x^2 \, dx = \frac{0.5}{2}\left\{f(x_0) + 2\left[f(x_1) + f(x_2) + f(x_3)\right] + f(x_4)\right\} \tag{22}$$

$$= \frac{0.5}{2}\{18 + 2[24.5 + 32 + 40.5] + 50\} \tag{23}$$

$$= 65.5 \tag{24}$$

From above the exact solution is 65.33, therefore the absolute error is

$$AE = |ES - AS| = |65.33 - 65.5| = 0.17$$

By comparison, we realize that the composite trapezium is more accurate than the simple trapezium method.

Simple Simpson's 1/3 Rule

1. This is based on a quadratic curve through equally spaced point rather than a line as is the case of the simple trapezium rule.
2. The interval (a,b) is subdivided into two equal parts with the step length $h = \frac{b-a}{2}$.
3. We approximate the integral curve by the parabola joining these points.
4. The formula of the Simpson's 1/3 rule is deduced from interpolation techniques, and it is given by
$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \tag{25}$$
5. The Simpson's rule integrates exactly polynomials of degree ≤ 3.

Example

Find the derivative of the following functions using the simple Simpson's 1/3 rule

1. $\int_3^5 2x^2 dx$
2. $\int_1^3 \frac{1}{1+x} dx$

For 2 sub-intervals $\implies h = \frac{b-a}{2} = \frac{5-3}{2} = 1.$

Therefore the x points are

$$[x_0, x_1,\ x_2] = [3,\ 4,\ 5]$$

The functional value are

$$f(x_0) = f(3) = 18 = f(a) \tag{26}$$

$$f(x_1) = f(4) = 32 = f\left(\frac{a+b}{2}\right) \tag{27}$$

$$f(x_2) = f(5) = 50 = f(b) \tag{28}$$

Substituting into the formula

$$\int_a^b f(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \tag{29}$$

$$\int_3^5 2x^2 dx = \frac{5-3}{6}\left[18 + 4(32) + 50\right] \tag{30}$$

$$= \frac{1}{3}(196) \tag{31}$$

$$= 65.33 \tag{32}$$

Composite Simpson's 1/3 Rule

1. This is an extension of the simple Simpson's rule.
2. Here, the given interval $[a,b]$ can be divided into any finite sub-intervals of equal length say h.
3. For N sub-intervals the formula is given as

$$\int_a^b f(x)dx = \frac{h}{3}\Big\{f(x_0) + 4\Big[f(x_1) + f(x_3) + f(x_5) + \cdots + f(x_{N-1})\Big] + 2\Big[f(x_2) + f(x_4) + f(x_6) + \cdots + f(x_{N-2})\Big] + f(x_N)\Big\} \tag{33}$$

4. The composite Simpson's 1/3 rule is also of order 3, that is the composite Simpson's 1/3 rule produces exact results for polynomials of degree ≤ 3.

Example

Find the derivative of the following functions using the composite Simpson's 1/3 rule using 4 sub-intervals

1. $\int_3^5 2x^2\,dx$
2. $\int_1^3 \frac{1}{1+x}\,dx$

Solution

For 4 sub-intervals $\implies h = \dfrac{b-a}{4} = \dfrac{5-3}{4} = 0.5$.

Therefore the x points are

$$x_0 = 3,\ x_1 = 3.5,\ x_2 = 4,\ x_3 = 4.5,\ x_4 = 5$$

The functional value are

$$f(x_0) = f(3) = 18 \tag{34}$$

$$f(x_1) = f(3.5) = 24.5 \tag{35}$$

$$f(x_2) = f(4) = 32 \tag{36}$$

$$f(x_3) = f(4.5) = 40.5 \tag{37}$$

$$f(x_4) = f(5) = 50 \tag{38}$$

Substituting into the formula

$$\int_a^b f(x)dx = \frac{h}{3}\Big\{f(x_0) + 4\Big[f(x_1) + f(x_3) + f(x_5) + \cdots + f(x_{N-1})\Big] \tag{39}$$

$$+ 2\Big[f(x_2) + f(x_4) + f(x_6) + \cdots + f(x_{N-2})\Big] + f(x_N)\Big\} \tag{40}$$

$$\int_3^5 2x^2 dx = \frac{h}{3}\Big\{f(x_0) + 4\Big[f(x_1) + f(x_3)\Big] + 2\Big[f(x_2)\Big] + f(x_4)\Big\}$$

$$= \frac{0.5}{3}\Big\{18 + 4(24.5 + 40.5) + 2(32) + 50\Big\} \tag{41}$$

$$= 0.167(392) \tag{42}$$

$$= 65.474 \tag{43}$$

Simple Simpson's 3/8 Rule

1. To derive the Simpson's 1/3 rule, we have approximated $f(x)$ by a quadratic polynomial.
2. To derive the Simpson's 3/8 rule, we approximate $f(x)$ by a cubic polynomial.
3. For interpolating by a cubic polynomial, we require four nodal points. Hence, we subdivide the given interval $[a, b]$ into 3 equal parts so that we obtain four nodal points.
4. Let $h = (b-a)/3$, then the nodal points are given by $x_0 = a,\ x_1 = x_0 + h,\ x_2 = x_0 + 2h,\ x_3 = x_0 + 3h$.
5. Using the Newton's forward difference formula, the integral of the cubic polynomial approximation to f(x) gives the Simpson's 3/8 rule as

$$\int_a^b f(x)dx = \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] \tag{44}$$

Composite Simpson's 3/8 Rule

1. This is an extension of the simple Simpson's 3/8 rule.
2. In this case, we subdivide $[a, b]$ into a number of subintervals of equal length such that the number of subintervals is divisible by 3.
3. For example, if we divide $[a, b]$ into 6 parts, then we get 7 nodal points with Simpson's 3/8 rule as

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x^3} f(x)dx + \int_{x_3}^{x_6} f(x)dx \\ &= \frac{3h}{8}[\{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\}+\{f(x_3)+3f(x_4)+3f(x_5)+f(x_6)\}] \\ &= \frac{3h}{8}[f(x_0)+3f(x_1)+3f(x_2)+2f(x_3)+3f(x_4)+3f(x_5)+f(x_6)]\end{aligned}$$

Example

Using the Simpson's 3/8 rule, evaluate $\int_1^2 \frac{1}{5+3x}dx$ with 3 and 6 subintervals. Compare with the exact solution.

When $n=3$, we have the following step lengths and nodal points.

$$h = \frac{b-a}{n} = \frac{2-1}{3} = \frac{1}{3} \tag{45}$$

The nodes are

$$x_0 = 1,\ x_1 = x_0 + h = 4/3,\ x_2 = x_1 + h = 5/3, x_2 = 2.0.$$

We have the following tables of values

x	1.0	4/3	5/3	2.0
$f(x)$	0.125	0.11111	0.10000	0.09091

n =3

$$\int_a^b f(x)\,dx = \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right] \tag{46}$$

$$\int_1^2 \frac{1}{5+3x}\,dx = \frac{3}{8}\frac{1}{3}[0.125+3(0.11111)+3(0.10000)+0.09091] \tag{47}$$

$$= 0.10616 \tag{48}$$

Exact Solution

$$F(x) = \frac{1}{3}\ln(5+3x) \tag{49}$$

$$F(x)\Big|_1^2 = \frac{1}{3}[\ln 11 - \ln 8] = 0.10615. \tag{50}$$

$$\tag{51}$$

The magnitude of the error is 0.00001

When n=6

$$h = \frac{b-a}{6} = \frac{2-1}{6} = \frac{1}{6} \tag{52}$$

We have the following tables of values

x	1.0	7/6	8/6	9/6	10/6	11/6	2.0
$f(x)$	0.125	0.11765	0.11111	0.10526	0.10000	0.09524	0.09091

$$\int_a^b f(x)dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + 2f(x_3) + 3f(x_4) + 3f(x_5) + f(x_6)] \tag{53}$$

$$\int_1^2 \frac{1}{5+3x}dx = \frac{3}{8}\frac{1}{6}[0.125 + 3(0.11765 + 0.11111 + 0.10000 + 0.09524) + 2(0.10526) + 0.09091] \tag{54}$$

$$= 0.10615 \tag{55}$$

Romberg Method

1. Romberg integration uses the composite trapezium/Simpson's(1/3) rule to give preliminary approximations and then applies the Richardson extrapolation process to improve the approximations.
2. Usually, we start with a coarse step length, then reduce the step lengths and recompute the value of the integral.
3. The sequence of these values converges to the exact value of the integral.

Definition

The Richardson extrapolation is a sequence acceleration method used to improve the rate of convergence of a sequence of estimates of some value say A.

Romberg method for the trapezium rule

1. The Romberg extrapolation procedure for the composite trapezium rule is

$$I^{(m)}(h) = \frac{4^m I^{(m-1)}(h/2) - I^{(m-1)}(h)}{4^m - 1}; \qquad m = 1, 2, 3, \cdots \tag{56}$$

2. where $I^{(0)}(h) = I(h)$. Note these initial values are computed from the trapezium method discussed earlier.
3. This often uses the step lengths $h, \ \dfrac{h}{2}, \ \dfrac{h}{2^2}, \cdots$

Example

Solve $\int_0^1 \frac{1}{1+x}\,dx$ using Romberg method with two sub-interval. Compute your initial values using the composite trapezium method.
Perform two iterations.

Recall that the composite trapezium formula is
$\int_a^b f(x)dx = \frac{h}{2}\left\{f(x_0) + 2\left[f(x_1) + f(x_2) + \cdots + f(x_{N-1})\right] + f(x_N)\right\}$ where $h = (b-a)/N$ The approximations using the trapezium rule to the integral with various values of the step lengths were obtained as follows:

$$\text{1st h: } N = 2 \implies h_0 = 1/2, \implies I^{(0)}(1/2) = 0.708334 \quad (57)$$

$$\text{2nd h: } h = h_0/2 = 1/4, \implies N = 4 \implies I^{(0)}(1/4) = 0.697024 \quad (58)$$

$$\text{3rd h: } h = h_0/2^2 = 1/8, \implies N = 8 \implies I^{(0)}(1/8) = 0.694122. \quad (59)$$

When $m = 1, h = 1/2$

$$I^{(m)}(h) = \frac{4^m I^{(m-1)}(h/2) - I^{(m-1)}(h)}{4^m - 1}; \qquad m = 1, 2, 3, \cdots \tag{60}$$

$$I^{(1)}(1/2) = \frac{4I^{(0)}(1/4) - I^{(0)}(1/2)}{4 - 1} \tag{61}$$

$$= \frac{4(0.697024) - 0.708334}{3} \tag{62}$$

$$= 0.693254 \tag{63}$$

When $m = 2, h = 1/2$

$$I^{(2)}(1/2) = \frac{4^2 I^{(1)}(1/4) - I^{(1)}(1/2)}{4^2 - 1} \tag{64}$$

But $I^{(1)}(1/4)$ is not known. This should be computed with the same formula with $h = 1/4$

When $m = 1, h = 1/4$

$$I^{(1)}(1/4) = \frac{4I^{(0)}(1/8) - I^{(0)}(1/4)}{4-1} \tag{65}$$

$$= \frac{4(0.694122) - 0.697024}{3} \tag{66}$$

$$= 0.693155 \tag{67}$$

Thus eq. (64) becomes

When $m = 2, h = 1/2$

$$I^{(2)}(1/2) = \frac{4^2 I^{(1)}(1/4) - I^{(1)}(1/2)}{4^2-1} \tag{68}$$

$$= \frac{16(0.693155) - 0.693254}{15} \tag{69}$$

$$= 0.693148 \tag{70}$$

Exact Solution

$$F(x) = \ln(1 + x) \tag{71}$$

$$F(x)\Big|_0^1 = \ln(2) - \ln(1) \tag{72}$$

$$= 0.693147 \tag{73}$$

Magnitude of the error is 0.000001.

Romberg method for the Simpson's 1/3 rule

1. The Romberg extrapolation procedure for the composite Simpson's 1/3 rule is

$$I^{(m)}(h) = \frac{4^{m+1} I^{(m-1)}(h/2) - I^{(m-1)}(h)}{4^{m+1} - 1}; \qquad m = 1, 2, 3, \cdots \tag{74}$$

2. where $I^{(0)}(h) = I(h)$. Note these initial values are computed from the Simpson's 1/3 method discussed earlier.
3. This also uses the step lengths $h, \dfrac{h}{2}, \dfrac{h}{2^2}, \cdots$

Example

Solve $\int_0^1 \frac{1}{1+x}dx$ using Romberg method with two sub-interval. Compute your initial values using the composite Simpson's 1/3 method.
Perform two iterations.

The approximations using the Simpson's 1/3 rule to the integral with various values of the step lengths were obtained as follows:

$$\text{1st h: } N=2 \implies h_0 = 1/2, \implies I^{(0)}(1/2) = 0.694444 \tag{75}$$

$$\text{2nd h: } h = h_0/2 = 1/4, \implies N=4 \implies I^{(0)}(1/4) = 0.693254 \tag{76}$$

$$\text{3rd h: } h = h_0/2^2 = 1/8, \implies N=8 \implies I^{(0)}(1/8) = 0.693155 \tag{77}$$

When $m=1, h=1/2$

$$I^{(m)}(h) = \frac{4^{m+1} I^{(m-1)}(h/2) - I^{(m-1)}(h)}{4^{m+1}-1}; \qquad m = 1,2,3,\cdots \tag{78}$$

$$I^{(1)}(1/2) = \frac{16 I^{(0)}(1/4) - I^{(0)}(1/2)}{16-1} \tag{79}$$

$$= \frac{16(0.693254) - 0.694444}{15} \tag{80}$$

$$= 0.693175 \tag{81}$$

When $m=2, h=1/2$

$$I^{(2)}(1/2) = \frac{4^3 I^{(1)}(1/4) - I^{(1)}(1/2)}{4^3-1} \tag{82}$$

But $I^{(1)}(1/4)$ is not known. This should be computed with the same formula with $h=1/4$

When $m = 1, h = 1/4$

$$I^{(1)}(1/4) = \frac{16I^{(0)}(1/8) - I^{(0)}(1/4)}{16-1} \tag{83}$$
$$= \frac{16(0.693155) - 0.693244}{15} \tag{84}$$
$$= 0.693148 \tag{85}$$

Thus eq. (82) becomes

When $m = 2, h = 1/2$

$$I^{(2)}(1/2) = \frac{4^3 I^{(1)}(1/4) - I^{(1)}(h)}{4^3 - 1} \tag{86}$$
$$= \frac{64(0.693148) - 0.693175}{63} \tag{87}$$
$$= 0.693148 \tag{88}$$

Exact Solution

$$F(x) = \ln(1+x) \tag{89}$$

$$F(x)\Big|_0^1 = \ln(2) - \ln(1) \tag{90}$$

$$= 0.693147 \tag{91}$$

Magnitude of the error is 0.000001.

Gaussian Integration (Quadrature)

We have defined the general integration rule as

$$I = \int_a^b \omega(x)\ f(x)\ d(x) \tag{92}$$

We have the following Gaussian integration rules depending on the limits of integration and on the expression for the weight function $w(x)$.

1. **Gauss-Legendre integration rule**: $[a,\ b] = [-1,\ 1]$ and $w(x) = 1$.
2. **Gauss-Chebychev integration rule:**$[a,\ b] = [-1,1]$ and $w(x) = \dfrac{1}{\sqrt{1-x^2}}$
3. **Gauss-Laguerre integration rule**: $[a,\ b] = [0,\ \infty)$ and $w(x) = e^{-x}$
4. **Gauss-Hermite integration rule:**$[a,\ b] = (-\infty,\infty)$ and $w(x) = e^{-x^2}$

Exercise

Evaluate the function

$$\int_3^6 \frac{1}{1+x^2}, \qquad \int_0^6 \cos(e^x)$$

using

1. Simple trapezium rule
2. Composite trapezium rule with 6 sub-intervals
3. Simple Simpson's 1/3 rule
4. Composite Simpson's 1/3 rule with 8 sub-intervals
5. Romberg method with two sub-interval for three iterations. Compute your initial values using the Simpson's 1/3 method.
6. Romberg method with two sub-interval. Compute your initial values using the Trapezium method. Take $\epsilon = 1^{-5}$

END OF LECTURE

THANK YOU