Contents

Unit 3

Numerical Differentiation and Integration

3.1 Numerical Differentiation

The method of obtaining the derivative of a function using a numerical technique is known as numerical differentiation. There are mainly two situations where numerical differentiation is required. They are

(i) The function value f_i at some points x_i are known but the function f itself is unknown. Such functions are called tabulated functions.

(ii) The function f to be differentiated is known but is quite complicated and therefore difficult to differentiate.

When the function is given in tabulated form as (x_i, f_i), $i = 0, 1, \cdots, n$, the general method for deriving the numerical differentiation formulae is to differentiate the corresponding interpolating polynomial. So corresponding to each of the interpolation formulae we have derived, we can derive a formula for the derivative.

3.1.1 Numerical Differentiation using Divided Differences

Suppose that the tabulated values of a function $f(x)$ are given at $n+1$ points as (x_i, f_i), $i = 0, 1, \cdots, n$. The polynomial (Newton's form) that interpolates these data points is

$$\begin{aligned} P_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \cdots \\ \cdots + f[x_0, x_1, \cdots, x_n](x - x_0)(x - x_1)\cdots(x - x_{n-1}) \cdots\cdots (1) \end{aligned}$$

If $P_n(x)$ is a good approximation of $f(x)$, then we can assume that $P_n'(x)$ is a good approximation of $f'(x)$. Therefore differentiating (1) with respect to x, we get

$$\begin{aligned} P_n'(x) = f[x_0, x_1] + f[x_0, x_1, x_2][(x - x_1) + (x - x_0)] + \cdots \\ \cdots + f[x_0, x_1, \cdots, x_n] \sum_{i=0}^{n-1} \frac{(x - x_0)(x - x_1)\cdots(x - x_{n-1})}{x - x_i} \end{aligned}$$

Substituting for different values of x in the above expression, we can approximate the derivative of $f(x)$ for those values of x.

3.1.2 Error in Numerical Differentiation

The error in approximating $f(x)$ by the interpolating polynomial $P_n(x)$ is given by

$$E(x) = (x - x_0)(x - x_1)\cdots(x - x_n)\frac{f^{(n+1)}(\xi)}{(n+1)!}$$

where ξ is a point that depends on x. When this error term is differentiated, then we get the error for approximating $f'(x)$ by $P_n'(x)$ as follows:

$$E'(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\sum_{i=0}^{n}\frac{(x - x_0)(x - x_1)\cdots(x - x_n)}{(x - x_i)} + \frac{(x - x_0)\cdots(x - x_n)}{(n+1)!}\frac{d}{dx}f^{(n+1)}(\xi)$$

When $x = x_j$, $j = 0, 1, \cdots, n$, then

$$\begin{aligned} E'(x_j) &= (x_j - x_0)(x_j - x_1)\cdots(x_j - x_{j-1})(x_j - x_{j+1})\cdots(x_j - x_n)\frac{f^{(n+1)}(\xi)}{(n+1)!} \\ &= \prod_{i=0, i\neq j}^{n}(x_j - x_i)\frac{f^{(n+1)}(\xi)}{(n+1)!} \end{aligned}$$

which is the error of the approximation to $f'(x)$ when $x = x_j$.

3.1.3 Derivatives for evenly-spaced data

Suppose that the tabulated values of a function $f(x)$ are given at $n + 1$ points as (x_i, f_i), $i = 0, 1, \cdots n$, where $x_0, x_1, \cdots x_n$ are equal distance h apart i.e., $x_k = x_0 + kh$, $k = 0, 1, \cdots, n$. The Newton-Gregory forward difference interpolation polynomial for interpolating these points is

$$P_n(x) = f_0 + s\Delta f_0 + s(s-1)\frac{\Delta^2 f_0}{2!} + \cdots + s(s-1)\cdots(s-n+1)\frac{\Delta^n f_0}{n!} \cdots\cdots (1)$$

where $s = \dfrac{x - x_0}{h}$. Differentiating (1) with respect to x, we get $P_n'(x)$ which approximates $f'(x)$ as follows:

$$\begin{aligned} P_n'(x) &= \frac{d}{dx}P_n(x) = \frac{d}{ds}P_n(x)\cdot\frac{ds}{dx} \\ &= \frac{1}{h}\left[\Delta f_0 + \frac{\Delta^2 f_0}{2!}[s + (s-1)] + \cdots + \frac{\Delta^n f_0}{n!}\sum_{i=0}^{n-1}\frac{s(s-1)\cdots(s-n+1)}{s-i}\right] \end{aligned}$$

Substituting for different values of x in the above expression, we can approximate the derivative of $f(x)$ for different values of x.

3.1.4 Numerical Differentiation for Explicitly Defined Functions

The derivative of a function $f(x)$ at some point $x = a$ is given as the limit

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}.$$

When the function $f(x)$ is known but complicated, then we can approximate the value of $f'(a)$ as the value of the ratio given by

$$f'(a) \approx \frac{f(a+h) - f(a)}{h}$$

for some very small positive value of h. This formula is known as the forward difference formula for $f'(a)$. Note that $f'(a)$ is approximated in this formula by approaching a from the right side of a. If $f'(a)$ is approximated by approaching a from the left of a, we obtain the backward difference formula which is given by

$$f'(a) \approx \frac{f(a) - f(a-h)}{h}.$$

A more accurate formula known as central difference formula can also be used as

$$f'(a) \approx \frac{f(a+h) - f(a-h)}{2h}.$$

Second derivative central difference formula at $x = a$:

$$f''(a) \approx \frac{f(a+h) - 2f(a) + f(a-h)}{h^2}$$

3.1.5 Exercise

1. Find the derivative of the following tabulated function at $x = 4.1$ using divided differences table.

x	2	3	5	6
f	3	7	21	31

Solution: Here $n = 3$, so the formula for the derivation of above tabulated function is

$$P_3'(x) = f[x_0, x_1] + f[x_0, x_1, x_2][(x - x_0) + (x - x_1)]$$
$$+ f[x_0, x_1, x_2, x_3][(x - x_0)(x - x_1) + (x - x_1)(x - x_2) + (x - x_0)(x - x_2)] \cdots\cdots (1)$$

x_i	$f[x_i]$	$f[x_i, x_{i+1}]$	$f[x_i, x_{i+1}, x_{i+2}]$	$f[x_0, x_1, x_2, x_3]$
2	3			
		4		
3	7		1	
		7		0
5	21		1	
		10		
6	31			

Therefore from (1), we have

$$P_3'(x) = 4 + 1[(x-2) + (x-3)] + 0 = 2x - 1$$

When $x = 4.1$, we have

$$P_3'(4.1) = 2 \times 4.1 - 1 = 7.2.$$

2. Find the derivative of the following tabulated function at $x = 0.242$ using divided differences table.

x	0.21	0.23	0.27	0.32
f	0.3222	0.3617	0.4314	0.5051

3. For the function $f(x) = e^x\sqrt{\sin x + \ln x}$ estimate $f'(6.3)$ and $f''(6.3)$ taking $h = 0.01$. HINT: Use central difference formula.

4. How do you find the derivative if the function values are given in a tabulated form? The distance traveled by a vehicle at the intervals of 2 minutes are given as follows. Evaluate the velocity and acceleration of the vehicle at time $t = 5, 10, 13$.

$Time$	0	2	4	6	8	10	12	14	16
$Distance$	0	0.25	1	2.2	4	6.5	8.5	11	13

5. Let $f(x) = 3xe^x - \cos x$. Compute $f''(1.3)$ using $h = 0.1$ and $h = 0.01$.

6. Consider the following table of data:

x	0.2	0.4	0.6	0.8	1.0
$f(x)$	0.9798652	0.9177710	0.808038	0.6386093	0.3843735

Use appropriate formula to compute $f'(0.4)$, $f'(0.6)$, $f''(0.4)$, $f''(0.6)$, $f'(0.2)$, $f'(1)$.

3.2 Numerical Integration

Many times we need to calculate the value of definite integrals of the type

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

If $f(x)$ is a continuous function on the interval $[a, b]$, then this definite integrals must exist. But the class of functions $f(x)$ for which such integrals can be calculated easily are limited. For many functions $f(x)$, it is extremely hard to find the integral using analytical techniques. Also the function $f(x)$ may be given in tabulated form. So in these cases we have to use numerical methods for integration. In these numerical methods, we approximate the integrand $f(x)$ by a suitable polynomial function $P(x)$ and then approximate the integral $\int_a^b f(x)dx$ by $\int_a^b P(x)dx$. Since polynomials are easily integrable, so the latter can always be evaluated.

3.2.1 Newton-Cotes Method

To approximate the value of

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

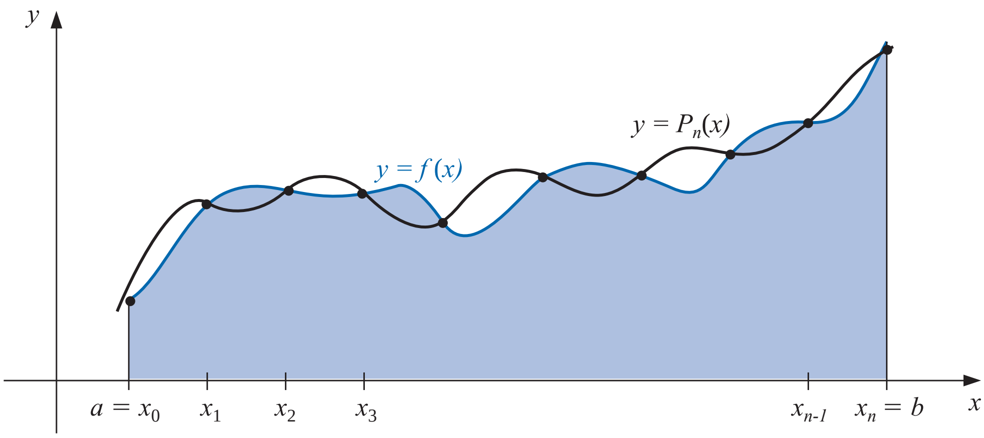
numerically using Newton-Cotes method, we first of all divide the interval $[a, b]$ into n equal parts of length h by points $x_i = a + ih$, $i = 0, 1, \cdots, n$ where $h = \frac{b-a}{n}$. Then

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b$$

forms a partition of $[a, b]$. Let $P_n(x)$ be the interpolating polynomial of $f(x)$ interpolating at $n+1$ points (x_i, f_i), $i = 0, 1, \cdots, n$ where $f_i = f(x_i)$. Then $P_n(x)$ is given by the formula

$$P_n(x) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \cdots + \frac{s(s-1)\cdots(s-n+1)}{n!}\Delta^n f_0$$

where $s = \frac{x - x_0}{h}$ and $\Delta^j f_0 = \Delta^{j-1} f_1 - \Delta^{j-1} f_0$ are the j^{th} forward differences. We now approximate the value of $\int_a^b f(x)dx$ by $\int_a^b P_n(x)dx$.



Therefore

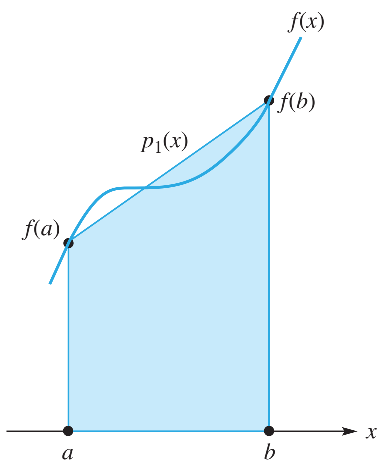
$$\begin{aligned}\int_a^b f(x)dx &\approx \int_a^b P_n(x)dx \\ &= \int_a^b \left[f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \cdots + \frac{s(s-1)\cdots(s-n+1)}{n!}\Delta^n f_0 \right] dx\end{aligned}$$

which is the Newton-Cotes formula for numerically evaluating $\int_a^b f(x)dx$.

Derivation of Trapezoidal rule from Newton-Cotes formula

The trapezoidal rule for numerically evaluating $\int_a^b f(x)dx$ results from Newton-Cotes formula when $n = 1$. Then $h = b - a$ and $x_0 = a$, $x_1 = a + h = b$ and so we have

$$\begin{aligned}
\int_a^b f(x)dx &\approx \int_a^b P_1(x)dx = \int_a^b [f_0 + s\Delta f_0]dx \\
&= f_0 \int_a^b dx + \Delta f_0 \int_a^b s dx = f_0 \, [x]_a^b + \Delta f_0 \int_a^b \frac{x - x_0}{h} dx \\
&= f_0(b-a) + \frac{\Delta f_0}{h} \left[\frac{(x-x_0)^2}{2} \right]_a^b = f_0(b-a) + \frac{\Delta f_0}{h} \left[\frac{(b-x_0)^2}{2} - \frac{(a-x_0)^2}{2} \right] \\
&= f_0 h + \frac{\Delta f_0}{h} \frac{(b-a)^2}{2} = f_0 h + \frac{\Delta f_0 h}{2} = f_0 h + \frac{(f_1 - f_0)h}{2} \\
&= \frac{h}{2}(f_0 + f_1).
\end{aligned}$$



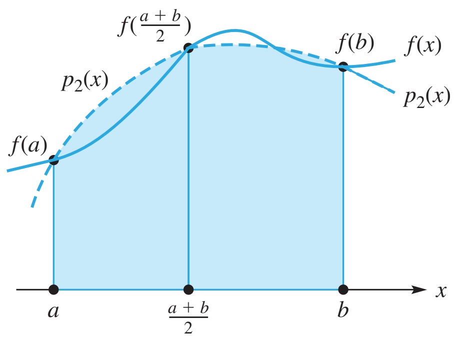
Therefore

$$\int_a^b f(x)dx \approx \frac{h}{2}(f_0 + f_1).$$

Derivation of Simpson's 1/3 rule from Newton-Cotes formula

The Simpson's 1/3 rule for numerically evaluating $\int_a^b f(x)dx$ results from Newton-Cotes formula when $n = 2$. Then $h = \frac{b-a}{2}$ and $x_0 = a$, $x_1 = a + h = \frac{a+b}{2}$, $x_2 = a + 2h = b$ and so we have

$$\begin{aligned}
\int_a^b f(x)dx &\approx \int_a^b P_2(x)dx \\
&= \int_a^b \left[f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 \right] dx \\
&= \int_a^b \left[f_0 + \frac{3s}{2}\Delta f_0 + \frac{s^2}{2}(\Delta f_1 - \Delta f_0) - \frac{s}{2}\Delta f_1 \right] dx \\
&= \frac{h}{3}(f_0 + 4f_1 + f_2).
\end{aligned}$$



Therefore

$$\int_a^b f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2).$$

Derivation of Simpson's 3/8 rule from Newton-Cotes formula

The Simpson's 3/8 rule for numerically evaluating $\int_a^b f(x)dx$ results from Newton-Cotes formula when $n = 3$. Then $h = \dfrac{b-a}{3}$ and $x_0 = a$, $x_1 = a + h = \dfrac{2a+b}{3}$, $x_2 = a + 2h = \dfrac{a+2b}{3}$, $x_3 = a + 3h = b$ and so we have

$$\begin{aligned}
\int_a^b f(x)dx &\approx \int_a^b P_3(x)dx \\
&= \int_a^b \left[f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_0 \right] dx \\
&= \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)
\end{aligned}$$

Therefore

$$\int_a^b f(x)dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3).$$

3.2.2 Composite formulas for evaluating integrals

Composite Trapezoidal Rule

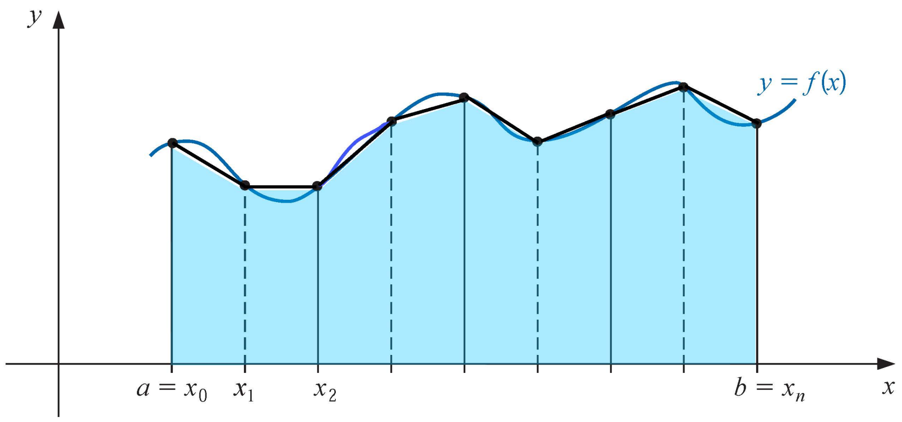
Suppose we have to evaluate the integral $\int_a^b f(x)dx$. We first divide the interval $[a,b]$ into n equally spaced subintervals by points $x_i = a + ih$, $i = 0, 1, \cdots, n$ where $h = \dfrac{b-a}{n}$. Then in each subinterval $[x_{i-1}, x_i]$, $i = 1, 2, \cdots, n$, we approximate the integral $\int_{x_{i-1}}^{x_i} f(x)dx$ by the trapezoidal formula $\frac{h}{2}[f(x_{i-1}) + f(x_i)]$ so that

$$\begin{aligned}
\int_a^b f(x)dx &= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx \\
&\approx \frac{h}{2}[f(x_0) + f(x_1)] + \frac{h}{2}[f(x_1) + f(x_2)] + \cdots + \frac{h}{2}[f(x_{n-1}) + f(x_n)] \\
&= \frac{h}{2}\left[f(x_0) + 2(f(x_1) + \cdots + f(x_{n-1})) + f(x_n)\right]
\end{aligned}$$

Therefore

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f_0 + 2(f_1 + \cdots + f_{n-1}) + f_n\right]$$

which is the composite trapezoidal rule for calculating $\int_a^b f(x)dx$.



Algorithm (Composite Trapezoidal Rule):

INPUT: A function $f(x)$, limits of integration a and b and the number of intervals n.

PROCESS:

SET $h = \dfrac{b-a}{n}$

SET $sum = 0$

FOR $i = 1$ to $n - 1$ {

SET $x = a + hi$
SET $sum = sum + 2f(x)$

}
SET $sum = sum + f(a) + f(b)$
SET $ans = sum \times \frac{h}{2}$

OUTPUT: Approximate value of the integral equal to ans.

Theorem (Error in Composite Trapezoidal Rule): If f is twice continuously differentiable on the interval $[a, b]$, then the error in approximating the integral $\int_a^b f(x)dx$ by composite trapezoidal rule with subinterval length h is

$$E = -\frac{1}{12}(b-a)h^2 f''(\xi)$$

for some $\xi \in (a, b)$.

Exercise

1. Calculate the integral value of the following function from $x = 1.8$ to $x = 3.4$ using composite trapezoidal rule.

x	1.6	1.8	2.0	2.2	2.4	2.6	2.8	3.0	3.2	3.4
$f(x)$	4.953	6.050	7.389	9.025	11.023	13.464	16.445	20.086	24.533	29.964

Solution: Here $h = 0.2$. So using the composite trapezoidal rule, the integral value of the given tabulated function from $x = 1.8$ to $x = 3.4$ is given by

$$\int_{1.8}^{3.4} f(x)\,dx \approx \frac{0.2}{2}[6.050+2(7.839+9.025+11.023+13.464+16.445+20.086+24.533)+29.964]$$
$$= 0.1 \times 239.944 = 23.9944.$$

2. Evaluate the integral of the following function from $x = 1.0$ to $x = 1.8$ using composite trapezoidal rule with $h = 0.1$, $h = 0.2$ and $h = 0.4$

x	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8
$f(x)$	1.543	1.669	1.811	1.971	2.151	2.352	2.577	2.828	3.107

Solution: If $h = 0.2$, then the composite trapezoidal rule gives the following value of the integral:

$$\int_{1.0}^{1.8} f(x)\,dx \approx \frac{0.2}{2}[1.543+2(1.811+2.151+2.577)+3.107] = 0.1 \times 17.728 = 1.7728.$$

Similarly we can calculate approximations for $h = 0.1$ and $h = 0.4$.

3. Evaluate $\int_0^1 e^{-x^2}\, dx$ using composite trapezoidal rule with $n = 5$ up to 6 decimal places.

   Solution: Here $a = 0$, $b = 1$ and $n = 5$. So $h = \frac{b-a}{5} = \frac{1}{5} = 0.2$. So we get the following table:

x	0	0.2	0.4	0.6	0.8	1.0
$f(x)$	1	0.960789	0.852144	0.697676	0.527292	0.367879

   Therefore the approximation of $\int_0^1 e^{-x^2}\, dx$ using composite trapezoidal rule is

   $$\int_0^1 e^{-x^2}\, dx \approx \frac{0.2}{2}[1 + 2(0.960789 + 0.852144 + 0.697676 + 0.527292) + 0.367879)]$$
   $$= 0.1 \times 7.443681 = 0.7443681.$$

4. Use composite trapezoidal rule to evaluate the following up to 5 decimal places.

   a. $\int_0^{\pi} (3\cos x + 5)\, dx$ with $n = 5$

   b. $\int_0^1 \frac{dx}{1+x^2}$ with $n = 5$

   c. $\int_{-0.5}^{0.5} \cos^2 x dx$ with $n = 4$

   d. $\int_e^{e+2} \frac{dx}{x \ln x}$ with $n = 8$

   e. $\int_{0.75}^{1.75} (\sin^2 x - 2x \sin x + 1) dx$ with $n = 8$

   f. $\int_{-0.5}^{0.5} x \ln(x+1) dx$ with $n = 6$. ≈ 0.09363

   g. $\int_0^2 e^{2x} \sin 3x dx$ with $n = 8$. ≈ -13.7560

   h. $\int_0^{\pi} x^2 \cos x dx$ with $n = 6$. ≈ -6.42872

   i. $\int_1^2 \frac{e^x}{x} dx$ with $n = 4$.

Composite Simpson's 1/3 Rule

Suppose we have to evaluate the integral $\int_a^b f(x)dx$. We first divide the interval $[a, b]$ into n equally spaced subintervals by points $x_i = a + ih$, $i = 0, 1, \cdots, n$ where $h = \frac{b-a}{n}$. However, here we assume that the number of such subintervals is even i.e., n is even. Then for each subinterval $[x_{2i}, x_{2i+2}]$, $i = 0, 1, \cdots, \frac{n}{2} - 1$, we approximate the integral $\int_{x_{2i}}^{x_{2i+2}} f(x)dx$ by the Simpson's 1/3 formula

$$\frac{h}{3}[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})]$$

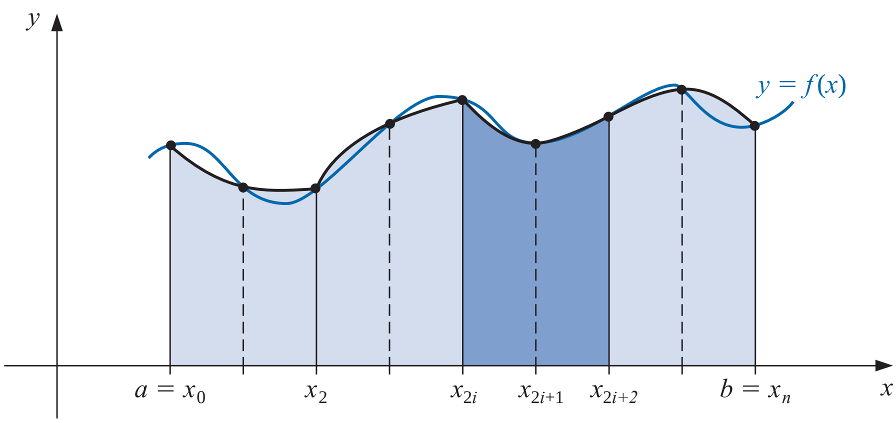
so that

$$\begin{aligned}
\int_a^b f(x)dx &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx \\
&\approx \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + \frac{h}{3}[f(x_2) + 4f(x_3) + f(x_4)] \\
&\qquad + \cdots + \frac{h}{3}[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)] \\
&= \frac{h}{3}[f(x_0) + 4(f(x_1) + f(x_3) + \cdots + f(x_{n-1})) + \\
&\qquad 2(f(x_2) + f(x_4) + \cdots + f(x_{n-2})) + f(x_n)]
\end{aligned}$$

Therefore

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

which is the composite Simpson's 1/3 rule for approximating $\displaystyle\int_a^b f(x)dx$.



Algorithm (Composite Simpson's 1/3 Rule):

INPUT: A function $f(x)$, endpoints a and b and an even number of intervals n.

PROCESS:

SET $h = \dfrac{b-a}{n}$

SET $sum = 0$

FOR $i = 1$ to $\dfrac{n}{2}$ {

SET $x = a - h + 2hi$
SET $sum = sum + 4f(x)$
IF $i \neq \frac{n}{2}$ THEN SET $sum = sum + 2f(x + h)$

}
SET $sum = sum + f(a) + f(b)$
SET $ans = sum \times \frac{h}{3}$

OUTPUT: Approximate value of the integral equal to ans.

Theorem (Error in Composite Simpson's 1/3 Rule): If f is four times continuously differentiable on the interval $[a, b]$, then the error in approximating the integral $\int_a^b f(x)dx$ by composite Simpson's 1/3 rule with subinterval length h is

$$E = -\frac{1}{180}(b - a)h^4 f^{(4)}(\xi)$$

for some $\xi \in (a, b)$.

Exercise

1. Calculate the integral value of the following function from $x = 0$ to $x = 1.6$ using Simpson's $1/3$ rule:

x	0	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
$f(x)$	0	0.24	0.55	0.92	1.63	1.84	2.37	2.95	3.56

Solution: Here $h = 0.2$. So using the composite Simpson's $1/3$ rule, the integral value of the given function is approximated as

$$\int_0^{1.6} f(x)\, dx \approx \frac{0.2}{3}[0 + 4(0.24 + 0.92 + 1.84 + 2.95) + 2(0.55 + 1.63 + 2.37) + 3.56]$$

$$= \frac{0.2}{3} \times 36.46 = 2.43.$$

2. Evaluate the integral of the following function from $x = 0.7$ to $x = 1.9$ using Simpson's $1/3$ rule:

x	0.7	0.9	1.1	1.3	1.5	1.7	1.9	2.1
$f(x)$	0.64835	0.91360	1.16092	1.36178	1.49500	1.55007	1.52882	1.44513

(Ans: 1.51938)

3. Compute the integral of $f(x) = \dfrac{\sin x}{x}$ between $x = 0$ to $x = 1$ using Simpson's $1/3$ rule with $h = 0.5$ and then $h = 0.25$.

   Solution: Taking $h = 0.25$, we get the following table:

x	0	0.25	0.5	0.75	1
$\frac{\sin x}{x}$	1	0.98962	0.95885	0.90885	0.84147

   Here we have use the fact that $\lim_{x\to 0} \dfrac{\sin x}{x} = 1$. Now for $h = 0.5$, the value of the integral $\displaystyle\int_0^1 \frac{\sin x}{x}\, dx$ is approximated as

$$\int_0^1 \frac{\sin x}{x}\, dx \approx \frac{0.5}{3}[1 + 4 \times 0.95885 + 0.84147] = \frac{0.5}{3} \times 5.67687 = 0.946145.$$

   Similarly we can approximate the integral taking $h = 0.25$.

4. Use composite Simpson's $1/3$ rule to evaluate the following up to 5 decimal places using $n = 4$:

   a. $\displaystyle\int_0^\pi (3\cos x + 5)\, dx$ b. $\displaystyle\int_0^1 \frac{dx}{1 + x^2}$ c. $\displaystyle\int_1^2 \frac{e^x}{x}\, dx$

   Solution:

   a. Here $a = 0$, $b = \pi$ and $n = 4$. So $h = \dfrac{b-a}{n} = \dfrac{\pi}{4}$. Therefore we get the following table:

x	0	$\frac{\pi}{4}$	$\frac{\pi}{2}$	$\frac{3\pi}{4}$	π
$3\cos x + 5$	8	7.12132	5	2.87868	2

   Hence the approximation of the integral $\displaystyle\int_0^\pi (3\cos x + 5)\, dx$ using composite Simpson's $1/3$ rule is

$$\int_0^\pi (3\cos x+5)\, dx \approx \frac{\pi/4}{3}[8+4(7.12132+2.87868)+2\times 5+2] = \frac{\pi}{12}\times 60 = 5\pi = 15.70796.$$

5. Calculate with 5 decimal places the problems $4(c)$-$4(i)$ of previous problem.

Composite Simpson's 3/8 Rule

Suppose we have to evaluate the integral $\displaystyle\int_a^b f(x)dx$. We first divide the interval $[a, b]$ into n equally spaced subintervals by points $x_i = a + ih$, $i = 0, 1, \cdots, n$ where $h = \dfrac{b-a}{n}$. However, here we assume that the number of such subintervals is divisible by 3. Then for each subinterval

$[x_{3i}, x_{3i+3}]$, $i = 0, 1, \cdots, \dfrac{n}{3} - 1$, we approximate the integral $\int_{x_{3i}}^{x_{3i+3}} f(x)dx$ by the Simpson's 3/8 formula $\dfrac{3h}{8}[f(x_{3i}) + 3f(x_{3i+1}) + 3f(x_{3i+2}) + f(x_{3i+3})]$ so that

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_3} f(x)dx + \int_{x_3}^{x_6} f(x)dx + \cdots + \int_{x_{n-3}}^{x_n} f(x)dx \\ &\approx \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] + \frac{3h}{8}[f(x_3) + 3f(x_4) + 3f(x_5) + f(x_6)] \\ &\qquad + \cdots + \frac{3h}{8}[f(x_{n-3}) + 3f(x_{n-2}) + 3f(x_{n-1}) + f(x_n)] \\ &= \frac{3h}{8}[f(x_0) + 3(f(x_1) + f(x_4) + \cdots + f(x_{n-2})) + 3(f(x_2) + f(x_5) + \cdots + f(x_{n-1})) \\ &\qquad + 2(f(x_3) + f(x_6) + \cdots + f(x_{n-3})) + f(x_n)]\end{aligned}.$$

Therefore

$$\begin{aligned}\int_a^b f(x)dx \approx \frac{3h}{8}[&f_0 + 3(f_1 + f_4 + \cdots + f_{n-2}) + 3(f_2 + f_5 + \cdots + f_{n-1}) \\ &+ 2(f_3 + f_6 + \cdots + f_{n-3}) + f_n]\end{aligned}$$

which is the composite Simpson's 3/8 rule for approximating $\displaystyle\int_a^b f(x)dx$.

Algorithm (Composite Simpson's 3/8 Rule):

INPUT: A function $f(x)$, endpoints a and b and number of intervals n which is divisible by 3.

PROCESS:

SET $h = \dfrac{b-a}{n}$
SET $sum = 0$
FOR $i = 1$ to $\dfrac{n}{3}$ {
  SET $x = a - 2h + 3hi$
  SET $sum = sum + 3f(x)$
  SET $sum = sum + 3f(x+h)$
  IF $i \neq \dfrac{n}{3}$ THEN SET $sum = sum + 2f(x+2h)$
}
SET $sum = sum + f(a) + f(b)$
SET $ans = sum \times \dfrac{3h}{8}$

OUTPUT: Approximate value of the integral equal to ans.

Exercise

1. Apply Simpson's $3/8$ rule to integrate $f(x) = e^{-x^2}$ from $x = 0.2$ to $x = 1.4$ with $n = 6$.

   Solution: Here $f(x) = e^{-x^2}$ $a = 0.2$, $b = 1.4$ and $n = 6$. Therefore $h = \dfrac{b-a}{n} = \dfrac{1.2}{6} = 0.2$. So we get the following table:

x	0.2	0.4	0.6	0.8	1.0	1.2	1.4
$f(x)$	0.960789	0.852144	0.697676	0.527292	0.367879	0.236928	0.140858

   Therefore the approximation of $\displaystyle\int_{0.2}^{1.4} e^{-x^2}\,dx$ using composite Simpson's $3/8$ rule is

   $$\int_{0.2}^{1.4} e^{-x^2}\,dx \approx \frac{3 \times 0.2}{8}[0.960789 + 3(0.852144 + 0.367879) + 3(0.697676 + 0.236928)$$

   $$+2 \times 0.527292 + 0.140858] = 0.075 \times 8.620112 = 0.6465084.$$

2. Evaluate $\displaystyle\int_1^7 f(t)\,dt$ using composite Simpson's $3/8$ rule using the following table.

t	1	2	3	4	5	6	7
$f(t)$	81	75	80	83	78	70	60

   Solution: Here $n = 6$, and $a = 1$, $b = 7$. So $h = \dfrac{b-a}{n} = \dfrac{7-1}{6} = 1$. Therefore, using composite Simpson's $3/8$ rule, we get

   $$\int_1^7 f(t)\,dt \approx \frac{3h}{8}[81 + 3(75 + 78) + 3(80 + 70) + 2 \times 83 + 60] = \frac{3}{8} \times 1216 = 456.$$

3. Use Simpson's $3/8$ rule to evaluate

   a. $\displaystyle\int_1^{2.8} (x^3 + 1)\,dx$ with $n = 9$

   b. $\displaystyle\int_0^{\pi/2} \sin x\,dx$ with $n = 6$

3.2.3 Numerical Double Integration

Suppose we have to evaluate the double integral

$$\int_a^b \int_c^d f(x, y)dydx$$

where a, b, c and d are constants. For this, we write it as an iterated integral as

$$\int_a^b \left(\int_c^d f(x,y)dy \right) dx.$$

This can be evaluated by first holding x variable constant while integrating with respect to y variable to obtain the inner integral and then integrating with respect to the x variable to obtain the outer integral. While integrating, we can use any of the trapezoidal, Simpson's $\frac{1}{3}$ or Simpson's $\frac{3}{8}$ rule for both the x and y variables or any combination of these rules as required.

3.2.4 Romberg Integration

Let $\int_a^b f(x)\ dx$ be the integral that has to be evaluated. Let the interval $[a, b]$ be divided into subintervals of equal length h and $T(h)$ denote the approximation of the integral $\int_a^b f(x)\ dx$ using composite trapezoidal rule with subinterval length h. A better approximation of $\int_a^b f(x)\ dx$ can be obtained by taking subintervals of length $\frac{h}{2}$ which we denote by $T\left(\frac{h}{2}\right)$. Then the Romberg method of integration uses $T(h)$ and $T\left(\frac{h}{2}\right)$ to obtain a better approximation $R(h)$ using extrapolation as follows:

$$R(h) = T\left(\frac{h}{2}\right) + \frac{1}{4^n - 1}\left[T\left(\frac{h}{2}\right) - T(h)\right]$$

where n is the order of the error.

Algorithm (Romberg Integration):

INPUT: A function $f(x)$, limits of integration $x = a$ to $x = b$, and maximum number of stages NST.

PROCESS:

SET $h = \dfrac{(b-a)}{2}$

SET sum$= f(a) + 2f(a+h) + f(b)$

SET $T(0,0) =$sum$\times \dfrac{h}{2}$

SET $d = 2h$

FOR ST$= 1$ TO NST {

SET $h = \dfrac{h}{2}$

Set $d = \dfrac{d}{2}$
FOR $i = 1$ to 2^{ST} {
  SET $x = a - h + di$
  SET sum= sum+$2 \times f(x)$
}
SET $T(ST, 0)$ =sum$\times \dfrac{h}{2}$
FOR $j = 1$ TO ST {
  SET $T(ST, j) = T(ST, j-1) + \dfrac{T(ST, j-1) - T(ST-1, j-1)}{4^j - 1}$
}
}

OUTPUT: Romberg integral table

Exercise

1. Use Romberg integration to find the integral of e^{-x^2} between the limits of $a = 0.2$ and $b = 1.5$ with initial subinterval size as $h = \dfrac{b-a}{2} = 0.65$ and final size $h = \dfrac{b-a}{16} = 0.08125$.

   Solution: Let $T(h)$ denote the approximation of the integral $\displaystyle\int_{0.2}^{1.5} e^{-x^2}\, dx$ using composite trapezoidal rule with subinterval length h. We need to calculate $T(h)$ for $h = 0.65, 0.325, 0.1625$ and 0.08125. We make the table as follows:

x	$f(x)$
0.2	0.96079
0.28125	0.92395
0.3625	0.87686
0.44375	0.82126
0.525	0.75910
0.60625	0.69244
0.6875	0.62334
76875	0.55379
0.85	0.48554
0.93125	0.42012
1.10125	0.35874
1.09375	0.30231
1.175	0.25142
1.25625	0.20635
1.3375	0.16714
1.41875	0.13361
1.5	0.10540

Therefore

$$T(0.08125) = \frac{0.08125}{2}[0.96979+2(0.92395+0.87686+0.82126+0.75910+0.69244+0.62334 +0.55379+0.48554+0.42012+0.35874+0.30231+0.25142+0.20635 +0.16714+0.13361)+0.10540] = 0.65886$$

$$T(0.1625) = \frac{0.1625}{2}[0.96979+2(0.87686+0.75910+0.62334+0.48554 +0.35874+0.25142+0.16714)+0.10540] = 0.6589$$

$$T(0.325) = \frac{0.325}{2}[0.96979+2(0.75910+0.48554+0.25142)+0.10540] = 0.65948$$

$$T(0.65) = \frac{0.65}{2}[0.96979+2\times 0.48554+0.10540] = 0.66211$$

Using the above approximations, we can calculate more accurate approximations as shown in the table below:

Romberg Table of Integrals

$$\begin{array}{cccc}
0.66211 & & & \\
 & 0.65860 & & \\
0.65948 & & 0.65882 & \\
 & 0.65881 & & 0.65882 \\
0.65898 & & 0.65882 & \\
 & 0.65882 & & \\
0.65886 & & &
\end{array}$$

Calculation of approximations in second column:

$$0.65948 + \frac{1}{4^1-1}[0.65948-0.66211] = 0.65860$$
$$0.65898 + \frac{1}{4^1-1}[0.65898-0.65948] = 0.65881$$
$$0.65886 + \frac{1}{4^1-1}[0.65886-0.65898] = 0.65882$$

Calculation of approximations in third column:

$$0.65881 + \frac{1}{4^2-1}[0.65881-0.65860] = 0.65882$$
$$0.65882 + \frac{1}{4^2-1}[0.65882-0.65881] = 0.65882$$

Calculation of approximations in fourth column:

$$0.65882 + \frac{1}{4^3-1}[0.65882-0.65882] = 0.65882$$

Therefore, the approximation of the integral $\int_{0.2}^{1.5} e^{-x^2}\ dx$ using Romberg integration is 0.65882.

2. Use the following data table to get the integral by Romberg method between the limits $x = 1.8$ to $x = 3.4$ and beginning with $h = 0.8$.

x	$f(x)$
1.6	4.953
1.8	6.050
2.0	7.389
2.2	9.025
2.4	11.025
2.6	13.464
2.8	16.445
3.0	20.086
3.2	24.533
3.4	29.964
3.6	36.598
3.8	44.701

Solution:

Romberg Table of Integrals

25.1768		
	23.9181	
24.2328		23.9147
	23.9149	
23.9944		

3.2.5 Gaussian Integration

All the integration formulas discussed so far (eg., composite trapezoidal rule, composite Simpson's $1/3$ rule, composite Simpson's $3/8$ rule) use function values at predetermined equidistant x-values. Gaussian integration technique is based on the concept that the accuracy of numerical integration can be improved by using function values at x-values selected wisely rather than on equidistant basis.

Given a function $f(x)$, we first evaluate the integral $\int_{-1}^{1} f(x)\ dx$. The Gaussian n-point formula for evaluating this integral is given by

$$\int_{-1}^{1} f(x)\ dx \approx \sum_{i=1}^{n} w_i f(x_i) \cdots\cdots (1).$$

There are $2n$ unknowns in the above formula, namely w_i, x_i, $i = 1, 2, \cdots, n$. To find these $2n$ unknowns, we first assume that the formula (1) is exact when $f(x)$ are polynomials of degree up to $2n-1$ i.e.,

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

when $f(x) = x^{2n-1}$, $f(x) = x^{2n-2}$, $\cdots$, $f(x) = x^2$, $f(x) = x$, $f(x) = 1$. This gives

$$\int_{-1}^{1} x^k\, dx = \sum_{i=1}^{n} w_i x_i^k$$

for each $k = 0, 1, 2, \cdots, 2n-1$. But

$$\int_{-1}^{1} x^k\, dx = \begin{cases} 0 & \text{for} \quad k = 1, 3, 5, \cdots, 2n-1 \\ \dfrac{2}{k+1} & \text{for} \quad k = 0, 2, 4, \cdots, 2n-2 \end{cases}$$

So

$$\sum_{i=1}^{n} w_i x_i^k = \begin{cases} 0 & \text{for} \quad k = 1, 3, 5, \cdots, 2n-1 \\ \dfrac{2}{k+1} & \text{for} \quad k = 0, 2, 4, \cdots, 2n-2 \end{cases}$$

Solving these $2n$ equations, we get the required $2n$ parameters for the Gaussian n-point formula (1).

When $n = 2$, we get the Gaussian 2-point formula by solving the 4 equations below:

$$w_1 x_1^0 + w_2 x_2^0 = \frac{2}{1} = 2 \Rightarrow w_1 + w_2 = 2 \cdots\cdots (A)$$

$$w_1 x_1^1 + w_2 x_2^1 = 0 \cdots\cdots (B)$$

$$w_1 x_1^2 + w_2 x_2^2 = \frac{2}{3} \cdots\cdots (C)$$

$$w_1 x_1^3 + w_2 x_2^3 = 0 \cdots\cdots (D)$$

Multiplying (B) by x_1^2 and subtracting (D) from it, we get

$$w_2 x_2 x_1^2 - w_2 x_2^3 = 0 \Rightarrow w_2 x_2 (x_1 - x_2)(x_1 + x_2) = 0.$$

If $w_2 = 0$, then from (B), $w_1 x_1 = 0$. But this contradicts (C) because we would get $0 = \frac{2}{3}$. If $x_2 = 0$, then $w_1 x_1 = 0$ from (B) which again contradicts (C). If $x_1 - x_2 = 0$ i.e., $x_1 = x_2$, then from (B) $(w_1 + w_2)x_1 = 0$ which implies $x_1 = x_2 = 0$ again contradicting (C). So we must have $x_1 + x_2 = 0$ i.e., $x_1 = -x_2$. So from (B), $w_1 x_1 - w_2 x_1 = 0 \Rightarrow w_1 - w_2 = 0$ since $x_1 = 0$ will contradict (C). From (A), we have therefore, $w_1 = w_2 = 1$. Now from (C),

$$x_1^2 + x_2^2 = \frac{2}{3} \Rightarrow (-x_2)^2 + x_2^2 = \frac{2}{3} \Rightarrow x_2 = \frac{1}{\sqrt{3}}$$

and so $x_1 = -x_2 = \dfrac{-1}{\sqrt{3}}$. Therefore

$$\int_{-1}^{1} f(x)\,dx = w_1 f(x_1) + w_2 f(x_2) = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

which is the 2-point Gaussian formula.

Similarly, one can calculate 3-point, 4-point and in general n-point Gaussian formula. The following table lists the weights w_i and nodes x_i for different values of n.

n	i	w_i	x_i
2	1	1	-0.57735
	2	1	0.57735
3	1	0.55556	-0.77460
	2	0.88889	0
	3	0.55556	0.77460
4	1	0.34785	-0.86114
	2	0.65215	-0.33998
	3	0.65215	0.33998
	4	0.34785	0.86114
5	1	0.23693	-0.90618
	2	0.47863	-0.53847
	3	0.56889	0
	4	0.47863	0.53847
	5	0.23693	0.90618

Changing the limits of integration: Gaussian integration requires the limit of integration to be from -1 to 1. If the limits of integration are from a to b and not from -1 to 1, then we must change the interval of integration to $(-1, 1)$ by a change of variable as follows:

If $\displaystyle\int_a^b f(x)\,dx$ is to be evaluated, let the variable x be changed to y as

$$x = \frac{(b-a)y + b + a}{2} \cdots\cdots (1)$$

Then, when $x = a$, we get $y = -1$ and when $x = b$, we get $y = 1$. Also from (1),

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

so $dx = \dfrac{b-a}{2}\,dy$. Therefore

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_{-1}^{1} f\left(\frac{(b-a)y+b+a}{2}\right)\left(\frac{b-a}{2}\right)\,dy \\ &= \frac{(b-a)}{2}\int_{-1}^{1} f\left(\frac{(b-a)y+b+a}{2}\right)\,dy.\end{aligned}$$

Now the integral

$$\int_{-1}^{1} f\left(\frac{(b-a)y+b+a}{2}\right)\,dy$$

can be evaluated using the Gaussian technique.

Exercise

1. Evaluate $\displaystyle\int_{0.2}^{1.5} e^{-x^2}\,dx$ using Gaussian integration 3-point formula.

   Solution: Let
   $$x = \frac{(1.5-0.2)y+1.5+0.2}{2} = 0.65y + 0.85$$
   Then the limits of integration changes from $(0.2, 1.5)$ to $(-1, 1)$ so that
   $$\int_{0.2}^{1.5} e^{-x^2}\,dx = \frac{1.5-0.2}{2}\int_{-1}^{1} e^{-(0.65y+0.85)^2}\,dy$$
   Now, using the Gaussian 3-point formula, we get
   $$\int_{-1}^{1} e^{-(0.65y+0.85)^2}\,dy$$
   $$= 0.55556\times e^{-(0.65\times -0.77460+0.85)^2} + 0.88889\times e^{-(0.65\times 0+0.85)^2} + 0.55556\times e^{-(0.65\times 0.77460+0.85)^2}$$
   $$= 0.55556\times 0.88686 + 0.88889\times 0.48554 + 0.55556\times 0.16010 = 1.01324.$$
   Therefore
   $$\int_{0.2}^{1.5} e^{-x^2}\,dx = \frac{1.5-0.2}{2}\times 1.01324 = 0.65861.$$

2. Evaluate $\displaystyle\int_{0}^{\pi/2} \sin x\,dx$ using 2-point Gaussian formula. (Ans: ≈ 0.99847)

3. Evaluate $\displaystyle\int_{-1}^{1} \frac{dx}{1+x^2}$ using 3-point Gaussian formula. (Ans: ≈ 1.5)

4. Evaluate $\displaystyle\int_{0}^{1} \frac{\sin x}{x}$ using 4-point Gaussian formula. (Ans: ≈ 0.946085)

5. Evaluate $\displaystyle\int_{1}^{2} (\ln x + x^2\sin x)dx$ using 3-point Gaussian formula.

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