GAUSSIAN QADRATURE

http://www.phys.uconn.edu/~rozman/Courses/m3510_18f/

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1 Introduction

A quadrature rule is the approximation of a definite integral by a finite sum of the form

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} w_i f(x_i), \tag{1}$$

where $x_1, \ldots, x_n$ and $w_1, \ldots, w_n$ are referred to as the quadrature nodes and weights, respectively. In 1814 Gauss described a choice for the nodes and weights that is optimal in the sense that for each n it exactly integrates polynomials up to degree $2n-1$. It can be shown that no other quadrature rule with n nodes can do this or better.

In this notes we illustrate the idea of Gaussian quadrature by several simple examples. Let's consider the three point quadrature:

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3). \tag{2}$$

This three point rule contains six parameters — three nodes x_i and three weights w_i, $i = 1, 2, 3$. Determine the parameters from the requirements that Eq. (2) is exact for the integrand $f(x) = x^k$, $k = 0, \dots, 5$:

$$
\begin{aligned}
\int_{-1}^{1} \mathrm{d}x &= w_1 + w_2 + w_3 = 2, &(3)\\
\int_{-1}^{1} x\,\mathrm{d}x &= w_1 x_1 + w_2 x_2 + w_3 x_3 = 0, &(4)\\
\int_{-1}^{1} x^2\,\mathrm{d}x &= w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2 = \frac{2}{3}, &(5)\\
\int_{-1}^{1} x^3\,\mathrm{d}x &= w_1 x_1^3 + w_2 x_2^3 + w_3 x_3^3 = 0, &(6)\\
\int_{-1}^{1} x^4\,\mathrm{d}x &= w_1 x_1^4 + w_2 x_2^4 + w_3 x_3^4 = \frac{2}{5}, &(7)\\
\int_{-1}^{1} x^5\,\mathrm{d}x &= w_1 x_1^5 + w_2 x_2^5 + w_3 x_3^5 = 0. &(8)
\end{aligned}
$$

The system of the nonlinear equations (3)–(8) can be solved as it is written. However, the solution process can be greatly simplified if we notice that if the integration range in Eq. (2) is symmetric with respect to the origin, so must be the coordinates of the nodes and the weights:

$$x_1 = -x_3, \quad x_2 = 0, \tag{9}$$

$$w_1 = w_3. \tag{10}$$

Using the symmetry property, we notice that Eq. (4), (6), (8) are satisfied automatically. Only three equations for three unknowns — x_1, w_1 and w_2 — remain:

$$
\begin{aligned}
2w_1 + w_2 &= 2, &(11)\\
2w_1 x_1^2 &= \frac{2}{3}, &(12)\\
2w_1 x_1^4 &= \frac{2}{5}. &(13)
\end{aligned}
$$

Dividing Eq. (13) by Eq. (12), we obtain: $x_1^2 = \frac{3}{5}$,

$$x_1 = \sqrt{\frac{3}{5}}, \quad \text{hence} \quad x_3 = -\sqrt{\frac{3}{5}}. \tag{14}$$

Next, from Eq. (12),

$$w_1 = \frac{5}{9} = w_2. \tag{15}$$

Finally, from Eq. (11)

$$w_2 = \frac{8}{9}. \tag{16}$$

The three point quadrature rule is as following:

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \frac{1}{9}\left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right)\right]. \tag{17}$$

2 Gauss-Hermite quadrature

Gauss-Hermite quadrature is a form of Gaussian quadrature for approximating the value of integrals of the following form:

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,\mathrm{d}x. \tag{18}$$

In this case

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} w_i f(x_i). \tag{19}$$

where n is the number of sample points used.

Consider the two-point Gauss-Hermite quadrature

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,\mathrm{d}x \approx w_1 f(x_1) + w_2 f(x_2). \tag{20}$$

The symmetry conditions give

$$x_1 = -x_2, \qquad w_1 = w_2. \tag{21}$$

Thus two-point rule contains two parameters:

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,\mathrm{d}x \approx w f(x) + w f(-x). \tag{22}$$

Determine the unknown parameters from the requirements that Eq. (22) is exact for $f(x) = 1$ and $f(x) = x^2$:

$$\int_{-\infty}^{+\infty} e^{-x^2}\,\mathrm{d}x = 2w, \qquad \int_{-\infty}^{+\infty} e^{-x^2} x^2\,\mathrm{d}x = 2wx^2. \tag{23}$$

The integrals in Eq. (23) are evaluated in (46). We obtain

$$2w = \sqrt{\pi}, \qquad 2wx^2 = \frac{\sqrt{\pi}}{2}. \tag{24}$$

Thus,

$$w = \frac{\sqrt{\pi}}{2}, \qquad x = \frac{1}{\sqrt{2}}, \tag{25}$$

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,\mathrm{d}x \approx \frac{\sqrt{\pi}}{2}\left[f\left(-\frac{1}{\sqrt{2}}\right) + f\left(\frac{1}{\sqrt{2}}\right)\right]. \tag{26}$$

3 Gauss-Chebyshev quadrature

Gauss-Chebyshev quadrature is a form of Gaussian quadrature for approximating the value of integrals of the following form:

$$\int_{-1}^{1} \frac{f(x)\,\mathrm{d}x}{\sqrt{1-x^2}}. \tag{27}$$

In this case

$$\int_{-1}^{1} \frac{f(x)\,\mathrm{d}x}{\sqrt{1-x^2}} \approx \sum_{i=1}^{n} w_i f(x_i). \tag{28}$$

where n is the number of sample points used.

Consider the two-point Gauss-Chebyshev quadrature

$$\int_{-1}^{1} \frac{f(x)\,\mathrm{d}x}{\sqrt{1-x^2}} \approx w_1 f(x_1) + w_2 f(x_2). \tag{29}$$

The symmetry conditions give

$$x_1 = -x_2, \qquad w_1 = w_2. \tag{30}$$

Thus two-point rule contains two parameters:

$$\int_{-1}^{1} \frac{f(x)\,\mathrm{d}x}{\sqrt{1-x^2}} \approx w f(x) + w f(-x). \tag{31}$$

Determine the unknown parameters from the requirements that Eq. (31) is exact for $f(x) = 1$ and $f(x) = x^2$:

$$\int_{-1}^{1} \frac{\mathrm{d}x}{\sqrt{1-x^2}} = 2w, \qquad \int_{-1}^{1} \frac{x^2\,\mathrm{d}x}{\sqrt{1-x^2}} = 2wx^2. \tag{32}$$

The integrals in Eq. (23) are evaluated in (46). We obtain

$$2w = \pi, \qquad 2wx^2 = \frac{\pi}{2}. \tag{33}$$

Thus,

$$w = \frac{\pi}{2}, \qquad x = \frac{1}{\sqrt{2}}, \tag{34}$$

$$\int_{-1}^{1} \frac{x^2\,\mathrm{d}x}{\sqrt{1-x^2}} \approx \frac{\pi}{2}\left[f\left(-\frac{1}{\sqrt{2}}\right) + f\left(\frac{1}{\sqrt{2}}\right)\right]. \tag{35}$$

4 Evaluating the integrals

4.1 Gauss-Hermite integrals

Consider the integral

$$H(n) = \int_{-\infty}^{\infty} x^n e^{-x^2}\,\mathrm{d}x \tag{36}$$

for integer $n = 0, 1, 2, \ldots$.

Notice that the integral is identically zero for odd values of n:

$$H(2k+1) = 0. \tag{37}$$

For even values of $n = 2k$,

$$H(2k) = \int_{-\infty}^{\infty} x^{2k} e^{-x^2} \mathrm{d}x = 2 \int_{0}^{\infty} x^{2k} e^{-x^2} \mathrm{d}x. \tag{38}$$

Introducing the integration variable u,

$$u = x^2, \quad 0 \le u \le 1, \quad x = u^{\frac{1}{2}}, \quad \mathrm{d}x = \frac{1}{2} u^{-\frac{1}{2}} \mathrm{d}u, \tag{39}$$

$$H(2k) = \int_{0}^{\infty} u^{k-\frac{1}{2}} e^{-u} \mathrm{d}u = \Gamma\left(k + \frac{1}{2}\right), \tag{40}$$

where $\Gamma()$ is Gamma function. For the reference, using the property of Gamma function

$$\Gamma(x+1) = x\Gamma(x), \tag{41}$$

we obtain:

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \tag{42}$$

$$\Gamma\left(\frac{3}{2}\right) = \Gamma\left(1 + \frac{1}{2}\right) = \frac{1}{2}\Gamma\left(\frac{1}{2}\right) = \frac{\sqrt{\pi}}{2}, \tag{43}$$

$$\Gamma\left(\frac{5}{2}\right) = \Gamma\left(1 + \frac{3}{2}\right) = \frac{3}{2}\Gamma\left(\frac{3}{2}\right) = \frac{3\sqrt{\pi}}{4}, \tag{44}$$

$$\Gamma\left(\frac{7}{2}\right) = \Gamma\left(1 + \frac{5}{2}\right) = \frac{5}{2}\Gamma\left(\frac{5}{2}\right) = \frac{15\sqrt{\pi}}{8}. \tag{45}$$

Therefore,

$$H(0) = \int_{-\infty}^{\infty} e^{-x^2}\mathrm{d}x = \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \tag{46}$$

$$H(2) = \int_{-\infty}^{\infty} x^2 e^{-x^2}\mathrm{d}x = \Gamma\left(\frac{3}{2}\right) = \frac{\sqrt{\pi}}{2}, \tag{47}$$

$$H(4) = \int_{-\infty}^{\infty} x^4 e^{-x^2}\mathrm{d}x = \Gamma\left(\frac{5}{2}\right) = \frac{3\sqrt{\pi}}{4}, \tag{48}$$

$$H(6) = \int_{-\infty}^{\infty} x^6 e^{-x^2}\mathrm{d}x = \Gamma\left(\frac{7}{2}\right) = \frac{15\sqrt{\pi}}{8}. \tag{49}$$

In general,

$$\Gamma\left(k+\frac{1}{2}\right) = \frac{(2k-1)!!\sqrt{\pi}}{2^k} = \frac{(2k)!\sqrt{\pi}}{4^k k!}, \tag{50}$$

thus

$$H(2k) = \int_{-\infty}^{\infty} x^{2k} e^{-x^2}\mathrm{d}x = \Gamma\left(k+\frac{1}{2}\right) = \frac{(2k)!\sqrt{\pi}}{4^k k!} = \frac{(2k-1)!!\sqrt{\pi}}{2^k}. \tag{51}$$

4.2 Gauss-Chebyshev integrals

Consider the integral

$$C(n) = \int_{-1}^{1} x^n \left(1-x^2\right)^{-\frac{1}{2}} \mathrm{d}x \tag{52}$$

for integer $n = 0, 1, 2, \ldots$.

Notice that the integral is identically zero for odd values of n:

$$C(2k+1) = 0. \tag{53}$$

For even values of $n = 2k$,

$$C(2k) = \int_{-1}^{1} x^{2k} \left(1-x^2\right)^{-\frac{1}{2}} \mathrm{d}x = 2\int_{0}^{1} x^{2k} \left(1-x^2\right)^{-\frac{1}{2}} \mathrm{d}x. \tag{54}$$

Introducing the integration variable u,

$$u = x^2, \quad 0 \le u \le 1, \quad x = u^{\frac{1}{2}}, \quad \mathrm{d}x = \frac{1}{2} u^{-\frac{1}{2}} \mathrm{d}u, \tag{55}$$

$$C(2k) = \int_0^1 u^k (1-u)^{-\frac{1}{2}} \,\mathrm{d}u = \int_0^1 u^{\left(k+\frac{1}{2}\right)-1} (1-u)^{\frac{1}{2}-1} \,\mathrm{d}u = B\left(k + \frac{1}{2}, \frac{1}{2}\right), \tag{56}$$

where $B(p,q)$ is beta function. Using the identity

$$B(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}, \tag{57}$$

where $\Gamma(x)$ is the Gamma function. Therefore,

$$C(2k) = \frac{\Gamma\left(k+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma(k+1)}, \tag{58}$$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \tag{59}$$

$$\Gamma(k+1) = k!, \tag{60}$$

$$\Gamma\left(k + \frac{1}{2}\right) = \frac{(2k)!\sqrt{\pi}}{4^k k!}, \tag{61}$$