# Gauss Quadrature for Improper Integral

kenn

## 1 Exact Analytical Integration

We have definite integral

$$I = \int_0^\infty e^{-ax^2 - \frac{b}{x^2}} \mathrm{d}x \tag{1}$$

where $a$ and $b$ are positive real. By change of variable

$$x = \frac{\sqrt{b}}{\sqrt{a}t}$$

we obtain

$$I = \sqrt{\frac{b}{a}} \int_0^\infty e^{-at^2 - \frac{b}{t^2}} \frac{1}{t^2} \mathrm{d}t \tag{2}$$

Equations (1) and (2) can be, respectively, rearranged as

$$\sqrt{a}I = \int_0^\infty e^{-ax^2 - \frac{b}{x^2}} \sqrt{a} \mathrm{d}x \tag{3a}$$

$$\sqrt{a}I = \int_0^\infty e^{-ax^2 - \frac{b}{x^2}} \frac{\sqrt{b}}{x^2} \mathrm{d}x \tag{3b}$$

Adding Eqs. (3a) and (3b) together, we arrive at

$$2\sqrt{a}I = \int_0^\infty e^{-(\sqrt{a}x - \frac{\sqrt{b}}{x})^2 - 2\sqrt{ab}} \left(\sqrt{a} + \frac{\sqrt{b}}{x^2}\right) \mathrm{d}x$$

That is,

$$2\sqrt{a}I = e^{-2\sqrt{ab}} \int_0^\infty e^{-(\sqrt{a}x - \frac{\sqrt{b}}{x})^2} \mathrm{d}(\sqrt{a}x - \frac{\sqrt{b}}{x}) \tag{4}$$

Another change of variable

$$u = \sqrt{a}x - \frac{\sqrt{b}}{x}$$

recasts Eq. (4) into the well known Gauss integral

$$2\sqrt{a}I = e^{-2\sqrt{ab}} \int_{-\infty}^\infty e^{-u^2} \mathrm{d}u = e^{-2\sqrt{ab}} \sqrt{\pi}$$

Thus, the original integral

$$I = \frac{1}{2}\sqrt{\frac{\pi}{a}} e^{-2\sqrt{ab}} \tag{5}$$

## 2 Numerical Integration with Gauss Quadrature

Gauss quadrature reads

$$I = \int_a^b f(x)w(x)\mathrm{d}x = \sum_{j=0}^{N} W_j f(x_j) \tag{6}$$

where $w(x)$ denotes the weight function, $x_j$ denotes integration points, and $W_j$ denotes integration weights. As some examples,

Legendre Gauss Quadrature: $$I = \int_{-1}^{1} f(x)\mathrm{d}x = \sum_{j=0}^{N} W_j f(x_j)$$

Hermite Gauss Quadrature: $$I = \int_{-\infty}^{\infty} f(x)e^{-x^2/2}\mathrm{d}x = \sum_{j=0}^{N} W_j f(x_j)$$

Laguerre Gauss Quadrature: $$I = \int_{0}^{\infty} f(x)e^{-x}\mathrm{d}x = \sum_{j=0}^{N} W_j f(x_j)$$

Chebyshev Gauss Quadrature: $$I = \int_{-1}^{1} f(x)\frac{1}{\sqrt{1-x^2}}\mathrm{d}x = \sum_{j=0}^{N} W_j f(x_j)$$

The integration points $x_j$ are selected as $N+1$ roots of $(N+1)^{th}$ orthogonal polynomial, and the integration weights $W_j$ are $N+1$ solutions to the linear system

$$\sum_{j=0}^{N} (x_j)^k W_j = \int_a^b x^k w(x)\mathrm{d}x \qquad 0 \le k \le N$$

Here is the power of Gauss quadrature: the quadrature formula Eq. (6) is exact for a polynomial of degree $\le 2N+1$. In comparison, Newton-Cotes quadrature (such as Simpson's rule) is exact only for $N$ or $N+1$ degrees of polynomials. In other words, in real life the Gauss quadrature is more accurate by several orders of magnitude.

## 3 Chebyshev Gauss Quadrature for Improper Integral

Let us first try Chebyshev Gauss Lobatto quadrature, which is more popular in numerical computation of partial differential equations. The integration points and weights are

$$x_j = \cos\frac{\pi j}{N}, \qquad W_j = \frac{\pi}{N\tilde{c}_j}$$

where

$$\tilde{c}_j = \begin{cases} 2, & j = 0, N \\ 1, & j = 1, 2, ...N-1 \end{cases}$$

| $j$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| $x_j$ | 0.97390652 | 0.86506336 | 0.67940956 | 0.43339539 | 0.14887433 | $-x_4$ | $-x_3$ | $-x_2$ | $-x_1$ | $-x_0$ |
| $W_j$ | 0.06667134 | 0.14945134 | 0.21908636 | 0.26926671 | 0.29552422 | $W_4$ | $W_3$ | $W_2$ | $W_1$ | $W_0$ |

Table 1: Integration points and weights for Legendre Gauss quadrature with $N = 9$ (10 points).

| $a = 1.0$, $b = 1.0$ | Values for the integral | Relative errors |
|---|---|---|
| Exact | 0.119938 | |
| Simpson Rule (11 points) | 0.110880 | 7.55% |
| Legendre Gauss Quadrature (10 points) | 0.119617 | 0.268% |

Table 2: Accuracy comparison between Legendre Gauss quadrature and Simpson rule.

Note that two boundary points are included as integration points and this makes imposition of boundary conditions for partial differential equations easier; as a side effect, the accuracy of Lobatto approach drops by two orders of polynomials. A change of variable

$$x = \tan\left(\frac{\pi}{2}t\right)$$

converts the original integral Eq. (1) into

$$I = \frac{\pi}{4}\int_{-1}^{1}\sqrt{1-t^2}\sec^2\left(\frac{\pi}{2}t\right)\exp\left(-a\tan^2(\frac{\pi}{2}t) - \frac{b}{\tan^2(\frac{\pi}{2}t)}\right)\frac{1}{\sqrt{1-t^2}}\mathrm{d}t \tag{7}$$

While the singularity in the weight function will be automatically taken care of by quadrature, the singularities in the kernel require special handling. Hence, we go back to the original Chebyshev Gauss quadrature, where integration points are all in the interior domain

$$x_j = \cos\frac{(2j+1)\pi}{2N+2}, \qquad W_j = \frac{\pi}{N+1}$$

# 4 Legendre Gauss Quadrature for Improper Integral

Table 1 shows the integration points and weights for 10-point Legendre Gauss quadrature. Integral Eq. (1) or Eq. (7) should be rearranged as

$$I = \frac{\pi}{4}\int_{-1}^{1}\sec^2\left(\frac{\pi}{2}t\right)\exp\left(-a\tan^2(\frac{\pi}{2}t) - \frac{b}{\tan^2(\frac{\pi}{2}t)}\right)\mathrm{d}t$$

Table 2 shows the advantage of Legendre gauss quadrature over Simpson rule.