MC3010: Differential Equations & Numerical Methods

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NUMERICAL COMPUTATION

Lecture – 05: Numerical Integration

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Numerical Methods : Syllabus Outline

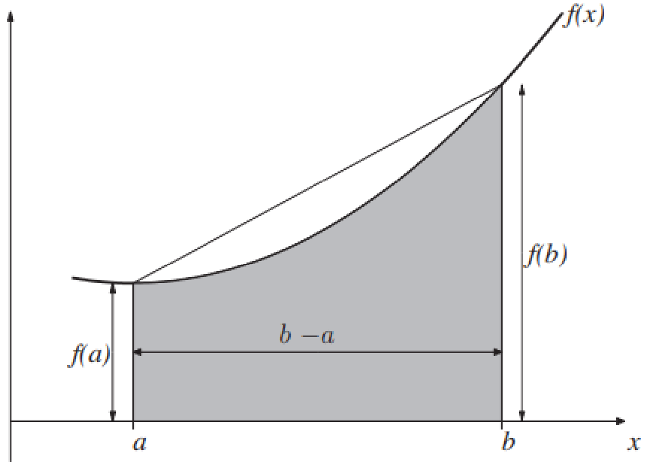
1. Numerical Errors
2. Roots of Equations
3. Numerical Interpolation
4. Numerical Differentiation
5. **Numerical Integration**
6. Numerical Solution for Ordinary Differential Equations

Integrals

We encounter definite integrals in a wide range of applications, generally in the form

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

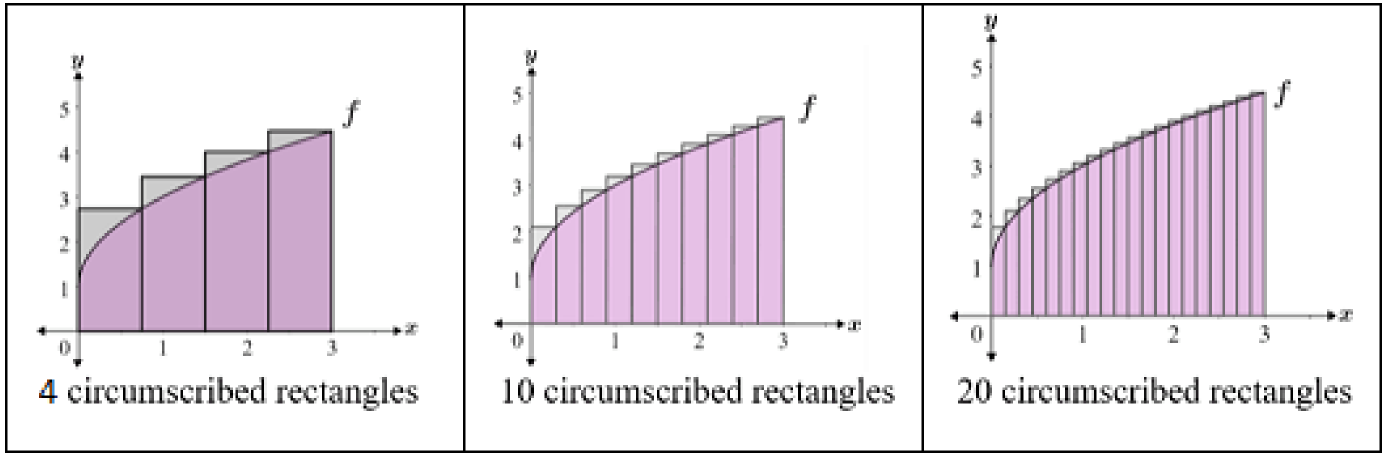
where $f(x)$ is the integrand and a and b are the limits of integration. The value of this definite integral is the area of the region between the graph of $f(x)$ and the x-axis, bounded by the lines $x = a$ and $x = b$.



$$\int_a^b f(x)\,dx \quad = \quad \text{grey shaded area}$$

Introduction to Numerical integration

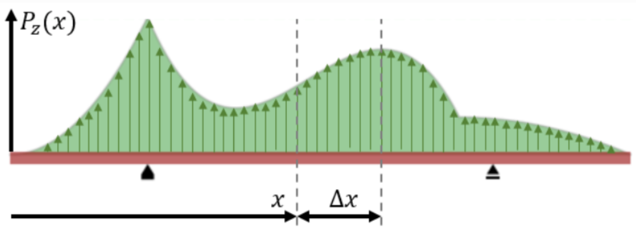
Numerical integration is a mathematical technique for approximating the value of a definite integral of a function using numerical methods.



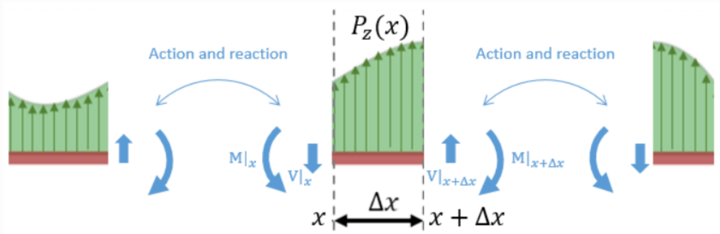
It involves dividing the interval of integration into small subintervals, and then approximating the area under the curve of the function over each subinterval using a simple geometric shape, such as a rectangle or trapezoid. These approximations are then summed together to give an estimate of the overall area under the curve, and hence an approximation to the value of the definite integral.

Numerical Integrations

Let's consider an arbitrarily loaded beam as shown in the figure below, where $\mathbf{P_z}(x)$ is an arbitrarily distributed load applied to the beam.



Let's zoom-in and draw a free-body diagram of a given beam segment $[x_0 \le x \le x_0 + \Delta x]$.



Free body diagram of a differential segment of the beam

The equilibrium of vertical forces yields then the following:

$$
\begin{aligned}
\sum \mathbf{F_z} &= 0 \\
V(x+\Delta x) - V(x) + \overline{\mathbf{P_z}}(x)\Delta x &= 0 \\
\frac{V(x+\Delta x) - V(x)}{\Delta x} &= -\overline{\mathbf{P_z}}(x) \\
\lim_{\Delta x \to 0} \quad \boxed{\frac{dV(x)}{dx} = -\mathbf{P_z}(x)}
\end{aligned}
$$

The equilibrium of moments can be written as:

$$
\begin{aligned}
\sum \mathbf{M}|_{\mathbf{x}+\Delta \mathbf{x}} &= 0 \\
M(x+\Delta x) - M(x) - V(x)\Delta x + (\overline{\mathbf{P_z}}(x)\Delta x \cdot \tfrac{\Delta x}{2}) &= 0 \\
\frac{M(x+\Delta x) - M(x)}{\Delta x} + \underbrace{(\overline{\mathbf{P_z}}(x)\Delta x \cdot \tfrac{\Delta x}{2})}_{\Delta x^2 \to 0} &= V(x) \\
\lim_{\Delta x \to 0} \quad \boxed{\frac{dM(x)}{dx} = V(x)}
\end{aligned}
$$

$$V = \frac{dM}{dx}$$

$$\frac{dV}{dx} = \frac{d^2M}{dx^2} = q$$

$$\int_{V_A}^{V_B} dV = V_B - V_A = \int_{x_A}^{x_B} q\, dx$$

$$\int_{M_A}^{M_B} dM = M_B - M_A = \int_{x_A}^{x_B} V\, dx$$

- The change in shear force from A to B is equal to the area of the loading diagram between x_A and x_B.
- The change in moment from A to B is equal to the area of the shear-force diagram between x_A and x_B.

Numerical integration is a primary tool used by engineers and scientists to obtain approximate answers for definite integrals that cannot be solved analytically.

Numerical integration is used **when the integrand is given as a set of data or, the integrand is an analytical function, but the antiderivative is not easily found.**

$$f(x) = \int_0^x \frac{t^3}{e^t - 1} dt$$

$$f(x) = \int_a^b \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx$$

Applications of Numerical integration in Engineering field

1. Computational fluid dynamics: used to approximate the integrals that arise in the discretization of the partial differential equations, allowing engineers to simulate the flow of fluids in complex geometries and obtain insights into aerodynamics, heat transfer, and other important engineering applications.
2. Control system analysis and design: In control system analysis and design, numerical integration is used to simulate the behavior of dynamic systems and obtain time-domain response, frequency response, and other system characteristics

1. Electromagnetic simulations: In electromagnetic simulations, numerical integration is used to compute the electric and magnetic fields, currents, and other electromagnetic quantities in complex structures.
2. Signal processing: Numerical integration is used in various signal processing applications, such as digital filters, Fourier analysis, and spectral analysis.
3. Finite element analysis: Numerical integration is used to approximate the integrals that arise in the formulation of finite element equations, allowing engineers to simulate the behavior of structures under different loads and boundary conditions.

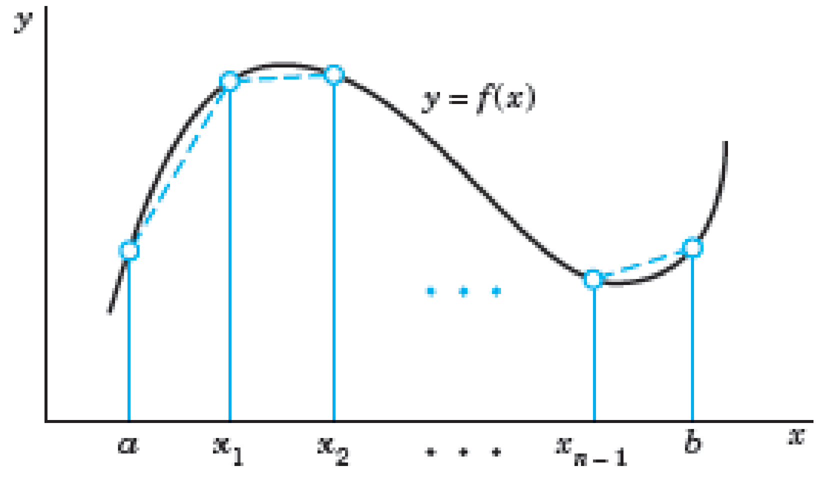
Approaches of Numerical Integrations

- Trapezoidal Rule
- Simpson's Rule
- Gauss-Legendre Rule

1. Trapezoidal Rule

- The trapezoidal rule is a numerical integration method that approximates the area under a curve by dividing it into trapezoids and computing the sum of their areas.
- This approximation assumes that the function is linear between the two endpoints and provides a better approximation to the area under the curve than the rectangular rule.
- One advantage of the trapezoidal rule is that it is easy to implement and can be applied to a wide range of functions.
- However, it may not be very accurate for functions that have significant curvature or oscillations over the interval. To improve the accuracy of the approximation, other methods such as Simpson's rule or Gaussian quadrature can be used.

If we take the same subdivisions and approximate f by a broken line segments (chords) with endpoints $[a, f(a)]$, $[x_1, f(x_1)]$, ….. $[b, f(b)]$ on the curve of f .
Then the area under the curve of f between a and b is approximated by n trapezoids of areas,



Trapezoidal rule

$$\frac{1}{2}[f(a)+f(x_1)]h, \quad \frac{1}{2}[f(x_1)+f(x_2)]h \;, \; .... \;, \quad \frac{1}{2}[f(x_{n-1})+f(b)]h$$

The **formula for the Trapezoidal rule** can be expressed as:

$$\boxed{J = \int_a^b f(x)dx \;\approx h\,[\frac{1}{2}f(a)+f(x_1)+f(x_2)+..+f(n-1)+\frac{1}{2}f(b)]}$$

Where $h = (b-a)/n$ and x_i , a and b are nodes.

Example : 01

Evaluate $J = \int_0^1 e^{-x^2} dx$ using Trapezoidal rule with $n = 10$.

Note that this integral cannot be evaluated by elementary calculus,

j	x_j	x_j^2	$e^{-x_j^2}$	
0	0	0	1.000000	
1	0.1	0.01		0.990050
2	0.2	0.04		0.960789
3	0.3	0.09		0.913931
4	0.4	0.16		0.852144
5	0.5	0.25		0.778801
6	0.6	0.36		0.697676
7	0.7	0.49		0.612626
8	0.8	0.64		0.527292
9	0.9	0.81		0.444858
10	1.0	1.00	0.367879	
Sums			1.367879	6.778167

$$J = \int_a^b f(x)dx \approx h\left[\frac{1}{2}f(a) + f(x_1) + f(x_2) + .. + f(n-1) + \frac{1}{2}f(b)\right]$$

$$J \approx 0.1\,(0.5x1.367879 + 6.778167) = 0.746211$$

Example : 02

Evaluate the definite integral, $J = \int_{-1}^{1} \frac{1}{x+2} dx$ using trapezoidal rule with $n = 8$.

Solution :

With the limits of integration at $b = 1, a = -1$, we find the spacing size as

$$h = (b - a)/n = 2/8 = 0.25.$$

The nine nodes are thus defined as $x_1 = -1, -0.75, -0.5, \ldots, 0.75, 1 = x_9$.

$$\int_{-1}^{1} \frac{1}{x+2} dx = \frac{0.25}{2}[f(-1) + 2f(-0.75) + 2f(-0.5) + \cdots + 2f(0.75) + f(1)] = 1.1032$$

Program (**Composite Trapezoidal Rule**). To approximate the integral

$$\int_a^b f(x)\,dx \approx \frac{h}{2}(f(a)+f(b)) + h\sum_{k=1}^{M-1} f(x_k)$$

by sampling $f(x)$ at the $M+1$ equally spaced points $x_k = a + kh$, for $k = 0, 1, 2, \ldots, M$. Notice that $x_0 = a$ and $x_M = b$.

```
function s=traprl(f,a,b,M)

%Input   - f is the integrand input as a string 'f'
%        - a and b are upper and lower limits of integration
%        - M is the number of subintervals
%Output  - s is the trapezoidal rule sum

h=(b-a)/M;
s=0;
for k=1:(M-1)
   x=a+h*k;
   s=s+feval(f,x);
end
s=h*(feval(f,a)+feval(f,b))/2+h*s;
```

Exercises

Apply the trapezoid rule with $h = 1/4$ to approximate the following integrals

1. $$I = \int_0^1 x(1-x^2)dx = \frac{1}{4}.$$

2. $$I = \int_0^1 \frac{1}{\sqrt{1+x^4}}dx = 0.92703733865069.$$

3. $$I = \int_0^1 \ln(1+x)dx = 2\ln 2 - 1.$$

4. $$I = \int_0^1 \frac{1}{1+x^3}dx = \frac{1}{3}\ln 2 + \frac{1}{9}\sqrt{3}\pi.$$

5. $$I = \int_1^2 e^{-x^2}dx = 0.1352572580.$$

Error Estimate for Trapezoidal Rule

The error in the trapezoidal rule approximation can be estimated using the following formula:

$$\epsilon = -\frac{(b-a)^3}{12n^2} f''(\hat{t}) = -\frac{b-a}{12} h^2 f''(\hat{t})$$

Where, $\hat{t}$ is a (suitable ,unknown) value between x_0 and x_1

Error Bound

Error Bounds are obtained by taking the largest value for f'', say M_2 and the smallest value M_2^*, in the interval of integration. Then

$$KM_2 \leqq \epsilon \leqq KM_2^* \quad \text{where} \quad K = -\frac{(b-a)^3}{12n^2} = -\frac{b-a}{12} h^2.$$

Example : 03

Estimate the error in the computation of $J = \int_0^1 e^{-x^2}\,dx$ using Trapezoidal rule with $n = 10$.

By differentiation, $f''(x) = 2(2x^2 - 1)e^{-x^2}$.

$f'''(x) > 0$ if $0 < x < 1$,

so that the minimum and maximum occur at the ends of the interval.

We compute $M_2 = f''(1) = 0.735759$ and $M_2^* = f''(0) = -2$.

Furthermore, $K = -1/1200$,

$-0.000614 \leqq \epsilon \leqq 0.001667$.

Hence the exact value of J must lie between

$$0.746211 - 0.000614 = 0.745597 \quad \text{and} \quad 0.746211 + 0.001667 = 0.747878.$$

Example : 04

Consider $f(x) = 2 + \sin(2\sqrt{x})$. Investigate the error when the Trapezoidal rule is used over [1,6] and the number of sub-intervals 10, 20, 40, 80 and 160.

M	h	$\mathrm{T}(f,h)$	$E_T(f,h) = \boldsymbol{O}(h^2)$
10	0.5	8.19385457	-0.01037540
20	0.25	8.18604926	-0.00257006
40	0.125	8.18412019	-0.00064098
80	0.0625	8.18363936	-0.00016015
160	0.03125	8.18351924	-0.00004003

true value of the definite integral is

$$\int_1^6 f(x)\,dx = F(x)\Big|_{x=1}^{x=6} = 8.1834792077.$$

This is important to observe that when h is reduced by a factor of ½ successive errors $E_T(f,h)$ are diminished by approximately ¼ . This confirms that the order is $\boldsymbol{O}(h^2)$

2. Simpson’s Rule of Integration

- **Simpson’s one third rule** approximates the function with a **quadratic polynomial (second-degree polynomial i.e., three points needed to determine this polynomial)** over each subinterval, and then integrates the polynomial exactly over that subinterval.
- This makes it more accurate than the trapezoidal rule, which approximates the function with a straight line over each subinterval.
- It is based on the idea of approximating the area under a curve by fitting parabolic arcs to three consecutive points on the curve.

Simpson's Rule of Integration cont'd

The second-degree Lagrange interpolating polynomial

$$p_2(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} f(x_1) + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} f(x_2) + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} f(x_3)$$

The definite integral will then be evaluated with this polynomial replacing the integrand

$$\int_a^b f(x)\,dx \cong \int_a^b p_2(x)\,dx$$

Substituting for $p_2(x)$, integrating from a to b, and simplifying, yields

$$\int_a^b f(x)\,dx \cong \frac{h}{3}[f(x_1) + 4f(x_2) + f(x_3)], \quad h = \frac{b-a}{2}$$

Simpson's Rule of Integration cont'd

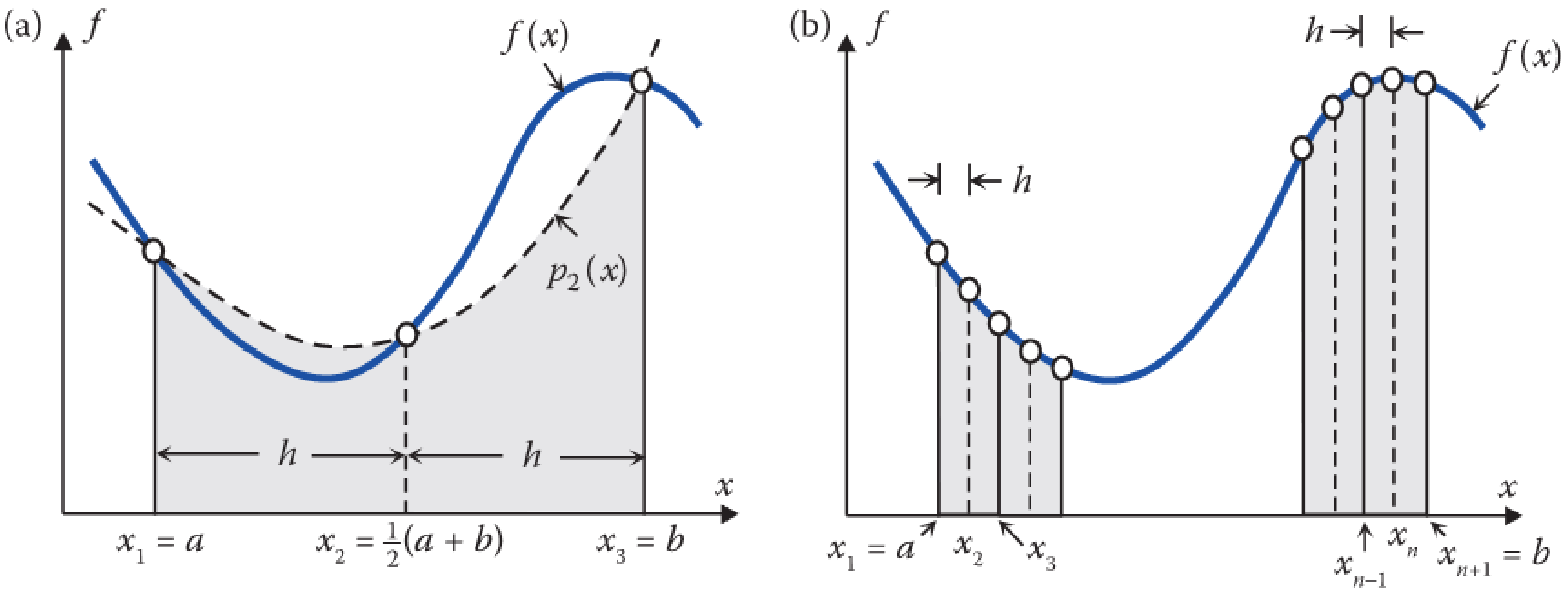
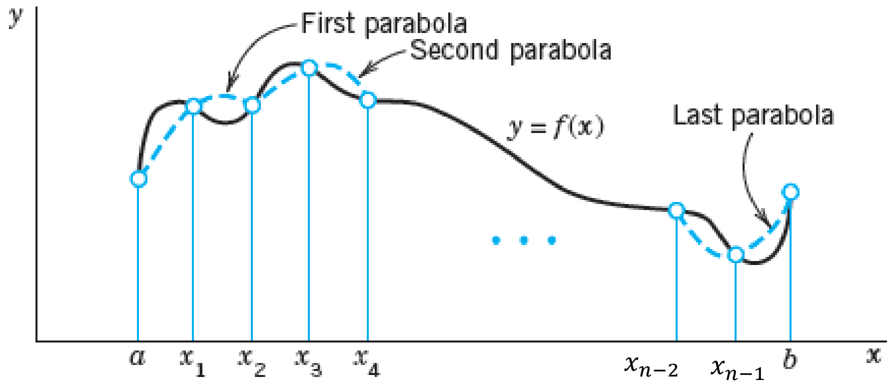


FIGURE 6.6
(a) Simpson's 1/3 rule and (b) composite Simpson's 1/3 rule.

Simpson's One third Rule



The interval $[a, b]$ is divided into $\boldsymbol{n}$ **subintervals** defined by $n + 1$ points labelled $a = x_0, x_1, x_2, \dots, x_{n-1}, x_n = b$.

The formula for the Simpson's can be expressed as:

$$\int_a^b f(x)dx = \frac{h}{3}[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + 4f_5 + \cdots + 2f_{n-2} + 4f_{n-1} + f_n]$$

<u>Or</u>

$$\int_a^b f(x)dx = \frac{h}{3}[f_0 + f_n + 4(f_1 + f_3 + f_5 + \cdots + f_{n-1}) + 2(f_2 + f_4 + \cdots + f_{n-2})]$$

where $h = \frac{(b-a)}{n}$

Example : 05

Using 4 subintervals in the composite Simpson's rule approximate $\int_1^2 \ln(x)\,dx$.

Answer

In this case $h = (2-1)/4 = 0.25$. There will be five x-values and the results are tabulated below to 6 d.p.

x_n	$f_n = \ln(x_n)$
1.00	0.000000
1.25	0.223144
1.50	0.405465
1.75	0.559616
2.00	0.693147

It follows that

$$\begin{aligned}\int_1^2 \ln(x)\,dx &\approx \frac{1}{3}h\left(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4\right)\\ &= \frac{1}{3}(0.25)\left(0 + 4\times 0.223144 + 2\times 0.405465 + 4\times 0.559616 + 0.693147\right)\\ &= 0.386260 \quad \text{to 6 d.p.}\end{aligned}$$

Program **(Composite Simpson Rule).** To approximate the integral

$$\int_a^b f(x)\,dx \approx \frac{h}{3}(f(a)+f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1})$$

by sampling $f(x)$ at the $2M+1$ equally spaced points $x_k = a + kh$, for $k = 0, 1, 2, \ldots, 2M$. Notice that $x_0 = a$ and $x_{2M} = b$.

```
function s=simprl(f,a,b,M)
%Input    - f is the integrand input as a string 'f'
%         - a and b are upper and lower limits of integration
%         - M is the number of subintervals
% Output  - s is the simpson rule sum
h=(b-a)/(2*M);
s1=0;
s2=0;
for k=1:M
   x=a+h*(2*k-1);
   s1=s1+feval(f,x);
end
for k=1:(M-1)
   x=a+h*2*k;
   s2=s2+feval(f,x);
end
s=h*(feval(f,a)+feval(f,b)+4*s1+2*s2)/3;
```

Error Estimation for Simpson's one third Rule

If the fourth derivative $f^{(4)}$ exists and is continuous on $a \leqq x \leqq b$, the **error**, call it ϵ_S, is

$$\epsilon_S = -\frac{(b-a)^5}{180\ (n)^4} f^{(4)}(\hat{t}) = -\frac{b-a}{180} h^4 f^{(4)}(\hat{t});$$

here $\hat{t}$ is a suitable unknown value between a and b.
With this we may also write Simpson's rule as

$$\int_a^b f(x)\,dx = \frac{h}{3}\left(f_0 + 4f_1 + \cdots + f_n\right) - \frac{b-a}{180} h^4 f^{(4)}(\hat{t}).$$

Error Bounds

Error Bounds are obtained by taking the largest value for f^4, say M_4 and the smallest value M_4^*, in the interval of integration.

$$CM_4 \leqq \epsilon_S \leqq CM_4^* \qquad \text{where} \qquad C = -\frac{(b-a)^5}{180\,(n)^4} = -\frac{b-a}{180}h^4.$$

Example : 06

Consider $f(x) = 2 + \sin(2\sqrt{x})$. Investigate the error when the Simpson's rule is used over [1,6] and the number of sub-interval 5,10,20,40 and 80

M	h	$S(f,h)$	$E_S(f,h) = \boldsymbol{O}(h^4)$
5	0.5	8.18301549	0.00046371
10	0.25	8.18344750	0.00003171
20	0.125	8.18347717	0.00000204
40	0.0625	8.18347908	0.00000013
80	0.03125	8.18347920	0.00000001

The true value of the integral is 8.1834792077, which was used to compute the values $E_S(f,h) = 8.1834792077 - S(f,h)$. It is important to observe that when h is reduced by a factor of 1/2 , the successive errors $E_S(f,h)$ are diminished by approximately 1/16. this confirms that the order is $\boldsymbol{O}(h^4)$.

3. Gauss-Legendre Integration

Gauss-Legendre integration is a numerical integration method that **uses a set of weights and nodes** to approximate the integral of a function over a given interval.

$$\int_{-1}^{1} f(x)\,dx \cong \sum_{i=1}^{n} c_i f(x_i) = c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n)$$

It is a more advanced method than the trapezoidal rule, Simpson's rule, and other simple numerical integration methods, as it can provide more accurate approximations for integrals that are difficult or impossible to evaluate analytically.

Theorem (Gauss-Legendre Two-Point Rule)

If f is continuous on $[-1,1]$ then,

$$\int_{-1}^{1} f(x)dx \;\approx\; G_2(f) = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

The Gauss-Legendre rule $G_2(f)$ has degree of precision $n = \; 3$.

If $f \in C^4[-1,1]$.

$$\int_{-1}^{1} f(x)dx \;= f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) + \; E_2(f)$$

where, $E_2(f) = \dfrac{f^4(c)}{135}$

Example : 07

Use the two-point Gauss-Legendre rule to approximate

$$\int_{-1}^{1} \frac{dx}{x+2} = \ln 3 - \ln 1 \approx 1.09861$$

And compare the result with the trapezoidal rule $T(f,h)$ with $h = 2$ and Simpson's rule $S(f,h)$ with $h = 1$.

Solution

Two-point Gauss- Legendre rule:

$$G_2(f) = f(-0.57735) + f(0.57735) = 0.70291 + 0.388 = 1.09091$$

Trapezoidal rule:

$$T(f,2) = \frac{h}{2}[f(a) + f(b)] = f(-1.00000) + f(1.00000) = 1.00000 + 0.33333 = 1.33333$$

Simpson's one third rule:

$$S(f,h) = S(f,1) = \frac{f(-1) + 4f(0) + f(1)}{3} = \frac{1 + 2 + \frac{1}{3}}{3} = 1.11111$$

The errors are 0.00770, -0.23472, and -0.01250, respectively, so the Gauss-Legendre rule is seen to be best.

Theorem (Gauss-Legendre Three-Point Rule)

If f is continuous on [-1,1] then,

$$\int_{-1}^{1} f(x)dx \;\approx\; G_3(f) = \frac{5f\left(-\sqrt{3/5}\right) + 8f(0) + 5f\left(\sqrt{3/5}\right)}{9}$$

The Gauss-Legendre rule $G_3(f)$ has degree of precision n= 5. If $f \in C^6[-1,1]$, then

$$\int_{-1}^{1} f(x)dx \;= \frac{5f\left(-\sqrt{3/5}\right) + 8f(0) + 5f\left(\sqrt{3/5}\right)}{9} + \; E_3(f)$$

where, $E_3(f) = \frac{f^6(c)}{15750}$

Example : 08

Show that the three-point Gauss-Legendre rule is exact for

$$\int_{-1}^{1} 5x^4 \, dx = 2 = G_3(f)$$

Solution

Since the integrand is $f(x) = 5x^4$ and $f^6(x) = 0, E_3(f) = 0.$

$$G_3(f) = \frac{5f\left(-\sqrt{3/5}\right) + 8f(0) + 5f\left(\sqrt{3/5}\right)}{9}$$

$$G_3(f) = \frac{5(5)(0.6)^2 + 0 + 5(5)(0.6)^2}{9} = \frac{18}{9} = 2$$

Theorem (Gauss-Legendre Translation)

Suppose that the abscissas $\{x_{N,k}\}_{k=1}^{N}$ and weights $\{w_{N,k}\}_{k=1}^{N}$ are given for the N-point Gauss-Legendre rule over [-1,1]. To apply the rule over the interval [a, b], use the change of variable

$$t = \frac{a+b}{2} + \frac{b-a}{2}x \text{ and } dt = \frac{b-a}{2}\, dx$$

Then the relationship

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

is used to obtain the quadrature formula

$$\int_a^b f(t)\,dt = \frac{b-a}{2}\sum_{k=1}^{N} w_{N,k} f\left(\frac{a+b}{2} + \frac{b-a}{2}x_{N,k}\right).$$

Example : 09

Use the three-point Gauss-Legendre rule to approximate

$$\int_1^5 \frac{dt}{t} = \ln 5 - \ln 1 \approx 1.609438$$

Solution

$$t = \frac{a+b}{2} + \frac{b-a}{2}x = \frac{1+5}{2} + \frac{5-1}{2}\mathrm{x} = 3 + 2x$$

$$dt = \frac{b-a}{2}\,dx = \frac{5-1}{2}dx = 2dx$$

$$G_3(f) = \frac{5f\left(-\sqrt{3/5}\right)+8f(0)+5f\left(\sqrt{3/5}\right)}{9} = 1.602694$$

Program (**Gauss-Legendre Quadrature**). To approximate the integral

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\sum_{k=1}^{N} w_{N,k} f(t_{N,k})$$

```
function quad=gauss(f,a,b,A,W)

%Input  - f is the integrand input as a string 'f'
%       - a and b are upper and lower limits of integration
%       - A is the 1 x N vector of abscissas from Table 7.9
%       - W is the 1 x N vector of weights from Table 7.9
%Output - quad is the quadrature value

N=length(A);
T=zeros(1,N);
T=((a+b)/2)+((b-a)/2)*A;
quad=((b-a)/2)*sum(W.*feval(f,T));
```

Exercises

In Exercises 1 through 4, show that the two integrals are equivalent and calculate $G_2(f)$.

1. $\displaystyle\int_0^2 6t^5\,dt = \int_{-1}^1 6(x+1)^5\,dx$

2. $\displaystyle\int_0^2 \sin(t)\,dt = \int_{-1}^1 \sin(x+1)\,dx$

3. $\displaystyle\int_0^1 \frac{\sin(t)}{t}\,dt = \int_{-1}^1 \frac{\sin((x+1)/2)}{x+1}\,dx$

4. $\displaystyle\frac{1}{\sqrt{2\pi}}\int_0^1 e^{-t^2/2}\,dt = \frac{1}{\sqrt{2\pi}}\int_{-1}^1 \frac{e^{-(x+1)^2/8}}{2}\,dx$

5. The three-point Gauss-Legendre rule is

$$\int_{-1}^1 f(x)\,dx \approx \frac{5f(-(0.6)^{1/2}) + 8f(0) + 5f((0.6)^{1/2})}{9}.$$

Show that the formula is exact for $f(x) = 1, x, x^2, x^3, x^4, x^5$. *Hint.* If f is an odd function (i.e., $f(-x) = f(x)$), the integral of f over $[-1, 1]$ is zero.

END OF

NUMERICAL INTEGRATION

Thank You