Lecture 18: Numerical Integration Contd..

Rajen Kumar Sinha

Department of Mathematics
IIT Guwahati

Gauss Quadrature Rule

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

All quadrature rule has the form

$$I(f) \approx A_0 f(x_0) + A_1 f(x_1) + \cdots + A_k f(x_k), \tag{1}$$

with nodes $x_0, \cdots, x_k$ and weights $A_0, \ldots, A_k$.

$$I(f) \approx (b-a)f(a) \quad \text{(Rectangle rule)}$$

$A_0 = b-a, \quad x_0 = a$

$\underline{A_0 f(a)}$

$$I(f) \approx \frac{(b-a)}{2}[f(a) + f(b)] \quad \text{(Trapezoidal rule)}$$

$$I(f) \approx \frac{(b-a)}{6}[f(a) + 4f(\frac{a+b}{2}) + f(b)] \quad \text{(Simpson's rule)}$$

$A_0 = \frac{b-a}{6}$

$A_1 = \frac{2}{3}(b-a)$

$A_2 = \frac{b-a}{6}$

$x_0 = a$

$x_1 = \frac{a+b}{2}$

$x_2 = b$

Observation. There is no freedom in choosing the nodes $x_0, x_1, \ldots, x_k$. The difficulty with the Newton-Cotes formulas (Composite rules) is that the nodes x_i must be evenly spaced. $x_i - x_{i-1} = h$

Q. Is it possible to make a rule exact for polynomial of degree $\leq 2k+1$ by choosing the nodes appropriately?

To discuss Gaussian rules in the more general context, we write the integral as

$$\int_a^b f(x)dx = \int_a^b w(x)g(x)dx,$$

where the weight function w(x) is assumed to be nonnegative and integrable on $[a, b]$, and

$$g(x) = \frac{f(x)}{w(x)}.$$

Here, $f(x)$ may behave like $(x-a)^{\alpha}$ near a for some $\alpha > -1$.

OR we may have a or/and b may be infinite.

Consider approximating the weighted integral

$$\begin{aligned} I(g) &= \int_a^b g(x)w(x)dx \\ &\approx A_0 g(x_0) + A_1 g(x_1) + \cdots + A_k g(x_k) \\ &= \sum_{j=0}^{k} A_j g(x_j) = I_k(g). \end{aligned}$$

Here the nodes x_j and weights A_j are to be chosen so that $I_k(g)$ equals $I(g)$ exactly for polynomials $g(x)$ of as higher degree as possible (This is the basic idea of Gaussian rule).

Consider the special case with $w(x) = 1$, and $[a, b] = [-1, 1]$

$$\int_{-1}^{1} g(x)\, dx \approx \sum_{j=0}^{k} A_j g(x_j).$$

Define the error

$$E_k(g) = \int_{-1}^{1} g(x)\, dx - \sum_{j=0}^{k} A_j g(x_j). \tag{2}$$

The weights A_j and nodes x_j are to be determined to make the error

$$E_k(g) = 0 \tag{3}$$

for as high a degree polynomial $g(x)$ as possible. Note that

$$E_k(a_0 + a_1 x + \cdots + a_n x^m) = a_0 E_k(1) + a_1 E_k(x) + \cdots + a_m E_k(x^m) \tag{4}$$

$E_k(g) = 0$ ∀ poly. g(x) of deg $\leq m$.

If $E_k(x^i) = 0$, $i = 0, 1, \cdots, m$.

$$E_k(g) = 0 \text{ for every polynomial of degree } \leq m$$
$$\iff E_k(x^i) = 0, \ i = 0, 1, 2, \ldots, m.$$

For $k = 0$, we have $\int_{-1}^{1} g(x)\,dx \approx A_0 g(x_0)$. We require $E_k(1) = 0$ and $E_k(x) = 0$.

$E_k(1) = \int_{-1}^{1} dx - A_0$

$$E_k(1) = 0 \implies \int_{-1}^{1} dx - A_0 = 0 \implies A_0 = 2$$

$$E_k(x) = 0 \implies \int_{-1}^{1} x\,dx - A_0 x_0 = 0 \implies x_0 = 0$$

This leads to the formula

$$\int_{-1}^{1} g(x)\,dx \approx 2g(0),$$

$$\boxed{\int_a^b f(x)\,dx \approx (b-a) f\left(\frac{a+b}{2}\right) \approx 2f(0)}$$

which is mid-point rule.

For $k = 1$, we have $\int_{-1}^{1} g(x)\,dx \approx A_0 g(x_0) + A_1 g(x_1)$. There are four unknown parameters to be determined. Thus, we require

That is,

$g(x) = 1.$

$$E_k(1) = 0 \implies \int_{-1}^{1} dx - (A_0 + A_1) = 0 \implies A_0 + A_1 = 2$$

$g(x) = x$

$$E_k(x) = 0 \implies \int_{-1}^{1} x\,dx - (A_0 x_0 + A_1 x_1) = 0 \implies A_0 x_0 + A_1 x_1 = 0$$

$g(x) = x^2$

$$E_k(x^2) = 0 \implies \int_{-1}^{1} x^2\,dx - (A_0 x_0^2 + A_1 x_1^2) = 0 \implies A_0 x_0^2 + A_1 x_1^2 = \frac{2}{3}$$

$g(x) = x^3$

$$E_k(x^3) = 0 \implies \int_{-1}^{1} x^3\,dx - (A_0 x_0^3 + A_1 x_1^3) = 0 \implies A_0 x_0^3 + A_1 x_1^3 = 0$$

On solving, we get $A_0 = A_1 = 1$ and $x_0 = \frac{1}{\sqrt{3}}$, $x_1 = -\frac{1}{\sqrt{3}}$. This leads to the formula

$$\int_{-1}^{1} g(x)\,dx \approx g\left(\frac{1}{\sqrt{3}}\right) + g\left(-\frac{1}{\sqrt{3}}\right),$$

which has degree of precision three.

For a general k, there are $2k+2$ parameters (weights $\{w_i\}_{i=0}^k$ and nodes $\{x_i\}_{i=0}^k$) to be determined. The equations to be solved are

$$E_k(x^i) = 0, \quad i = 0, 1, 2, \ldots, 2k+1.$$

This leads to the set of equations:

$$\sum_{j=0}^{k} A_j x_j^i = \begin{cases} 0 & i = 1, 3, \ldots, 2k+1 \\ \frac{2}{i+1} & i = 0, 2, \ldots, 2k. \end{cases} \tag{5}$$

Note: The equations in (5) are nonlinear equations, and their solvability is not at all obvious.

This procedure is called the method of undermined coefficients.

Example. Determine the parameters α and β so that the formula

$$\int_0^1 f(x)\,dx = \alpha f(0) + \beta f(1)$$

is exact for all polynomial of degree ≤ 1.

$$E(1) = 0 \implies \alpha + \beta = 1.$$

$$E(x) = 0 \implies \beta = \frac{1}{2}.$$

The desired quadrature formula is

$$\int_0^1 f(x)\,dx = \frac{1}{2} f(0) + \frac{1}{2} f(1).$$

$f(x) = 1.$

$E(1) = \int_0^1 dx - (\alpha + \beta)$

$\Rightarrow \alpha + \beta = 1.$

$f(x) = x.$

$\int_0^1 x\,dx - \alpha \cdot f(0) - \beta f(1)$

$= \int_0^1 x\,dx - \beta$

$\Rightarrow \beta = 1/2$

$\Rightarrow \alpha = 1/2$

An Alternate Approach. Choose $x_0, \ldots, x_k$ in (a, b) and write

$$g(x) = p_k(x) + g[x_0, \ldots, x_k, x]\psi_k(x),$$

where $p_k(x)$ is the polynomial of degree $\leq k$ which interpolates $g(x)$ at $x_0, \ldots, x_k$, and

$$\psi_k(x) = (x - x_0) \ldots (x - x_k).$$

This gives

$$I(g) = I(p_k) + \int_a^b g[x_0, \ldots, x_k, x]\psi_k(x)w(x)dx.$$

If we write $p_k(x)$ in Lagrange form

$$p_k(x) = g(x_0)L_0(x) + g(x_1)L_1(x) + \cdots + g(x_k)L_k(x)$$

with

$$L_i(x) = \prod_{\substack{j=0 \\ i \neq j}}^{k} \frac{(x - x_j)}{(x_i - x_j)}, \quad i = 0, \ldots, k$$

Then

$$
\begin{aligned}
I(p_k) &= \int_a^b p_k(x) w(x) dx \\
&= g(x_0) \underbrace{\int_a^b L_0(x) w(x) dx}_{A_0} + \cdots + g(x_k) \underbrace{\int_a^b L_k(x) w(x) dx}_{A_k.}
\end{aligned}
$$

Hence,

$$
I(p_k) = A_0 g(x_0) + A_1 g(x_1) + \cdots + A_k g(x_k),
$$

where

$$
A_i = \int_a^b L_i(x) w(x)\, dx, \quad i = 0, \ldots, k. \tag{6}
$$

Using the property of orthogonal polynomials, for many $w(x)$, we can find a polynomial $P_{k+1}(x)$ such that

$$\int_a^b P_{k+1}(x)q(x)w(x)dx = 0 \tag{7}$$

Example:
Legendre's polynomial - $w(x) = 1$, $a = -1$, $b = 1$

for all polynomial $q(x)$ of degree $\leq k$. Moreover,

$$P_{k+1}(x) = \alpha_{k+1}(x - \xi_0)(x - \xi_1)\cdots(x - \xi_k),$$

where $\xi_0, \ldots, \xi_k$ are the $k+1$ distinct points in the interval (a, b) at which P_{k+1} vanishes.
Set

$$x_j = \xi_j, \quad j = 0, \ldots, k.$$

$P_1, P_2, \ldots P_n \ldots$ Leg. Poly

$q(x) = c_1 P_1 + c_2 P_2 + \cdots + c_n P_n$

$\int_{-1}^{1} q(x) P_1 = c_0 \int_{-1}^{1} P_1^2 + c_2 \int_{-1}^{1} P_2 P_1 + \cdots + c_n \int_{-1}^{1} P_1 P_n = 0$

$c_0 = \dfrac{\int_{-1}^{1} q P_1}{\int_{-1}^{1} P_1^2 dx}$

- If we choose the points $x_0, \ldots, x_k$ as the zeros of the polynomial $P_{k+1}(x)$ of degree $k+1$ which is orthogonal to the weight function $w(x)$ over (a, b) to any polynomial of degree $\leq k$, and if the coefficients A_i $(i = 0, \ldots, k)$ are chosen according to (6), the resulting Gaussian formula will then be exact for all polynomials of degree $\leq 2k+1$.

Example. Let $w(x) = 1$. The change of variable

$\int_a^b f(x)dx \to \int_{-1}^1 g(z)dz$

$$x = [(b-a)t + (b+a)]/2$$

transform the limits of integration from $(a, b) \Longrightarrow (-1, 1)$.

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

$$\begin{aligned}
\int_a^b f(x)dx &= \int_{-1}^1 f(x(t))x'(t)dt \\
&= \int_{-1}^1 f(x(t))\frac{b-a}{2}dt \\
&= \int_{-1}^1 g(\tau)d\tau.
\end{aligned}$$

The appropriate orthogonal polynomials are the Legendre polynomials.

$$\begin{aligned}
P_1(x) &= x & \xi_0 &= 0 \\
P_2(x) &= \frac{3}{2}(x^2 - \frac{1}{3}) & \xi_0 &= -\frac{1}{\sqrt{3}},\ \xi_1 = \frac{1}{\sqrt{3}} \\
P_3(x) &= \frac{5}{2}(x^3 - \frac{3}{5}x) & \xi_0 &= -\sqrt{\frac{3}{5}},\ \xi_1 = 0\ \xi_2 = \sqrt{\frac{3}{5}}
\end{aligned}$$

If we choose $k = 1$, then $x_0 = \xi_0 = -\frac{1}{\sqrt{3}}$, $x_1 = \xi_1 = \frac{1}{\sqrt{3}}$. Then we obtain

$$\int_{-1}^{1} g(\tau) d\tau \approx A_0\, g\left(-\frac{1}{\sqrt{3}}\right) + A_1\, g\left(\frac{1}{\sqrt{3}}\right),$$

where

$$\begin{aligned} A_0 &= \int_{-1}^{1} \overbrace{\frac{x - (-1/\sqrt{3})}{1/\sqrt{3} - (-1/\sqrt{3})}}^{L_0(x),} dx = 1 \\ A_1 &= \int_{-1}^{1} \underbrace{\frac{x - 1/\sqrt{3}}{-1/\sqrt{3} - (1/\sqrt{3})}}_{L_1(x).} dx = 1 \end{aligned}$$

$w(x) = 1$

The gaussian two-point quadrature formula is given by

$$\int_{-1}^{1} g(\tau) d\tau \approx g\left(-\frac{1}{\sqrt{3}}\right) + g\left(\frac{1}{\sqrt{3}}\right).$$

Note: For $k > 1$, both the points ξ_i and the weights A_i become irrational. Their calculation, however, is straightforward.

*** Ends ***