CHAPTER 6 (4 LECTURES)
NUMERICAL INTEGRATION

1. Introduction

The general problem is to find the approximate value of the integral of a given function $f(x)$ over an interval $[a, b]$. Thus

$$I = \int_a^b f(x)dx. \tag{1.1}$$

Problem can be solved by using the Fundamental Theorem of Calculus by finding an anti-derivative F of f, that is, $F'(x) = f(x)$, and then

$$\int_a^b f(x)dx = F(b) - F(a).$$

But finding an anti-derivative is not an easy task in general. Hence, it is certainly not a good approach for numerical computations.
In this chapter we'll study methods for finding integration rules. We'll also consider composite versions of these rules and the errors associated with them.

2. Elements of numerical integration

The basic method involved in approximating the integration is called numerical quadrature and uses a sum of the type

$$\int_a^b f(x)dx \approx \lambda_i f(x_i). \tag{2.1}$$

The method of quadrature is based on the polynomial interpolation. We divide the interval $[a, b]$ in to a set of distinct nodes $\{x_0, x_1, x_2, \cdots, x_n\}$. Then we approximate the function $f(x)$ by an interpolating polynomial, say Lagrange interpolating polynomial is used to approximate $f(x)$, i.e.

$$\begin{aligned} f(x) &= P_n(x) + \text{Error} \\ &= \sum_{i=0}^{n} f(x_i) l_i(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i). \end{aligned}$$

Here $\xi = \xi(x) \in (a, b)$ and

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}, \ 0 \le i \le n.$$

Therefore

$$\begin{aligned} \int_a^b f(x)dx &= \int_a^b P_n(x)dx + \int_a^b e_n(x)dx \\ &= \sum_{i=0}^{n} f(x_i) \int_a^b l_i(x)dx + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi) \prod_{i=0}^{n} (x - x_i)dx \\ &= \sum_{i=0}^{n} \lambda_i f(x_i) + E \end{aligned}$$

where

$$\lambda_i = \int_a^b l_i(x)dx.$$

Error in the numerical quadrature is given by

$$E = \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi)\prod_{i=0}^{n}(x-x_i)dx.$$

We can also use Newton divided difference interpolation to approximate the function $f(x)$.

3. Newton-Cotes Formula

Let all nodes are equally spaced with spacing $h = \dfrac{b-a}{n}$. The number h is also called the step length.
Let $x_0 = a$ and $x_n = b$ then $x_i = a + ih,\ i = 0, 1, \cdots, n$.
The general quadrature formula is given by

$$\int_a^b f(x)dx = \sum_{i=0}^{n}\lambda_i f(x_i) + E.$$

This formula is called Newton-Cotes formula if all points are equally spaced. We now derive rules by taking one and two degree interpolating polynomials.

3.1. **Trapezoidal Rule.**

We derive the Trapezoidal rule for approximating $\int\limits_a^b f(x)dx$ using the linear Lagrange polynomial.
Let $x_0 = a$, $x_1 = b$, and $h = b - a$.

$$\int\limits_{a=x_0}^{b=x_1} f(x)\,dx = \int\limits_{x_0}^{x_1} P_1(x)dx + E.$$

We calculate both the integrals separately as:

$$\begin{aligned}
\int\limits_{x_0}^{x_1} P_1(x)dx &= \int\limits_{x_0}^{x_1}[l_0(x)f(x_0) + l_1(x)f(x_1)]\,dx \\
&= f(x_0)\int\limits_{x_0}^{x_1}\frac{x-x_1}{x_0-x_1}\,dx + f(x_1)\int\limits_{x_0}^{x_1}\frac{x-x_0}{x_1-x_0}\,dx \\
&= f(x_0)\left[\frac{(x-x_1)^2}{2(x_0-x_1)}\right]_{x_0}^{x_1} + f(x_1)\left[\frac{(x-x_0)^2}{2(x_1-x_0)}\right]_{x_0}^{x_1} \\
&= \frac{x_1-x_0}{2}[f(x_0)+f(x_1)] \\
&= \frac{h}{2}[f(a)+f(b)].
\end{aligned}$$

$$\begin{aligned}
E &= \int\limits_{x_0}^{x_1}\frac{f^{(2)}(\xi)}{2!}(x-x_0)(x-x_1)\,dx \\
&= \frac{1}{2}\int\limits_{x_0}^{x_1} f^{(2)}(\xi)(x-x_0)(x-x_1)\,dx.
\end{aligned}$$

Since $(x - x_0)(x - x_1)$ does not change its sign in $[x_0, x_1]$, therefore by the Weighted Mean-Value Theorem, there exists a point $\xi \in (x_0, x_1)$ such that

$$\begin{aligned} E &= \frac{f^{(2)}(\xi)}{2} \int_{x_0}^{x_1} (x - x_0)(x - x_1)\, dx \\ &= \frac{f^{(2)}(\xi)}{2} \left[\frac{(x_0 - x_1)^3}{6} \right] \\ &= -\frac{h^3}{12} f^{(2)}(\xi). \end{aligned}$$

Thus the integration formula is

$$\int_a^b f(x)dx = \frac{h}{2}[f(a) + f(b)] - \frac{h^3}{12} f^{(2)}(\xi).$$

Geometrically, it is the area of Trapezium (Trapezoid) with width h and ordinates $f(a)$ and $f(b)$.

3.2. **Simpson's Rule.** We take second degree Lagrange interpolating polynomial. We take $n = 2,\ x_0 = a,\ x_1 = \dfrac{a+b}{2},\ x_2 = b,\ h = (b-a)/2.$

$$\int_{a=x_0}^{b=x_2} f(x)\, dx = \int_{x_0}^{x_2} P_2(x)dx + E.$$

$$\begin{aligned} \int_{x_0}^{x_2} P_2(x)dx &= \int_{x_0}^{x_2} [l_0(x)f(x_0) + l_1(x)f(x_1) + +l_2(x)f(x_2)]\, dx \\ &= \lambda_0 f(x_0) + \lambda_1 f(x_1) + \lambda_2 f(x_2). \end{aligned}$$

The values of the multipliers λ_0, λ_1, and λ_2 are given by

$$\lambda_0 = \int_{x_0}^{x_2} \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}\, dx.$$

To simply this integral, we substitute $x = x_0 + ht,\ dx = h\ dt$ and change the limits from 0 to 2 accordingly. Therefore

$$\lambda_0 = \int_0^2 \frac{h(t-1)h(t-2)}{(-h)(-2h)}\, hdt = h/3.$$

Similarly

$$\begin{aligned} \lambda_1 &= \int_{x_0}^{x_2} \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}\, dx \\ &= \int_0^2 \frac{h(t-0)h(t-2)}{(h)(-h)}\, hdt = 4h/3. \end{aligned}$$

and

$$\begin{aligned} \lambda_2 &= \int_{x_0}^{x_2} \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}\, dx \\ &= \int_0^2 \frac{h(t-0)h(t-1)}{(2h)(h)}\, hdt = h/3. \end{aligned}$$

Now error is given by

$$E = \frac{1}{3!}\int_{x_0}^{x_2} f'''(\xi)(x-x_0)(x-x_1)(x-x_2)dx.$$

Since $(x-x_0)(x-x_1)(x-x_2)$ changes its sign in the interval $[x_0, x_2]$, therefore we cannot apply the Weighted Mean-Value Theorem (as we did in trapezoidal rule).
Also

$$\int_{x_0}^{x_2} (x-x_0)(x-x_1)(x-x_2)\,dx = 0.$$

We can add an interpolation point without affecting the area of the interpolated polynomial, leaving the error unchanged. We can therefore do our error analysis of Simpson's rule with any single point added, since adding any point in $[a, b]$ does not affect the area, we simply double the midpoint, so that our node set is $\{x_0 = a, x_1 = (a+b)/2, x_1 = (a+b)/2, x_2 = b\}$. We can now examine the value of the next interpolating polynomial. Therefore

$$E = \frac{1}{4!}\int_{x_0}^{x_2} f^{(4)}(\xi)(x-x_0)(x-x_1)^2(x-x_2)dx.$$

Now the product $(x-x_0)(x-x_1)^2(x-x_2)$ does not change its sign in $[x_0, x_2]$, therefore by the Weighted Mean-Value Theorem, there exists a point $\xi \in (x_0, x_2)$ such that

$$\begin{aligned} E &= \frac{1}{24}f^{(4)}(\xi)\int_{x_0}^{x_2}(x-x_0)(x-x_1)^2(x-x_2)dx \\ &= -\frac{f^{(4)}(\xi)}{2880}(x_2-x_0)^5 \\ &= -\frac{h^5}{90}f^{(4)}(\xi). \end{aligned}$$

Hence

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{h^5}{90}f^{(4)}(\xi).$$

This rule is called Simpson's $\frac{1}{3}$ rule.

Similarly by taking third order Lagrange interpolating polynomial with four nodes $a = x_0, x_1, x_2, x_3 = b$ with $h = \frac{b-a}{3}$, we get the next integration formula known as Simpson's $\frac{3}{8}$ rule given below.

$$\int_a^b f(x)dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3}{80}h^5 f^{(4)}(\xi).$$

Definition 3.1. *The degree of accuracy, or precision, or order of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \cdots, n$.*
In other words, an integration method of the form

$$\int_a^b f(x)dx = \sum_{i=0}^{n}\lambda_i f(x_i) + \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi)\prod_{i=0}^{n}(x-x_i)dx$$

is said to be of order n if it provides exact results for all polynomials of degree less than or equal to n and the error term will be zero for all polynomials of degree $\leq n$.

Trapezoidal rule has degree of precision one and Simpson's rule has three.

Example 1. *Find the value of the integral*

$$I = \int_0^1 \frac{dx}{1+x}$$

using trapezoidal and Simpson's rule. Also obtain a bound on the errors. Compare with exact value.

Sol.

$$f(x) = \frac{1}{1+x}.$$

By trapezoidal rule

$$I_T = h/2[f(a) + f(b)].$$

Here $a = 0, b = 1, h = b - a = 1$.

$$I = 1/2[1 + 1/2] = 0.75.$$

Exact value

$$I_{exact} = \ln 2 = 0.693147.$$

Error= $|0.75 - 0.693147| = 0.056853$
The error bound for the trapezoidal rule is given by

$$\begin{aligned} E &\leq h^3/12 \max_{0\leq\xi\leq 1} |f''(\xi)| \\ &= 1/12 \max_{0\leq\xi\leq 1} \left| \frac{2}{(1+\xi)^3} \right| \\ &= 1/6. \end{aligned}$$

Similarly by using Simpson's rule with $h = (b - a)/2 = 1/2$, we obtain

$$I_S = h/3[f(0) + 4f(1/2) + f(1)] = 1/6(1 + 8/3 + 1/2) = 0.69444.$$

Error= $|0.69444 - 0.693147| = 0.0013$.
The error bound for the Simpson's rule is given by

$$\begin{aligned} E &\leq \frac{h^5}{90} \max_{0\leq\xi\leq 1} |f^{(4)}(\xi)| \\ &= \frac{1}{2880} \max_{0\leq\xi\leq 1} \left| \frac{24}{(1+\xi)^5} \right| \\ &= 0.008333. \end{aligned}$$

Example 2. *Find the quadrature formula by method of undetermined coefficients*

$$\int_0^1 \frac{f(x)}{\sqrt{x(1-x)}} dx = af(0) + bf(1/2) + cf(1)$$

which is exact for polynomials of highest possible degree. Then use the formula to evaluate

$$\int_0^1 \frac{dx}{\sqrt{x - x^3}}.$$

Sol. We make the method exact for polynomials up to degree 2.

$$f(x) = 1 \ : \quad I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = a + b + c$$

$$f(x) = x \ : \quad I_2 = \int_0^1 \frac{x dx}{\sqrt{x(1-x)}} = b/2 + c$$

$$f(x) = x^2 \ : \quad I_3 = \int_0^1 \frac{x^2 dx}{\sqrt{x(1-x)}} = b/4 + c.$$

Now

$$I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = \int_0^1 \frac{dx}{\sqrt{1-(2x-1)^2}} = \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = [\sin^{-1} t]_{-1}^1 = \pi$$

Similarly

$$I_2 = \pi/2$$

$$I_3 = 3\pi/8.$$

Therefore

$$\begin{aligned} a+b+c &= \pi \\ b/2+c &= \pi/2 \\ b/4+c &= 3\pi/8. \end{aligned}$$

By solving these equations, we obtain $a=\pi/4,\ b=\pi/2,\ c=\pi/4$. Hence

$$\int_0^1 \frac{f(x)}{\sqrt{x(1-x)}}dx = \pi/4[f(0)+2f(1/2)+f(1)].$$

$$I = \int_0^1 \frac{dx}{\sqrt{x-x^3}} = \int_0^1 \frac{dx}{\sqrt{1+x}\sqrt{x(1-x)}} = \int_0^1 \frac{f(x)dx}{\sqrt{x(1-x)}}.$$

Here $f(x) = 1/\sqrt{1+x}$.
By using the above formula, we obtain

$$I = \pi/4\left[1+\frac{2\sqrt{2}}{\sqrt{3}}+\frac{\sqrt{2}}{2}\right] = 2.62331.$$

4. Composite Integration

As the order of integration method is increased, the order of the derivative involved in error term also increase. Therefore, we can use higher-order method if the integrand is differentiable up to required degree. We can apply lower-order methods by dividing the whole interval in to subintervals and then we use any Newton-Cotes or Gauss quadrature method for each subintervals separately.

Composite Trapezoidal Method: We divide the interval $[a,b]$ into N subintervals with step size $h = \dfrac{b-a}{N}$ and taking nodal points $a = x_0 < x_1 < \cdots < x_N = b$ where $x_i = x_0 + i\,h,\ i = 1,2,\cdots,N-1$. Now

$$\begin{aligned} I &= \int_a^b f(x)dx \\ &= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{N-1}}^{x_N} f(x)dx. \end{aligned}$$

Now use trapezoidal rule for each of the integrals on the right side, we obtain

$$\begin{aligned} I &= \frac{h}{2}[(f(x_0)+f(x_1))+(f(x_1)+f(x_2))+\cdots+(f(x_{N-1})+f(x_N)] \\ &\qquad -\frac{h^3}{12}[f^{(2)}(\xi_1)+f^{(2)}(\xi_2)+\cdots+f^{(2)}(\xi_N)] \\ &= \frac{h}{2}\left[f(x_0)+f(x_N)+2\sum_{i=1}^{N-1} f(x_i)\right] - \frac{h^3}{12}\sum_{i=1}^{N} f^{(2)}(\xi_i). \end{aligned}$$

This formula is composite trapezoidal rule where where $x_{i-1} \le \xi_i \le x_i,\ i = 1,2,\cdots,N$.
The error associated with this approximation is

$$E = -\frac{h^3}{12}\sum_{i=1}^{N} f^{(2)}(\xi_i).$$

If $f \in C^2[a,b]$, the Extreme Value Theorem implies that $f^{(2)}$ assumes its maximum and minimum in $[a,b]$. Since

$$\min_{x\in[a,b]} f^{(2)}(x) \le f^{(2)}(\xi_i) \le \max_{x\in[a,b]} f^{(2)}(x).$$

On summing, we have

$$N \min_{x\in[a,b]} f^{(2)}(x) \le \sum_{i=1}^{N} f^{(2)}(\xi_i) \le N \max_{x\in[a,b]} f^{(2)}(x)$$

and

$$\min_{x\in[a,b]} f^{(2)}(x) \le \frac{1}{N}\sum_{i=1}^{N} f^{(2)}(\xi_i) \le \max_{x\in[a,b]} f^{(2)}(x).$$

By the Intermediate Value Theorem, there is a $\xi \in (a,b)$ such that

$$f^{(2)}(\xi) = \frac{1}{N}\sum_{i=1}^{N} f^{(2)}(\xi_i).$$

Therefore

$$E = -\frac{h^3}{12} N f^{(2)}(\xi),$$

or, since $h = (b-a)/N$,

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

Composite Simpson's Method: Simpson's rule require three abscissas, choose an even integer N to produce odd number of nodes with $h = \dfrac{b-a}{N}$. Likewise before, we write

$$\begin{aligned} I &= \int_a^b f(x)dx \\ &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{N-2}}^{x_N} f(x)dx. \end{aligned}$$

Now use Simpson's rule for each of the integrals on the right side to obtain

$$\begin{aligned} I &= \frac{h}{3}[(f(x_0)+4f(x_1)+f(x_2)) + (f(x_2)+4f(x_3)+f(x_4)) + \cdots + (f(x_{N-2})+4f(x_{N-1})+f(x_N)] \\ &\qquad -\frac{h^5}{90}[f^{(4)}(\xi_1) + f^{(4)}(\xi_2) + \cdots + f^{(4)}(\xi_{N/2})] \\ &= \frac{h}{3}\left[f(x_0) + 2\sum_{i=1}^{N/2-1} f(x_{2i}) + 4\sum_{i=1}^{N/2} f(x_{2i-1}) + f(x_N)\right] - \frac{h^5}{90}\sum_{i=1}^{N/2} f^{(4)}(\xi_i). \end{aligned}$$

This formula is called composite Simpson's rule. The error in the integration rule is given by

$$E = -\frac{h^5}{90}\sum_{i=1}^{N} f^{(4)}(\xi_i).$$

If $f \in C^4[a,b]$, the Extreme Value Theorem implies that $f^{(4)}$ assumes its maximum and minimum in $[a,b]$. Since

$$\min_{x\in[a,b]} f^{(4)}(x) \le f^{(4)}(\xi_i) \le \max_{x\in[a,b]} f^{(4)}(x).$$

On summing, we have

$$\frac{N}{2}\min_{x\in[a,b]} f^{(4)}(x) \le \sum_{i=1}^{N/2} f^{(4)}(\xi_i) \le \frac{N}{2}\max_{x\in[a,b]} f^{(4)}(x)$$

and

$$\min_{x\in[a,b]} f^{(4)}(x) \le \frac{2}{N}\sum_{i=1}^{N/2} f^{(4)}(\xi_i) \le \max_{x\in[a,b]} f^{(4)}(x).$$

By the Intermediate Value Theorem, there is a $\xi \in (a,b)$ such that

$$f^{(4)}(\xi) = \frac{2}{N}\sum_{i=1}^{N/2} f^{(4)}(\xi_i).$$

Therefore

$$E = -\frac{h^5}{180} N f^{(4)}(\xi),$$

or, since $h = (b-a)/N$,

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

Example 3. *Determine the values of subintervals n and step-size h required to approximate*

$$\int_0^2 \frac{1}{x+4}\, dx$$

to within 10^{-5} and hence compute the approximation using composite Simpson's rule.

Sol. Here $f(x) = \dfrac{1}{x+4}$, therefore $f^{(4)}(x) = \dfrac{24}{(x+4)^5}$.

$$\therefore \max_{x\in[0,2]} |f^{(4)}(x)| = \frac{24}{4^5}.$$

Now error in Simpson's rule is given by

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

To get desire accuracy, we have

$$\frac{2h^4 \times 24}{4^5 \times 180} < 10^{-5}$$
$$\implies h < 0.44267.$$

Since $n = \frac{b-a}{h} > 2/0.44267 = 4.518$, and nearest even integer is 6, therefore we take minimum 6 subintervals to achieve the desired accuracy.
By taking 6 subintervals with $h = 2/6 = 1/3$ and using Simpson's rule, we obtain

$$I_S = \frac{1}{9}[f(0) + 4\{f(1/3) + f(1) + f(5/3)\} + 2\{f(2/3) + f(4/3)\} + f(2)] = 0.405466.$$

Example 4. *Determine the values of n and h required to approximate $\int_0^2 e^{2x}\sin 3x\, dx$ to within 10^{-4} using the*

(1) *composite trapezoid rule and*
(2) *composite Simpson's rule.*

Sol.

(1) The error form for the composite trapezoidal rule is

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

for some $\xi \in [0,2]$. Now

$$\begin{aligned}
|f''(x)| &= |12e^{2x}\cos 3x - 5e^{2x}\sin 3x| \\
&\le |12e^{2x}\cos 3x| + |5e^{2x}\sin 3x| \quad \text{(triangle inequality)} \\
&= 12e^{2x}|\cos 3x| + 5e^{2x}|\sin 3x| \\
&\le 12e^{2x} + 5e^{2x} = 17e^{2x}
\end{aligned}$$

which is increasing on $[0,2]$ so

$$|f''(\xi)| \le 17e^{2\cdot 2} = 17e^4.$$

Thus

$$\begin{aligned}
|E| &= \frac{1}{6}h^2|f''(\xi)| \le \frac{1}{6}h^2 \cdot 17e^4 \le 10^{-4} \\
\implies h &\le \left[\frac{(6)(10^{-4})}{17e^4}\right]^{1/2} \approx 8.04 \times 10^{-4} \\
\implies n &\ge \frac{2}{h} = \frac{2}{8.04 \times 10^{-4}} \approx 2487.5.
\end{aligned}$$

Hence $h \leq 8.04 \times 10^{-4}$ and $n \geq 2488$.

(2) The error form for the composite Simpson's rule is

$$|E| = \left| \frac{(b-a)h^4}{180} f^{(4)}(\xi) \right| = \frac{2h^4}{180} |f^{(4)}(\xi)|$$

for some $\xi \in [0, 2]$. Now

$$\begin{aligned} |f^{(4)}(x)| &= |-119e^{2x} \sin 3x - 120e^{2x} \cos 3x| \\ &\leq |119e^{2x} \sin 3x| + |120e^{2x} \cos 3x| \quad \text{(triangle inequality)} \\ &= 119e^{2x} |\sin 3x| + 120e^{2x} |\cos 3x| \\ &\leq 119e^{2x} + 120e^{2x} = 239e^{2x} \end{aligned}$$

which is increasing on $[0, 2]$ so

$$|f^{(4)}(\xi)| \leq 239e^{2 \cdot 2} = 239e^4.$$

Thus

$$\begin{aligned} |E| &= \frac{1}{90} h^4 |f^{(4)}(\xi)| \leq \frac{1}{90} h^4 \cdot 239e^4 \leq 10^{-4} \\ \Longrightarrow h &\leq \left[\frac{(90)(10^{-4})}{239e^4} \right]^{1/4} \approx 0.0288 \\ \Longrightarrow n &\geq \frac{2}{h} = \frac{2}{0.288} \approx 69.4. \end{aligned}$$

Hence $h \leq 0.0288$ and $n \geq 70$.

Example 5. *The area A inside the closed curve $y^2 + x^2 = \cos x$ is given by*

$$A = 4 \int_0^{\alpha} (\cos x - x^2)^{1/2} dx$$

where α is the positive root of the equation $\cos x = x^2$.
(a) Compute α with three correct decimals.
(b) Use trapezoidal rule to compute the area A with an absolute error less than 0.05.

Sol. (a) Using Newton method to find the root of the equation

$$f(x) = \cos x - x^2 = 0,$$

we obtain the following iteration scheme

$$x_{k+1} = x_k + \frac{\cos x_k - x_k^2}{\sin x_k + 2x_k}, \ k = 0, 1, 2, \cdots$$

Starting with $x_0 = 0.5$, we obtain

$$\begin{aligned} x_1 &= 0.5 + \frac{0.62758}{1.47942} = 0.92420 \\ x_2 &= 0.92420 + \frac{-0.25169}{2.64655} = 0.82911 \\ x_3 &= 0.82911 + \frac{-0.011882}{2.39554} = 0.82414 \\ x_4 &= 0.82414 + \frac{-0.000033}{2.38226} = 0.82413. \end{aligned}$$

Hence the value of α correct to three decimals is 0.824.

(b) Substituting the value of α, we obtain

$$A = 4 \int_0^{0.824} (\cos x - x^2)^{1/2} dx.$$

Using composite trapezoidal method by taking $h = 0.824,\ 0.412$, and 0.206 respectively, we obtain the following approximations of the area A.

$$
\begin{aligned}
A &= \frac{4(0.824)}{2}[1 + 0.017753] = 1.67725 \\
A &= \frac{4(0.412)}{2}[1 + 2(0.864047) + 0.017753] = 2.262578 \\
A &= \frac{4(0.206)}{2}[1 + 2(0.967688 + 0.864047 + 0.658115) + 0.017753] = 2.470951.
\end{aligned}
$$

5. Gauss Quadrature

In the numerical integration method if both nodes x_i and multipliers λ_i are unknown then method is called Gaussian quadrature. We can obtain the unknowns by making the method exact for polynomials of degree as high as required. The formulas are derived for the interval $[-1, 1]$ and any interval $[a, b]$ can be transformed to $[-1, 1]$ by taking the transformation $x = At + B$ which gives $a = -A + B$ and $b = A + B$ and after solving we get $x = \dfrac{b-a}{2}t + \dfrac{b+a}{2}$.
As observed in Newton-Cotes quadrature, we can write any integral as

$$
\int_{-1}^{1} f(x)dx = \sum_{i=0}^{n} \lambda_i f(x_i) + E.
$$

where E is the error.

Gauss-Legendre Integration Methods: The technique we have described could be used to determine the nodes and coefficients for formulas that give exact results for higher-degree polynomials.
One-point formula: The 1-point formula is given by

$$
\int_{-1}^{1} f(x)dx = \lambda_0 f(x_0).
$$

The method has two unknowns λ_0 and x_0. Make the method exact for $f(x) = 1, x$, we obtain

$$
f(x) = 1 \ : \quad \int_{-1}^{1} dx = 2 = \lambda_0
$$

$$
f(x) = x \ : \quad \int_{-1}^{1} x dx = 0 = \lambda_0 x_0 \implies x_0 = 0.
$$

Therefore one-point formula is given by

$$
\int_{-1}^{1} f(x)dx \approx 2f(0).
$$

Two-point formula: In this case, we write

$$
\int_{-1}^{1} f(x)dx = \lambda_0 f(x_0) + \lambda_1 f(x_1).
$$

The method has four unknowns. Make the method exact for $f(x) = 1, x, x^2, x^3$, we obtain

$$
f(x) = 1 \quad : \quad \int_{-1}^{1} dx = 2 = \lambda_0 + \lambda_1 \tag{5.1}
$$

$$
f(x) = x \quad : \quad \int_{-1}^{1} x dx = 0 = \lambda_0 x_0 + \lambda_1 x_1 \tag{5.2}
$$

$$
f(x) = x^2 \quad : \quad \int_{-1}^{1} x^2 dx = 2/3 = \lambda_0 x_0^2 + \lambda_1 x_1^2 \tag{5.3}
$$

$$
f(x) = x^3 \quad : \quad \int_{-1}^{1} x^3 dx = 0 = \lambda_0 x_0^3 + \lambda_1 x_1^3 \tag{5.4}
$$

Now eliminate λ_0 from second and fourth equation

$$\lambda_1 x_1^3 - \lambda_1 x_1 x_0^2 = 0$$

which gives

$$\lambda_1 x_1 (x_1 - x_0)(x_1 + x_0) = 0$$

Since $\lambda_1 \neq 0$, $x_0 \neq x_1$ and $x_1 \neq 0$ (if $x_1 = 0$ then by second equation $x_0 = 0$). Therefore $x_1 = -x_0$.
Substituting in second equation, we obtain $\lambda_0 = \lambda_1$.
By substituting these values in first equation, we get $\lambda_0 = \lambda_1 = 1$.
Third equation gives $x_0^2 = 1/3$ or $x_0 = \pm 1/\sqrt{3}$ and $x_1 = \mp 1/\sqrt{3}$.
Therefore, the two-point formula is given by

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

Three-point formula:

$$\int_{-1}^{1} f(x)dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) + \lambda_2 f(x_2).$$

The method has six unknowns. Make the method exact for $f(x) = 1, x, x^2, x^3, x^4, x^5$, we obtain

$$\begin{aligned}
f(x) = 1 \quad &: \quad 2 = \lambda_0 + \lambda_1 + \lambda_2 \\
f(x) = x \quad &: \quad 0 = \lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2 \\
f(x) = x^2 \quad &: \quad 2/3 = \lambda_0 x_0^2 + \lambda_1 x_1^2 + \lambda_2 x_2^2 \\
f(x) = x^3 \quad &: \quad 0 = \lambda_0 x_0^3 + \lambda_1 x_1^3 + \lambda_2 x_2^3 \\
f(x) = x^4 \quad &: \quad 2/5 = \lambda_0 x_0^4 + \lambda_1 x_1^4 + \lambda_2 x_2^4 \\
f(x) = x^5 \quad &: \quad 0 = \lambda_0 x_0^5 + \lambda_1 x_1^5 + \lambda_2 x_2^5
\end{aligned}$$

By solving these equations, we obtain $\lambda_0 = \lambda_2 = 5/9$ and $\lambda_1 = 8/9$. $x_0 = \pm\sqrt{3/5}$, $x_1 = 0$ and $x_2 = \mp\sqrt{3/5}$.
Therefore formula is given by

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

Note: Legendre polynomial $P_n(x)$ is a monic polynomial of degree n. The first few Legendre polynomials are

$$\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= x^2 - \frac{1}{3}, \\
P_3(x) &= x^3 - \frac{3}{5}x.
\end{aligned}$$

Nodes in Gauss-Legendre rules are roots of these polynomials.

Example 6. *Evaluate*

$$I = \int_1^2 \frac{2x}{1+x^4}\,dx$$

using Gauss-Legendre 1 and 2-point formula. Also compare with the exact value.

Sol. Firstly we change the interval $[1, 2]$ in to $[-1, 1]$ by taking $x = \dfrac{t+3}{2}$, $dx = dt/3$.

$$I = \int_1^2 \frac{2x}{1+x^4}dx = \int_{-1}^{1} \frac{8(t+3)}{16+(t+3)^4}dt.$$

Let

$$f(t) = \frac{8(t+3)}{16+(t+3)^4}.$$

By 1-point formula
$$I = 2f(0) = 0.4948.$$
By 2-point formula
$$I = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = f(-0.57735) + f(0.57735) = 0.5434.$$
Now exact value of the integral is given by
$$I = \int_1^2 \frac{2x}{1+x^4} dx = \tan^{-1} 4 - \frac{\pi}{4} = 0.5408.$$
Therefore errors by one and two points formula are $|0.4948 - 0.5408| = 0.046$ and $|0.5434 - 0.5408| = 0.0026$, respectively.

Example 7. *Evaluate*
$$I = \int_{-1}^{1} (1-x^2)^{3/2} \cos x \, dx$$
using Gauss-Legendre 3-point formula.

Sol. Using Gauss-Legendre 3-point formula with $f(x) = (1-x^2)^{3/2} \cos x$, we obtain
$$\begin{aligned} I &= \frac{1}{9}\left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right)\right] \\ &= \frac{1}{9}\left[5\left(\frac{2}{5}\right)^{3/2} \cos\left(\sqrt{\frac{3}{5}}\right) + 8 + 5\left(\frac{2}{5}\right)^{3/2} \cos\left(\sqrt{\frac{3}{5}}\right)\right] \\ &= 1.08979. \end{aligned}$$

Example 8. *Determine constants a, b, c, and d that will produce a quadrature formula*
$$\int_{-1}^{1} f(x)dx = af(-1) + bf(1) + cf'(-1) + df'(1)$$
that has degree of precision 3.

Sol. We want the formula
$$\int_{-1}^{1} f(x)dx = af(-1) + bf(1) + cf'(-1) + df'(1)$$
to hold for polynomials $1, x, x^2, \cdots$. Plugging these into the formula, we obtain:
$$\begin{aligned} f(x) = x^0 : &\qquad \int_{-1}^{1} dx = 2 = a \cdot 1 + b \cdot 1 + c \cdot 0 + d \cdot 0 \\ f(x) = x^1 : &\qquad \int_{-1}^{1} x dx = 0 = a \cdot (-1) + b \cdot 1 + c \cdot 1 + d \cdot 1 \\ f(x) = x^2 : &\qquad \int_{-1}^{1} x^2 dx = \frac{2}{3} = a \cdot 1 + b \cdot 1 + c \cdot (-2) + d \cdot 2 \\ f(x) = x^3 : &\qquad \int_{-1}^{1} x^3 dx = 0 = a \cdot (-1) + b \cdot 1 + c \cdot 3 + d \cdot 3. \end{aligned}$$
We have 4 equations in 4 unknowns:
$$\begin{aligned} a + b &= 2, \\ -a + b + c + d &= 0, \\ a + b - 2c + 2d &= \frac{2}{3}, \\ -a + b + 3c + 3d &= 0. \end{aligned}$$
Solving this system, we obtain:
$$a = 1, \; b = 1, \; c = \frac{1}{3}, \; d = -\frac{1}{3}.$$

Thus, the quadrature formula with accuracy 3 is

$$\int_{-1}^{1} f(x)dx = f(-1) + f(1) + \frac{1}{3}f'(-1) - \frac{1}{3}f'(1).$$

Example 9. *Evaluate*

$$I = \int_0^1 \frac{dx}{1+x}$$

by subdividing the interval $[0,1]$ *into two equal parts and then by using Gauss-Legendre three-point formula.*

Sol.

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

Let

$$I = \int_0^1 \frac{dx}{1+x} = \int_0^{1/2} \frac{dx}{1+x} + \int_{1/2}^{1} \frac{dx}{1+x} = I_1 + I_2.$$

Now substitute $x = \dfrac{t+1}{4}$ and $x = \dfrac{z+3}{4}$ in I_1 and I_2, respectively to change the limits to $[-1,1]$. We have $dx = dt/4$ and $dx = dz/4$ for integral I_1 and I_2, respectively.
Therefore

$$I_1 = \int_{-1}^{1} \frac{dt}{t+5} = \frac{1}{9}\left[\frac{5}{5-\sqrt{3/5}} + \frac{8}{5} + \frac{5}{5+\sqrt{3/5}}\right] = 0.405464$$

$$I_2 = \int_{-1}^{1} \frac{dz}{z+7} = \frac{1}{9}\left[\frac{5}{7-\sqrt{3/5}} + \frac{8}{7} + \frac{5}{7+\sqrt{3/5}}\right] = 0.287682$$

Hence

$$I = I_1 + I_2 = 0.405464 + 0.287682 = 0.693146.$$

Exercises

(1) Given

$$I = \int_0^2 x^2\, e^{-x^2}\, dx.$$

Approximate the value of I using trapezoidal and Simpson's one-third method.

(2) Approximate the following integrals using the trapezoidal and Simpson's formulas and compare with exact values.

(a) $I = \int\limits_{-0.25}^{0.25} (\cos x)^2\, dx.$

(b) $\int\limits_{e}^{e+1} \dfrac{1}{x\ln x}\, dx.$

(3) Approximate the integral $\int\limits_{1}^{1.5} x^2 \ln x dx$ using the (non-composite) trapezoidal rule. Give a rigorous error bound on this approximation.

(4) Approximate the integral $\int\limits_{0}^{0.5} \dfrac{2}{x-4} dx$ using the (non-composite) Simpson's rule. Give a rigorous error bound on this approximation.

(5) The Trapezoidal rule applied to $\int\limits_{0}^{2} f(x)dx$ gives the value 4, and Simpson's rule gives the value 2. What is $f(1)$?

(6) Suppose that $f(0) = 1$, $f(0.5) = 2.5$, $f(1) = 2$, and $f(0.25) = f(0.75) = \alpha$. Find α if the composite Trapezoidal rule with $n = 4$ gives the value 1.75 for $\int\limits_{0}^{1} f(x)dx$.

(7) Evaluate

$$I = \int_{-1}^{1} \frac{dx}{1+x^2}$$

using trapezoidal and Simpson's rule with 8 subintervals. Compare with the exact value of the integral.

(8) The quadrature formula $\int\limits_0^2 f(x)dx = c_0 f(0) + c_1 f(1) + c_2 f(2)$ is exact for all polynomials of degree less than or equal to 2. Determine c_0, c_1, and c_2.

(9) (a) Find the degree of precision of the quadrature formula

$$\int\limits_{-1}^{1} f(x)dx = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).$$

(b) Generalize the integration rule in part (a) to approximate the integral $\int\limits_a^b f(x)dx$.

(10) Find the constants c_0, c_1, and x_1 so that the quadrature formula

$$\int\limits_0^1 f(x)dx = c_0 f(0) + c_1 f(x_1)$$

has the highest possible degree of precision.

(11) The length of the curve represented by a function $y = f(x)$ on an interval $[a, b]$ is given by the integral

$$I = \int_a^b \sqrt{1 + [f'(x)]^2}\, dx.$$

Use the trapezoidal rule with $n = 20$, compute the length of the graph of the ellipse given with equation $4x^2 + 9y^2 = 36$.

(12) A car laps a race track in 84 seconds. The speed of the car at each 6-second interval is determined by using a radar gun and is given from the beginning of the lap, in feet/second, by the entries in the following table.

Time	0	6	12	18	24	30	36	42	48	54	60	66	72	78	84
Speed	124	134	148	156	147	133	121	109	99	85	78	89	104	116	123

How long is the track?

(13) Evaluate the integral

$$\int_{-1}^{1} e^{-x^2} \cos x \, dx$$

by using the Gauss-Legendre two and three point formula.

(14) Evaluate

$$I = \int_0^1 \frac{\sin x \, dx}{2+x}$$

by subdividing the interval $[0, 1]$ into two equal parts and then by using Gauss-Legendre two point formula.

(15) A particle of mass m moving through a fluid is subjected to a viscous resistance R, which is a function of the velocity v. The relationship between the resistance R, velocity v, and time t is given by the equation

$$t = \int\limits_{v(t_0)}^{v(t)} \frac{m}{R(u)}\, du$$

Suppose that $R(v) = -v\sqrt{v}$ for a particular fluid, where R is in newtons and v is in meters/second. If $m = 10$ kg and $v(0) = 10$ m/s, approximate the time required for the particle to slow to $v = 5$ m/s.

(16) In statistics it is shown that

$$\int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} e^{-\dfrac{x^2}{2\sigma^2}} \, dx = 1,$$

for any positive σ. The function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\dfrac{x^2}{2\sigma^2}}$$

is the normal density function with mean $\mu = 0$ and standard deviation σ. The probability that a randomly chosen value described by this distribution lies in $[a, b]$ is given by $\int_a^b f(x)dx$. Approximate to within 10^{-3} the probability that a randomly chosen value described by this distribution will lie in

(a) $[-\sigma, \sigma]$
(b) $[-2\sigma, 2\sigma]$
(c) $[-3\sigma, 3\sigma]$.

Appendix A. Algorithms

Algorithm (Composite Trapezoidal Method):
Step 1 : Inputs: function $f(x)$; end points a and b; and N number of subintervals.
Step 2 : Set $h = (b - a)/N$.
Step 3 : Set sum $= 0$
Step 4 : For $i = 1$ to $N - 1$
Step 5 : Set $x = a + h * i$
Step 6 : Set sum $=$ sum$+2 * f(x)$
end
Step 7 : Set sum $=$ sum$+f(a) + f(b)$
Step 8 : Set ans $=$ sum$*(h/2)$
End

Algorithm (Composite Simpson's Method):
Step 1 : Inputs: function $f(x)$; end points a and b; and N number of subintervals (even).
Step 2 : Set $h = (b - a)/N$.
Step 3 : Set sum $= 0$
Step 4 : For $i = 1$ to $N - 1$
Step 5 : Set $x = a + h * i$
Step 6 : If rem$(i, 2) = 0$
sum $=$ sum$+2 * f(x)$
else
sum $=$ sum$+4 * f(x)$
end
Step 7 : Set sum $=$ sum$+f(a) + f(b)$
Step 8 : Set ans $=$ sum$*(h/3)$
End

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