Chapter 4: Numerical Integration

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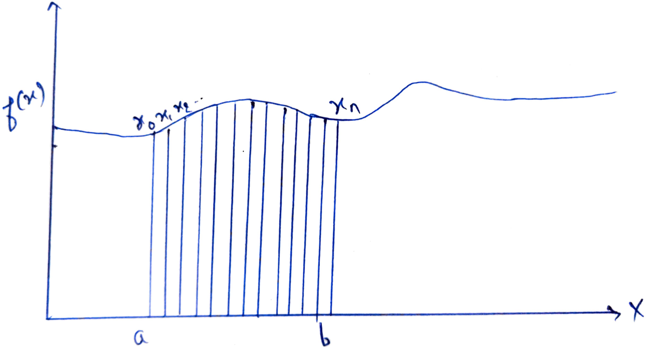
Newtonian Formulas

- Newton's various formulas rely on the philosophy of dividing the region of integration into small intervals and in each interval the function is approximated by a polynomial which is subsequently integrated.
- Finally, the values of the polynomials integrated over each interval are added to obtain the total integral. Now, we will describe various approaches.

(i) Trapezoidal Rule

- Trapezoidal rule relies upon dividing the integration region into n small intervals and in each interval the function is approximated by a straight line as shown below.
- Next we will derive the formula for both equally and unequally spaced arguments.



(a) Unequally Spaced Arguments

- In this case the i-th interval connecting x_{i-1} and x_i is approximated by a linear polynomial, i.e.,

$$f(x) \approx p_i(x) = f(x_{i-1}) + (x - x_{i-1}) f[x_{i-1}, x_i]$$

- Or

$$f(x) \approx f(x_{i-1}) + \frac{(x - x_{i-1})}{(x_i - x_{i-1})}(f(x_i) - f(x_{i-1}))$$

- Using the shorthand notation $f(x_i) = f_i$, we obtain the contribution of the i-th interval to the integral

$$I_i = \int_{x_{i-1}}^{x_i} p_i(x) dx$$

$$= f_{i-1}(x_i - x_{i-1}) - (f_i - f_{i-1}) x_{i-1} + \frac{(f_i - f_{i-1})}{2(x_i - x_{i-1})}(x_i^2 - x_{i-1}^2)$$

(a) Unequally Spaced Arguments (contd.)

- After simplification

$$I_i = \frac{1}{2}(f_i + f_{i-1})(x_i - x_{i-1}) \equiv \mathit{area\ of\ } i^{th} \mathit{\ trapezium}$$

- Thus

$$I = \int_a^b f(x)dx \approx \sum_i I_i \tag{1}$$

- Or

$$I = \frac{1}{2}\sum_{i=1}^{n}(f_i + f_{i-1})(x_i - x_{i-1}) \tag{2}$$

- In order to estimate the error, we recall that the error associated with linear interpolation is

$$E_i(x) = (x - x_{i-1})(x - x_i)f[x_{i-1}, x_i, x]$$

$$= \frac{(x - x_{i-1})(x - x_i)f^{(2)}(\xi_i)}{2!}$$

$$E_i(x) = \left[\frac{x^2}{2} - \frac{x(x_i + x_{i-1})}{2} + \frac{x_i x_{i-1}}{2}\right] f^2(\xi_i) \tag{3}$$

- Error in the integration is

$$\Delta I_i = \int_{x_{i-1}}^{x_i} E_i(x)dx$$

$$= \left\{\frac{(x_i^3 - x_{i-1}^3)}{6} - (x_i^2 - x_{i-1}^2)^2 \times \frac{(x_i + x_{i-1})}{4} + \frac{x_i x_{i-1}}{2}(x_i - x_{i-1})\right\} f^2(\xi_i)$$

$$= \left\{\frac{x_i^3}{6} - \frac{x_{i-1}^3}{6} - \frac{x_i^3}{4} - \frac{x_i^2 x_{i-1}}{4} + \frac{x_i x_{i-1}^2}{4} + \frac{x_{i-1}^2}{4} + \frac{x_i^2 x_{i-1}}{2} - \frac{x_i x_{i-1}^2}{2}\right\} f^2(\xi_i)$$

$$= \left\{ -\frac{x_i^3}{12} + \frac{x_{i-1}^3}{12} + \frac{x_i^2 x_{i-1}}{4} - \frac{x_i x_{i-1}^2}{4} \right\} f^2(\xi_i)$$

$$= -\frac{1}{12}\left\{ x_i^3 + 3x_i x_{i-1}^2 - 3x_i^2 x_{i-1} - x_{i-1}^3 \right\} f^2(\xi_i)$$

$$\Delta I_i = -\frac{1}{12}\{x_i - x_{i-1}\}^3 f^2(\xi_i) \tag{4}$$

- If we define

$$x_i - x_{i-1} = h_i \equiv \textit{spacing associated with the } i^{th} \textit{ interval}$$

- We get the total error associated with the trapezoidal rule to be

$$E = -\frac{1}{12}\sum_{i=1}^{n} h_i^3 f^2(\xi_i) \tag{5}$$

(b) Equally Spaced Arguments

- The results obtained in the previous section simplify tremendously when we assume that all the integration intervals are equispaced.
- In that case Eq.2 yields

$$I = \frac{1}{2}\sum_{i=1}^{n}(f_i + f_{i-1})h$$

- Or

$$I = \frac{(f_0 + f_n)}{2}h + (f_1 + f_2 + \ldots . f_{n-1})h$$

$$I = \sum_{i=0}^{n} f_i h - \frac{(f_0 + f_n)}{2}h \tag{6}$$

- The error is given by

$$E = -\frac{1}{12}\sum_i (x_i - x_{i-1})^3 f^{(2)}(\xi_i) = -\frac{h^3}{12}\sum_i f^{(2)}(\xi_i)$$

- If we make the approximation that $f^{(2)}(\xi_i) \approx f^{(2)}(\xi)$
- Then

$$E \approx -\frac{f^{(2)}(\xi) n h^3}{12}$$

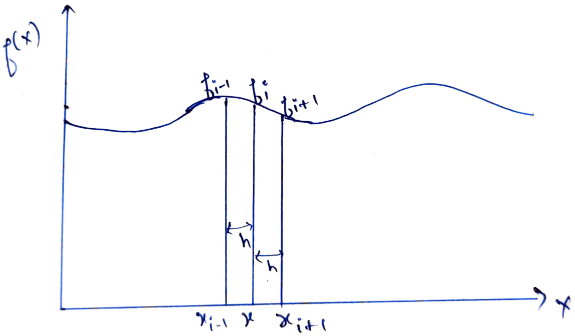
- Using the fact $b - a = nh$, we have

$$E \approx -\frac{(b-a)h^2 f^{(2)}(\xi)}{12} \tag{7}$$

- Which means that the error approximately scales as h^2 when the trapezoidal rule is used.

(ii) Simpson Rule

- Simpson rule is one of the most frequently used integration formulas.
- It is an improvement over the trapezoidal rule in the sense that instead of a linear polynomial, a quadratic polynomial is used to approximate the function in the subintervals.
- We will derive the necessary formulas for the case of equally spaced intervals.
- The case of unequally spaced intervals being straight forward but tedious.



- We consider two intervals – i^{th} and $(i+1)^{th}$, and approximate the function by a quadratic polynomial passing through the points x_{i-1}, x_i, and x_{i+1}

$$f(x) \approx f_{i-1} + (x - x_{i-1})\frac{\Delta f_{i-1}}{h} + \frac{(x - x_{i-1})(x - x_i)\Delta^2 f_{i-1}}{2h^2} \quad (8)$$

Simpson Rule (contd.)

- Using the fact that

$$\left.\begin{array}{r} x_{i-1} = x_i - h \\ \text{and defining } x - x_i = th \end{array}\right\} \tag{9}$$

where $t \in (-1, 1)$ is another variable

- We get

$$f(t) \approx f_{i-1} + (t+1)\Delta f_{i-1} + \frac{t(t+1)}{2}\Delta^2 f_{i-1} \tag{10}$$

- And the integral of the function over the two intervals

$$I_{i-1,i+1} = \int_{x_{i-1}}^{x_{i+1}} f(x)dx = h\int_{-1}^{1} f(t)dt$$

- Using Eq.9, we get

$$I_{i-1,i+1} = \left(2f_{i-1} + 2\Delta f_{i-1} + \frac{4}{3}\Delta^2 f_{i-1} - \Delta^2 f_{i-1}\right) h$$

- Or

$$I_{i-1,i+1} = \left(2f_{i-1} + 2\Delta f_{i-1} + \frac{1}{3}\Delta^2 f_{i-1}\right) h$$

$$= \left(2f_{i-1} + 2f_i - 2f_{i-1} + \frac{1}{3}[\Delta f_i - \Delta f_{i-1}\right) h$$

$$= \left(2f_i + \frac{1}{3}[f_{i+1} - f_i - f_i + f_{i-1}]\right) h$$

$$I_{i-1,i+1} = \left(\frac{1}{3}f_{i-1} + \frac{4}{3}f_i + \frac{1}{3}f_{i+1}\right) h \qquad (11)$$

Simpson Rule (contd.)

- Now clearly

$$I = \frac{1}{3}(f_0 + f_2 + f_4 + \ldots)\,h + \frac{4}{3}(f_1 + f_3 + f_5 + \ldots)\,h$$
$$+ \frac{1}{3}(f_2 + f_4 + f_6 + \ldots)\,h$$

- Or

$$I = \frac{h}{3}\{f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \ldots .2f_{n-2} + 4f_{n-1} + f_n\} \quad (12)$$

Error for Simpson Rule

- Let us try to estimate the error using the error formula

$$E_i(x) = \frac{(x - x_{i-1})(x - x_i)(x - x_{i+1})}{3!} f^{(3)}(\xi_i)$$

$$\Delta E_i = \int_{x_{i-1}}^{x_{i+1}} E_i(x) dx$$

with $x - x_i = t.h$

$$\Delta E_i = f^{(3)}(\xi) \frac{h^4}{3!} \int_{-1}^{1} (t+1)t(t-1)dt$$

$$\Delta E_i = \frac{h^4}{3} f^{(3)}(\xi) \int_{-1}^{1} t(t^2 - 1)dt = 0$$

- In other words, the error at the third order vanishes.

- Thus, error has to be computed differently for this case.
- We will do that using Taylor expansion around $x = x_i$

$$I_i = \frac{h}{3}(f_i + 4f_{i+1} + f_{i+2})$$

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2}f_i'' + \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i'''' + ...$$

$$f_{i+2} = f_i + 2hf_i' + \frac{(2h)^2}{2}f_i'' + \frac{(2h)^3}{3!}f_i''' + \frac{(2h)^4}{4!}f_i'''' + ...$$

- So

$$I_i = \frac{h}{3}\left(6f_i + 6hf_i' + 4h^2f_i'' + 2h^3f_i''' + \frac{5}{6}h^4f_i'''' + ...)\right)$$

Error for Simpson Rule (contd.)

- Assuming that $f(x) = F'(x)$
- We get the exact value

$$I_i^{ex} = \int_{x_i}^{x_{i+2}} F'(x)dx = F(x_{i+2}) - F(x_i)$$

$$F(x_{i+2}) - F(x_i) = 2hF_i' + \frac{(2h)^2}{2!}F_i'' + \frac{(2h)^3}{3!}F_i''' + \frac{(2h)^4}{4!}F_i'''' + \frac{(2h)^5}{5!}F_i'''''$$

$$= 2hf_i + 2h^2 f_i' + \frac{4}{3}f_i'' + \frac{2}{3}h^4 f_i''' + \frac{4}{15}h^5 f_i'''' + ...$$

Error for Simpson Rule (contd.)

$$I_i^{ex} - I_i^{simp} = \left(\frac{4}{15} - \frac{5}{18}\right) h^5 f_i^{(4)} + \ldots = -\frac{h^5}{90} f_i^{(4)} + \ldots.$$

- So total error

$$\Delta E = -(\frac{n}{2})\frac{h^5}{90} f^{(4)}(3) = -\frac{(b-a)}{180} h^4 f^{(4)}(\xi)$$

- There are $\frac{n}{2}$ terms in the above sum.

(iii) Recursive Integration

- If we apply a formula such as the Simpson rule or the trapezoidal rule just once to perform an integration numerically, we are never sure that the result that we obtain is convergent.
- Therefore, in practice a recursive computation is advisable which is based upon the following algorithm.

1. Choose an initial spacing which can be

$$h = h_{min} = \frac{b-a}{n_{min}}$$

where $a \equiv$ lower limit of integration
$b \equiv$ upper limit of integration
$n_{min} = 2$ for trapezoidal rule
$= 3$ for Simpson rule

Recursive Integration (contd.)

2. Compute the integral
3. Check if the result has converged compared to the previous iteration. If yes, then stop.
4. If result has not converged, halve the interval, i.e., set $h = \frac{h}{n}$, where usually $n = 2$.
5. Go to step 2.

- Application of this recursive procedure will ensure converges along with avoidance of unnecessary competition by needlessly choosing a very fine grid.
- In addition, in every iteration one can use the function values f_i computed in the previous equation.

(iv) Romberg Integration

- The idea of Romberg integration is to extrapolate to the exact result while performing recursive integration outlined above.
- Let us suppose that we want to numerically compute the integral

$$I = \int_a^b f(x)dx \tag{13}$$

- If we use a procedure such as the trapezoidal rule or the Simpson rule, then the error is of the form

$$E = C^{'} h^r f(r)(\xi) \tag{14}$$

where $\xi \in (a, b)$ and r is an integer.
- Recall $r = 2$ for trapezoidal rule and $r = 4$ for Simpson rule.

Romberg Integration (contd.)

- Let us compute the integral two times, say with spacing h_1 and h_2 so that results I_1 and I_2 are obtained.
- Clearly

$$I_1 = I - C' h_1^r f^{(r)}(\xi_1)$$
$$I_2 = I - C' h_2^r f^{(r)}(\xi_2)$$

- If we assume that $f^{(r)}(\xi)$ is sufficiently smoothly varying, we can approximate $f^{(r)}(\xi_1) \approx f^{(r)}(\xi_2)$.
- So that we can write

$$I_1 = I - Ch_1^r \tag{15}$$

$$I_2 = I - Ch_2^r \tag{16}$$

where $C = C' f^{(r)}(\xi_1) = C' f^{(r)}(\xi_2)$.

- Eqs. 15 and 16 can be solved to yield

$$I \approx \frac{I_2 h_1^r - I_1 h_2^r}{h_1^r - h_2^r}$$

- or, on rearranging terms

$$I \approx I_2 + \frac{I_2 - I_1}{\left(\frac{h_1}{h_2}\right)^r - 1} \tag{17}$$

- For the special case when $h_1 = 2h_2$, we get

$$I \approx I_2 + \frac{I_2 - I_1}{2^r - 1} \tag{18}$$

- Formula 18 is called Richardson extrapolation.

Romberg Integration (contd.)

- The idea behind Romberg integration is to combine the philosophy behind recursive integration and Richardson extrapolation to reach the correct answer.
- Romberg integration relies upon the knowledge of the dependence of the error associated with the method on h.
- For example, it can be shown that the error associated with the trapezoidal rule is

$$E = C_1 h^2 + C_2 h^4 + C_N h^{2N} - (b-a) h^{2N+2} \frac{B_{2N+2}}{(2N+2)!} f^{(2N+2)}(\xi) \tag{19}$$

where B_{2N+2} is the Bernoulli number.

- Above N can be taken to be arbitrarily large provided the derivative $f^{(2N+2)}(\xi)$ exists for $a \leq \xi \leq b$.
- Once we know the error series of type Eq.19, we can apply the Richardson extrapolation procedure on the computed integrals to remove errors involving successively higher order in h.

Algorithmically speaking:

- (i) We compute the trapezoidal approximations $T_k^{(0)}$ to the integral I, computed with spacings

$$h_k = \frac{b-a}{2^k}.$$

- (ii) To successive pairs $T_k^{(0)}, T_{k+1}^{(0)}$ we apply Richardson extrapolation (Eq.18) with $r = 2$ to generate numbers $T_k^{(1)}$.

- These numbers clearly are free of the error at order h^2, but have errors of the order h^4 and higher.
- (iii) To successive pairs $T_k^{(1)}$ and $T_{k+1}^{(1)}$ we apply Richardson extrapolation with $r = 4$ to generate numbers $T_k^{(2)}$......
- These are free of the error at the h^4 level.
- This procedure is continued and the following triangular Romberg array is generated

$$
\begin{array}{llll}
T_0^{(0)} & & & \\
T_1^{(0)} & T_0^{(1)} & & \\
T_2^{(0)} & T_1^{(1)} & T_0^{(2)} & \cdots \\
\vdots & & &
\end{array}
$$

- The process is terminated once the sequence of diagonal elements $T_0^{(i)}$ stop changing.
- Clearly, this procedure can be applied to any integration formula for which the form of the series 19 is known.

$$T_{k+1}^{(i)} = T_{k+1}^{(i-1)} + \frac{T_{k+1}^{(i-1)} - T_k^{(i-1)}}{2^{2i} - 1}$$

- Until now we discussed numerical methods for integration which involved the use of equidistant x-points distributed over the entire integration range.
- We also saw that generally a large number of x-points are needed to achieve high accuracy.
- It is clear that the generalization of these methods for integration in higher dimensions $(i.e. I = \int_{a_3}^{b_3} \int_{a_2}^{b_2} \int_{a_1}^{b_1} f(x,y,z)dxdydz)$ will be computationally very expensive.

Gaussian Quadrature (contd.)

- Thus the question arises that can one perform highly accurate integration using a rather smaller number of specially chosen sample points which may not be equispaced ?
- Gaussian quadrature (quadrature means integration) is precisely such an approach which we discuss next.
- But first we will introduce the concept of direct integration.

- Until now, while performing integration, we approximated the function by an interpolation polynomial.
- However, here we do not use such an approach, rather we try to obtain an approximate method for general function $f(x)$ which will yield exact results, when $f(x)$ is taken to be an specific polynomial depending upon the number of x-points.
- For example, using this approach let as derive the formula for the Simpson rule.
- We want to approximate the integral as

$$\int_{-1}^{1} f(x)dx \approx af(-1) + bf(0) + cf(1) \tag{20}$$

- We first take $f(x) = 1$ and get from Eq.20

$$a + b + c = 2 \tag{21}$$

Direct Integration (contd.)

- Similarly by taking $f(x)$ to be x and x^2, we, respectively, get

$$-a + c = 0 \tag{22}$$

and

$$a + c = \frac{2}{3} \tag{23}$$

- So on solving Eqs. 21-23, we get

$$\left.\begin{array}{c} a = c = \frac{1}{3} \\ b = \frac{4}{3} \end{array}\right\} \tag{24}$$

- And thus we recover the integration formula of Simpson rule

$$\int_0^2 f(x) \approx \frac{1}{3}\left(f(-1) + 4f(0) + f(1)\right) \tag{25}$$

Direct Integration (contd.)

- It is clear that the highest error in the approximation will be because of the next neglected term, i.e. x^3 which yields the result

$$\int_{-1}^{1} x^3 dx \approx \frac{1}{3}(-1+1) + E_3$$

$$\Rightarrow 0 \approx 0 + E_3 \Rightarrow E_3 = 0$$

- The next term is x^4 which yields

$$\frac{1}{2} \approx \frac{1}{3}(1+1) + E_4$$

$$\Rightarrow E_4 \approx \frac{-1}{6}$$

Gaussian Quadrature – Examples

- In the direct integration approach, if N sample x-points are used for integration, typically the error is of the order of next neglected power of x, i.e. x^N.
- Now, the question is, can we improve this situation, i.e. achieve even higher accuracy with the same number of sampling points?
- The answer is yes provided we use a special choice of x-points.
- This choice is the essence behind the Gaussian quadrature.
- Let us consider two examples

$$I_1 = \int_{-1}^{1} f(x)dx \tag{26}$$

$$I_2 = \int_{0}^{\infty} e^{-x} f(x)dx \tag{27}$$

- Let us try to approximate these integrals by using just two x-points, i.e.

$$I_{1/2} = w_1 f(x_1) + w_2 f(x_2) \tag{28}$$

Gaussian Quadrature – Example (contd.)

- But, we want the integral to yield exact results for up to cubic polynomials, i.e, for $f(x) = 1, x, x^2, x^3$
- Let us start out with calculation of I_1 by substituting respectively $f(x) = 1, x, x^2, x^3$ in Eqs. 26 and 28

$$\begin{aligned} w_1 + w_2 &= 2 \\ w_1 x_1 + w_2 x_2 &= 0 \\ w_1 x_1^2 + w_2 x_2^2 &= \frac{2}{3} \\ w_1 x_1^3 + w_2 x_2^3 &= 0 \end{aligned} \tag{29}$$

- Let us next take $f(x) = \pi^2(x) = (x - x_1)(x - x_2)$, i.e., a quadratic polynomial whose roots are x_1 and x_2
- Note that we can write $\pi^2(x) = x^2 - (x_1 + x_2)x + x_1 x_2 = x^2 + c_1 x + c_0$, where $\pi^2(x_1) = \pi^2(x_2) = 0$

Gaussian Quadrature for I_1

- Because $\pi^{(2)}(x)$ is a quadratic polynomial, therefore, we must get exact result if we substitute $f(x) = \pi^2(x)$ and $f(x) = x\pi^{(2)}(x)$ in Eqs. 26 and 28
- For $f(x) = \pi^2(x)$, we have

$$\int_{-1}^{1}(x^2 + c_1 x + c_0)dx = w_1\pi^{(2)}(x_1) + w_2\pi^{(2)}(x_2) = 0$$

$$\implies \frac{2}{3} + 0 + 2c_0 = 0$$

$$\implies c_0 = -\frac{1}{3}$$

- For $f(x) = x\pi^{(2)}(x) = x^3 + c_1 x^2 - \frac{1}{3}x$

$$\int_{-1}^{1}(x^3 + c_1 x^2 - \frac{1}{3}x)dx = w_1 x_1\pi^{(2)}(x_1) + w_2 x_2\pi^{(2)}(x_2) = 0$$

$$\implies 0 + \frac{2}{3}c_1 - 0 = 0$$

$$\implies c_1 = 0$$

Gaussian Quadrature for I_1(contd.)

- Now we can find the points x_1 and x_2 as the roots of $\pi^{(2)}(x)$

$$x^2 - \frac{1}{3} = 0$$
$$\implies x_1, x_2 = -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}$$

- Now we can easily determine the weights w_1 and w_2 by substituting the values of x_1 and x_2 in the Eqs. 29.
- Substituting these in the second of Eqs. 29, we obtain

$$-\frac{w_1}{\sqrt{3}} + \frac{w_2}{\sqrt{3}} = 0 \implies w_1 = w_2$$

- On substituting this in the first of Eqs. 29, we obtain

$$w_1 = w_2 = 1$$

- Thus yielding the two-point Gaussian quadrature formula

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

  which is accurate up to x^3
- This actually is an example of 2-point Gauss-Legendre quadrature

Gaussian Quadrature for I_2

- For cubic polynomial, the using Eqs. 27 and 28defining equations for $f(x) = 1, x, x^2, x^3$ are respectively

$$w_1 + w_2 = 1 \tag{30}$$

$$w_1 x_1 + w_2 x_2 = 1 \tag{31}$$

$$w_1 x_1^2 + w_2 x_2^2 = 2 \tag{32}$$

$$w_1 x_1^3 + w_2 x_2^3 = 6 \tag{33}$$

- Next we take $f(x) = \pi^2(x) = (x - x_1)(x - x_2)$
- Clearly

$$\pi^{(2)}(x) = x^2 - (x_1 + x_2)x + x_1 x_2 \tag{34}$$

- Or
$$\pi^{(2)}(x) = x^2 + c_1 x + c_0 \tag{35}$$
- Thus $\pi^2(x)$ is the polynomial whose roots are points x_1 and x_2 using the results of Eqs.30-33, we immediately get for Eq. 28.
$$\int_0^\infty e^{-x}\pi^{(2)}(x)dx = w_1\pi(x_1) + w_2\pi(x_2)$$
but $\pi(x_i) = 0$
- So we get
$$c_0 + c_1 + 2 = 0 \tag{36}$$
- Next we consider
$$f(x) = x\pi^{(2)}(x)$$
- So that we get
$$c_0 + 2c_1 + 6 = w_1 x_1 \pi^{(2)}(x_1) + w_2 x_2 \pi^{(2)}(x_2) = 0 \tag{37}$$

- Upon solving Eq.36 and Eq.37 we get

$$\left.\begin{aligned} c_1 &= -4 \\ c_0 &= 2 \end{aligned}\right\} \tag{38}$$

- So that

$$\pi^2(x) = x^2 - 4x + 2$$

and x_1 and x_2 are its roots given by

$$x_{1,2} = \frac{4 \pm \sqrt{16-8}}{2} = 2 \pm \sqrt{2}$$

- Now that we have determined points x_1 and x_2, we can determine weights w_1 and w_2 from Eqs.30 and 31.

$$w_1 + w_2 = 1$$

$$w_1(2+\sqrt{2}) + w_2(2-\sqrt{2}) = 1$$

- which leads to

$$w_1 + w_2 = 1$$

$$\sqrt{2}w_1 - \sqrt{2}w_2 = -1$$

- which can be solved to yield

$$w_1 = \frac{\sqrt{2}-1}{2\sqrt{2}}$$

$$w_2 = \frac{\sqrt{2}+1}{2\sqrt{2}}$$

- Thus our final integration formula accurate up to cubic power in x:

$$\int_0^\infty e^{-x} f(x) dx = \frac{\sqrt{2}-1}{2\sqrt{2}} f(2-\sqrt{2}) + \frac{\sqrt{2}+1}{2\sqrt{2}} f(2+\sqrt{2}) \quad (39)$$

This is an example of 2-point Gauss Laguerre quadrature

Gaussian Quadrature (contd.)

- Let us try to analyze as to how we have with just two points while in the direct formula approach to achieve this accuracy we would have needed four sample points.
- The reason behind this is that in the direct formula approach the points of integration are fixed while only undetermined quantities are the weights.
- Thus to determine N weights one would need N equation leading to an accuracy of the order of x^{N-1}.
- However, in the Gaussian quadrature approach, both the sample points as well as the weights are unknown.
- Thus, if we want to perform integration using N x points, we will have $2N$ unknowns in total leading to an accuracy of x^{2N-1}, with just N points.

- We consider the most general case here involving the integral

$$I = \int_a^b k(x) f(x) dx \tag{40}$$

with $k(x) \geq 0$ for $a \leq x \leq b$

- Our aim, using the method of Gaussian quadrature is to obtain an expression of the type

$$I \approx \sum_{k=1}^{N} w_k f(x_k) \tag{41}$$

- Clearly, Eq.41 involves $2N$ unknowns requiring $2N$ conditions. This means that we can make it exact for up to polynomial of degree $2N - 1$.

- As usual our defining equations will be obtained by approximating $f(x) = 1, x, x^2, ...x^{2N-1}$ leading to

$$m_j = \sum_{k=1}^{N} w_k x_k^j \tag{42}$$

for $j = 0, 1, 2, ..., 2N-1$, where $m_j \equiv j^{th}$ moment of k, is defined as

$$m_j = \int_a^b x^j k(x) dx \tag{43}$$

- Next we consider

$$\pi^{(N)}(x) = (x - x_1)(x - x_2).....(x - x_N) \tag{44}$$

that is a polynomial of degree N whose roots are the N sampling points of Eq.41.

- Clearly, we can write

$$\pi^{(N)}(x) = x^N + c_{N-1}x^{N-1} + ...c_0 = \sum_{j=0}^{N-1} c_j x^j + x^N \tag{45}$$

- Next we approximate $f(x) = \pi^{(N)}(x)$ in Eq.41 and use results of Eq.42, we get

$$\sum_{j=0}^{N-1} m_j c_j + m_N = \sum_{k=1}^{N} w_k \pi(x_k) = 0 \qquad (46)$$

- Repeating this procedure for choices of $f(x) = x^k \pi^{(N)}(x)$ with $k = 1, ..., N-1$, we get

$$\sum_{j=0}^{N-1} m_{j+k} c_j + m_{N+k} = 0 \quad k = 0, 1, ... N-1$$

which is a set of N inhomogeneous equations

$$\sum_{j=0}^{N-1} m_{j+k} c_j = -m_{N+k} \quad \text{for } k = 0, 1, ... N-1 \qquad (47)$$

whose coefficient matrix is made up of moments m_{j+k}, and c_j are the unknown coefficients

Gaussian quadrature (contd.)

- Now our aim is to demonstrate that N equations 47 will have non-trivial solutions.
- We will demonstrate this by considering a homogeneous equation, which has the same coefficient matrix as the inhomogeneous equation (Eq. 47)

$$\sum_{j=0}^{N-1} m_{j+k} a_j = 0 \quad \text{for } k = 0, 1, ..., N-1 \tag{48}$$

- and show that the only possible solution of the homogeneous equation is the trivial one, i.e., $a_j = 0$ for $j = 0, \ldots, N-1$.
- This would imply that the determinant of the coefficient matrix m_{j+k} is non-zero
- which, in turn, would imply that the inhomegeneous Eq. 47 will have nontrivial solutions

- Let us multiply the homogeneous equation by a_k and use the definition of $m_j's$

$$\sum_{j=0}^{N-1} m_{j+k} a_j a_k = \int_{j=0}^{N-1} k(x) x^{j+k} a_k a_j dx = 0 \quad \text{for } k = 0, 1, ..., N-1$$

- If we add all the N equations involving a_k we get

$$\int_a^b k(x) \left(\sum_{j=0}^{N-1} a_j x^j \right) \left(\sum_{k=0}^{N-1} a_k x^k \right) = 0 \tag{49}$$

- or

$$\int_a^b k(x) \left\{ \sum_{j=0}^{N-1} a_j x^j \right\}^2 = 0 \tag{50}$$

- Since $k(x) \geq 0$ in the range of integration, thus we conclude from Eq.50 that

$$\sum_{j=0}^{N-1} a_j x^j = 0 \;\; for\ all\ x$$

$$\Rightarrow a_j = 0 \;\; for\ j = 0, \ldots, N-1$$

- This solution is possible for a homogeneous Eqs. 48 only if the determinant of coefficients is non zero.
- This implies that the corresponding inhomogeneous equation (Eq.47) will have a nontrivial solution.

- Next thing we need to prove is that the polynomial $\pi_x^{(N)}$ will indeed have N zeros in the range of integration.
- Let us suppose that it is not the case and we have only k zero's $x_1, x_2, \ldots x_k \in (a, b)$, i.e., in the range of integration.
- Let us define a polynomial $p(x)$ of degree $k < N$.

$$p(x) = (x - x_1)(x - x_2).....(x - x_k)$$

- Then

$$\int_a^b k(x)\pi(x)p(x) = \sum_{j=1}^{N} w_j \pi(x_j)p(x_j) = 0$$

- R.H.S. is zero because $x_j's$ are roots of $\pi(x)$.

- But

$$\pi(x)p(x) = (x-x_1)^2(x-x_2)^2......(x-x_k)^2(x-x_{k+1})....(x-x_N)$$

- Therefore, $\int_a^b k(x)\pi(x)p(x)dx > 0$ because in the range of integration $k(x)\pi(x)p(x) > 0$, i.e., it does not change sign in the range of integration.
- Thus we have a contradiction because $\pi(x)p(x)$ is a polynomial of degree $N+k \leq 2N-1$ and for a polynomial of that degree we had exactly satisfied the defining equation, therefore, the integral must be zero.
- Thus, we have a contradiction.
- The only way to resolve it is to take $k = N$, i.e. the polynomial has N real roots in the range of integration.

Weights are positive numbers

- In the most general case the expression for weights is obtained rapidly by considering $f(x) = \pi_i(x)^2$, where $\pi_i(x) = (x - x_1)\dots(x - x_{i-1})(x - x_{i+1})\dots(x - x_N)$,

$$\Longrightarrow \int_a^b k(x)\pi_i^2(x)dx = w_i\pi_i^2(x_i)$$

  which immediately leads to the expression

$$w_i = \int_a^b k(x)\frac{\pi_i^2(x)}{\pi_i^2(x_i)}dx \tag{51}$$

- Recalling that

$$l_i(x) = \frac{\pi_i(x)}{\pi_i(x_i)} \tag{52}$$

  we get the alternative expression for the weights

$$w_i = \int_a^b k(x)l_i^2(x)dx \tag{53}$$

Weights are positive numbers (contd.)

- Since, in the range of integration both $k(x)$ and $l_i^2(x)$ are positive, hence w_i will be positive.
- Thus in Gaussian quadrature formulas, the round off problem will not be severe.

Useful General Expression for Weights

- Next we will derive a general expression for weights which is simpler than Eq.53.
- We start with the basic Gaussian quadrature formula

$$\int_a^b k(x)f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$

which is exact for all the polynomials of degree $2N-1$ or less.

- Next we consider $f(x)$ to be the Lagrangian interpolation formula for N points (or polynomial of degree N).

$$f(x) = \sum_{i=1}^{N} l_i(x) f(x_i) \tag{54}$$

and substitute above

Useful General Expression for Weights (contd.)

$$\sum_{i=1}^{N} \int_a^b k(x) l_i(x) f(x_i) dx = \sum_{i=1}^{N} w_i f(x_i) \quad (55)$$

leading to

$$w_i = \int_a^b k(x) l_i(x) dx \quad (56)$$

- Next, we will consider different specific quadratures .

- This is useful for the case where $k(x) = 1$, $a = -1$, and $b = 1$, i.e. integrals of the type

$$I = \int_{-1}^{1} f(x)dx \tag{57}$$

- In this case the polynomial $\pi(x)$ is chosen to be proportional to the Legendre polynomial of degree N, i.e.

$$\pi(x) = \frac{2^N(N!)}{2N!} P_N(x) \tag{58}$$

- It is a well known property of $P_N(x)$ that it has$N$ real roots in the interval (-1,1).
- There is no analytic expression for the roots of $P_N(x)$, thus they have to be computed numerically.

- Now for this case

$$l_i(x) = \frac{\pi_i(x)}{\pi_i(x_i)} = \frac{P_N(x)}{(x-x_i)P'_N(x_i)}$$

since

$$\pi_i(x_i) = \left.\frac{d\pi}{dx}\right|_{x=x_i} = \pi'(x_i)$$

- Thus, using Eq.56, we get

$$w_i = \int_{-1}^{1} \frac{P_N(x)dx}{(x-x_i)P'_N(x_i)} \quad (59)$$

- To perform this integral, we will use the Christoffel's identity for Legendre polynomials.

$$(t-x)\sum_{i=0}^{n}(2i+1)P_i(x)P_i(t) = (n+1)\left[P_{n+1}(t)P_n(x) - P_n(t)P_{n+1}(x)\right] \quad (60)$$

Gauss-Legendre Quadrature (contd.)

- Take t = x_i, and n = N so that the second term on the R.H.S. vanishes and we get

$$\frac{P_N(x)}{x-x_i} = -\sum_{k=0}^{N} \frac{(2k+1)P_k(x)}{(N+1)P_{N+1}(x_i)} P_k(x_i) \qquad (61)$$

- Substituting this in Eq.59, we get

$$w_i = -\frac{1}{P_N(x_i)P_{N+1}(x_i)(N+1)} \sum_{k=0}^{N} (2k+1)P_k(x_i) \int_{-1}^{1} P_k(x)dx$$

- Using the fact that $P_0(x) = 1$ and the orthogonality relation of $P_n(x)'s$, i.e.

$$\int_{-1}^{1} P_n(x)P_m(x)dx = \delta_{nm}\frac{2}{2n+1} \qquad (62)$$

- We see that only the k = 0 term survives above, i.e.

$$w_i = -\frac{2}{(N+1)P_{N+1}(x_i)P'_N(x_i)}$$

but recursion relation

$$(N+1)P_{N+1}(x) = -NP_{N-1}(x)$$

yields a positive expression

$$w_i = \frac{2}{NP'_N(x_i)P_{N-1}(x_i)} \tag{63}$$

- Now using the relation

$$(1-x^2)P'_n(x) = -nxP_n(x) + nP_{n-1}(x) \tag{64}$$

- we immediately get

$$NP_{N-1}(x_i) = (1 - x_i^2)P'_N(x_i)$$

- So that from Eq.63 we get an alternative expression for the weights

$$w_i = \frac{2}{(1 - x_i^2)[P'_N(x_i)]^2} \tag{65}$$

- It is the expression which is used to compute the weights w_i for Gauss-Legendre quadrature in the book "Numerical Recipes".

Gauss-Laguerre Quadrature

- When one has to integrate the function of the type

$$I = \int_0^\infty e^{-x} f(x) dx \tag{66}$$

  Gauss-Laguerre quadrature is useful.

- In this case, if we want an accuracy of up to x^{2N-1}, we need to use the Laguerre polynomial of degree N, i.e.

$$\pi(x) = (-1)^N L_N(x) \tag{67}$$

  so that

$$I \approx \sum_{i=1}^{N} w_i f(x_i) \tag{68}$$

  where x_i are the N roots of the Laguerre polynomial lying in the interval $(0, \infty)$.

- The weights are determined by

$$w_i = \int_0^\infty e^{-x} l_i(x)dx = \int_0^\infty \frac{e^{-x} L_N(x)}{(x - x_i) L'_N(x_i)} dx \tag{69}$$

- The Christoffel identity for Laguerre polynomials

$$\sum_{k=0}^{N} \frac{L_k(x)L_k(t)}{(k!)^2} = -\frac{L_{N+1}(x)L_N(t) - L_N(x)L_{N+1}(t)}{(N!)^2(x-t)} \tag{70}$$

- Setting $t = x_i$ in Eq.70, we get

$$\frac{L_N(x)}{x - x_i} = \frac{(N!)^2}{L_{N+1}(x_i)} \sum_{k=0}^{N} \frac{L_k(x)L_k(x_i)}{(k!)^2}$$

so that

$$w_i = \frac{(N!)^2}{L_{N+1}(x_i)L'_N(x_i)} \sum_{k=0}^{N} \frac{L_k(x_i)}{(k!)^2} \int_0^\infty L_k(x) e^{-x} dx$$

- Using the normalization condition:
$\int_0^\infty L_k(x)L_m(x)e^{-x}dx = \delta_{km}(m!)^2$ and $L_0(x) = 1$, we get

$$w_i = \frac{(N!)^2}{L_{N+1}(x_i)L'_N(x_i)} \tag{71}$$

- Using the relation

$$xL'_m(x) = (x - m - 1)L_m(x) + L_{m+1}(x)$$

we get

$$L_{N+1}(x_i) = x_i L'_N(x_i)$$

so that

$$w_i = \frac{(N!)^2}{x_i[L'_N(x_i)]^2} \tag{72}$$

Gauss-Hermite Quadrature

- In order to compute the integrals of the type

$$I = \int_{-\infty}^{\infty} e^{-x^2} f(x) dx \tag{73}$$

one resorts to Gauss-Hermite quadrature using

$$\pi(x) = \frac{H_N(x)}{2^N} \tag{74}$$

- So that

$$I = \sum_{i=1}^{N} w_i f(x_i) \tag{75}$$

where $x_i's$ are the roots of the Hermite polynomial of degree N which lie between -∞ and +∞.

- The weights will be

$$w_i = \int_{-\infty}^{\infty} \frac{e^{-x^2} H_N(x)}{(x - x_i) H'_N(x_i)} \tag{76}$$

- The Christoffel identity in this case is

$$\sum_{k=0}^{N} \frac{H_k(x)H_k(t)}{\sqrt{\pi}2^k k!} = \frac{H_{N+1}(x)H_N(t) - H_N(x)H_{N+1}(t)}{2\sqrt{\pi}2^N N!(x-t)}$$

for which

$$\frac{H_N(x)}{x-x_i} = -\frac{2^{N+1}N!}{H_{N+1}(x_i)} \sum_{k=0}^{N} \frac{H_k(x)H_k(x_i)}{2^k k!}$$

so that

$$w_i = -\frac{2^{N+1}N!}{H_{N+1}(x_i)H'_N(x_i)} \sum_{k=0}^{N} \sum_{-\infty}^{\infty} e^{-x^2} \frac{H_k(x_i)H_x(x)}{2^k k!} dx$$

- Using the fact

$$\sum_{-\infty}^{\infty} H_k(x)H_m(x)e^{-x^2} dx = \delta_{km}2^k k!\sqrt{\pi} \qquad (77)$$

and $H_0(x) = 1$

Gauss-Hermite Quadrature (contd.)

- We get

$$w_i = \frac{-2^{N+1} N! \sqrt{\pi}}{H_{N+1}(x_i) H'_N(x_i)} \tag{78}$$

- Using the relation

$$H'_m(x) = 2x H_m(x) - H_{m+1}(x) \tag{79}$$

we get

$$H_{N+1}(x_i) = H'_N(x_i)$$

- So that we get

$$w_i = \frac{2^{N+1} N! \sqrt{\pi}}{[H'_N(x_i)]^2}$$