Numerical Analysis

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Gaussian Quadrature

Suppose that w is a weight-function, defined, positive and integrable on the open interval (a, b) of $\mathbb{R}$.

Lemma

Let $\{\phi_0, \phi_1, \ldots, \phi_n, \ldots\}$ *be orthogonal polynomials for the inner product*

$$\langle f, g \rangle = \int_a^b w(x) f(x) g(x) \, \mathrm{d}x.$$

Then, for each $k = 0, 1, \ldots,$ ϕ_k *has* k *distinct roots in the interval* (a, b)*.*

Proof. Since $\phi_0(x) \equiv$ const. $\neq 0$, the result is trivially true for $k = 0$.

Suppose that $k \geq 1$. Then,

$$\langle \phi_k, \phi_0 \rangle = \int_a^b w(x)\phi_k(x)\phi_0(x)\,\mathrm{d}x = 0$$

with ϕ_0 constant implies that

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with $w(x) > 0$, $x \in (a, b)$;

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with $w(x) > 0$, $x \in (a, b)$; thus $\phi_k(x)$ must change sign in (a, b), i.e., ϕ_k has at least one root in (a, b).

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$$q(x) = \prod_{j=1}^{\ell}(x - r_j) \times \text{the sign of } \phi_k \text{ on } (r_\ell, b)$$

has the same sign as ϕ_k on (a, b).

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Hence $\langle \phi_k, q \rangle = \int_a^b w(x)\phi_k(x)q(x)\,\mathrm{d}x > 0$. Thus, from the previous lemma, q (which is of degree ℓ) must be of degree $\ge k$, i.e., $\ell \ge k$.

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Therefore $\ell = k$, and ϕ_k has k distinct roots in (a, b). □

Quadrature revisited. The above lemma leads to very efficient quadrature rules since it answers the question: how should we choose the quadrature points $x_0, x_1, \ldots, x_n$ in the quadrature rule

$$\int_a^b w(x) f(x) \, \mathrm{d}x \approx \sum_{j=0}^{n} w_j f(x_j)$$

so that the rule is exact for polynomials of degree as high as possible? (The case $w(x) \equiv 1$ is the most common.)

Recall that the Lagrange interpolating polynomial

$$p_n = \sum_{j=0}^{n} f(x_j) L_{n,j} \in \Pi_n$$

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is unique, so if $f \in \Pi_n \implies p_n \equiv f$ whatever interpolation points are used. Moreover, we have

$$\begin{aligned}
\int_a^b w(x) f(x)\,\mathrm{d}x &= \int_a^b w(x) p_n(x)\,\mathrm{d}x \\
&= \int_a^b w(x) \sum_{j=0}^{n} f(x_j) L_{n,j}(x)\,\mathrm{d}x \\
&= \sum_{j=0}^{n} f(x_j) \int_a^b w(x) L_{n,j}(x)\,\mathrm{d}x \\
&= \sum_{j=0}^{n} w_j f(x_j),
\end{aligned}$$

where $w_j = \int_a^b w(x) L_{n,j}(x)\,\mathrm{d}x$ exactly!

Theorem

Suppose that $x_0 < x_1 < \cdots < x_n$ *are the roots of the* $n+1$*-st degree orthogonal polynomial* ϕ_{n+1} *with respect to the inner product*

$$\langle g, h\rangle = \int_a^b w(x)g(x)h(x)\,\mathrm{d}x,$$

then the quadrature formula

$$\int_a^b w(x)f(x)\,\mathrm{d}x \approx \sum_{j=0}^{n} w_j f(x_j) \tag{13.1}$$

with weights $w_j = \int_a^b w(x)L_{n,j}(x)\,\mathrm{d}x$ *is exact whenever* $f \in \Pi_{2n+1}$.

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So

$$\begin{aligned}\int_a^b w(x)p(x)\,\mathrm{d}x &= \int_a^b w(x)q(x)\phi_{n+1}(x)\,\mathrm{d}x + \int_a^b w(x)r(x)\,\mathrm{d}x \\ &= \sum_{j=0}^{n} w_j r(x_j) \end{aligned} \tag{13.2}$$

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since the integral involving $q \in \Pi_n$ is zero by the lemma above and the other is integrated exactly since $r \in \Pi_n$. Finally, for all $p \in \Pi_{2n+1}$ we have

$$p(x_j) = q(x_j)\phi_{n+1}(x_j) + r(x_j) = r(x_j), \quad (j = 0, \ldots, n),$$

for as the x_j are the roots of ϕ_{n+1}, hence (13.2) yields

$$\int_a^b w(x)p(x)\,\mathrm{d}x = \sum_{j=0}^{n} w_j p(x_j). \square$$

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1. For $w(x) \equiv 1$, $(a, b) = (-1, 1)$
   we have Gauss–Legendre Quadrature.
2. For $w(x) = (1 - x^2)^{-1/2}$ and $(a, b) = (-1, 1)$
   we have Gauss–Chebyshev Quadrature.
3. For $w(x) = \mathrm{e}^{-x}$ and $(a, b) = (0, \infty)$
   we have Gauss–Laguerre Quadrature.
4. For $w(x) = \mathrm{e}^{-x^2}$ and $(a, b) = (-\infty, \infty)$
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   we have Gauss–Hermite Quadrature.

Gaussian Quadrature gives better accuracy than Newton–Cotes Quadrature for the same number of function evaluations.

Note that by the simple linear change of variable $t = (2x - a - b)/(b - a)$, which maps $[a, b] \to [-1, 1]$, we can evaluate for example

$$\int_a^b f(x)\,\mathrm{d}x = \int_{-1}^{1} f\left(\frac{(b-a)t + b + a}{2}\right)\frac{b-a}{2}\,\mathrm{d}t$$

$$\simeq \frac{b-a}{2}\sum_{j=0}^{n} w_j f\left(\frac{b-a}{2}t_j + \frac{b+a}{2}\right),$$

where $\simeq$ denotes "quadrature" and the t_j, $j = 0, 1, \ldots, n$, are the roots of the $n + 1$-st degree Legendre polynomial on $(-1, 1)$.

Example. 2-point Gauss–Legendre Quadrature:

$$\phi_2 = x^2 - \tfrac{1}{3} \implies t_0 = -\tfrac{1}{\sqrt{3}}, \quad t_1 = \tfrac{1}{\sqrt{3}},$$

and

$$w_0 = \int_{-1}^{1} \frac{x - \frac{1}{\sqrt{3}}}{-\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}} \, \mathrm{d}x = -\int_{-1}^{1} \left(\frac{\sqrt{3}}{2} x - \frac{1}{2} \right) \mathrm{d}x = 1$$

with $w_1 = 1$, similarly.

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$$\int_{1}^{2} \frac{1}{x}\,\mathrm{d}x = \frac{1}{2}\int_{-1}^{1} \frac{2}{t+3}\,\mathrm{d}t \simeq \frac{1}{3 + \frac{1}{\sqrt{3}}} + \frac{1}{3 - \frac{1}{\sqrt{3}}} = 0.6923077\ldots \ .$$

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Note that with the Trapezium Rule (i.e., also with two evaluations of the integrand):

$$\int_1^2 \frac{1}{x} \, \mathrm{d}x \simeq \frac{1}{2} \left[\frac{1}{2} + 1 \right] = 0.75,$$

whereas $\displaystyle\int_1^2 \frac{1}{x} \, \mathrm{d}x = \ln 2 = 0.6931472\ldots$.