MA579H Scientific Computing

Numerical Integration II

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Lecture outline

- Degree of exactness
- Method of undetermined coefficients
- Gaussian quadrature formula
- Orthogonal polynomials and Gauss quadrature

Degree of exactness

The error $E(f) = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\theta)$ shows that Simpson's rule $S(f)$ is exact for polynomials of degree ≤ 3, which is one degree more than Newton-Cotes quadrature formula of order 2 (i.e., $n = 2$) can guarantee.

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Fact: The degree of exactness of a Newton-Cotes rule of order m is $m + 1$ if m is even or zero. But the degree of exactness is m if m is odd.

Method of undetermined coefficients

The weights in the Simpson's rule

$$S(f) = \left[w_0 f(a) + w_1 f\left(\frac{a+b}{2}\right) + w_2 f(b)\right] \approx \int_a^b f(x)dx$$

can be determined by utilizing the fact that $S(f)$ is exact for $f(x) = 1, f(x) = x$, and $f(x) = x^2$.

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Method of undetermined coefficients

Solving the Vandermonde system

$$\begin{bmatrix} 1 & 1 & 1 \\ a & \frac{a+b}{2} & b \\ a^2 & \frac{(a+b)^2}{4} & b^2 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} b-a \\ \frac{b^2-a^2}{2} \\ \frac{b^3-a^3}{3} \end{bmatrix}$$

we obtain $w_0 = (b-a)/6 = w_2$ and $w_1 = 2(b-a)/3$.

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$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_0 & x_1 & \cdots & x_n \\ \vdots & \vdots & \ldots & \vdots \\ x_0^n & x_1^n & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} b-a \\ \frac{b^2-a^2}{2} \\ \vdots \\ \frac{b^{n+1}-a^{n+1}}{n+1} \end{bmatrix}.$$

Example

Once again consider the Simpson rule

$$\int_0^1 f(x)dx \approx w_0 f(0) + w_1 f(1/2) + w_2 f(1).$$

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Solving the system, we have $w_0 = 1/6 = w_2$ and $w_1 = 2/3$. Hence the Simpson's rule is given by

$$\int_0^1 f(x)dx \approx \frac{1}{6}[f(0) + 4f(1/2) + f(1)].$$

Approximation of weighted definite integrals

Newton-Cotes formulas can be used to approximate integral of the form

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

where $\mu \in C[a,b]$ is such that $\mu(x) > 0$ for all $x \in [a,b]$. The function μ is called a weight function.

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In this case, the weights $w_0, \ldots, w_n$ are given by

$$w_j = \int_a^b \ell_j(x)\mu(x)dx, \quad j = 0 : n.$$

Gaussian quadrature rules

Consider the quadrature rule

$$Q_n(f) = w_0 f(x_0) + \cdots + w_n f(x_n) \approx \int_a^b f(x)dx.$$

If $Q_n(f)$ is interpolatory, that is, $w_j = \int_a^b \ell_j(x)dx, j = 0 : n,$ then the degree of exactness $Q_n(f)$ is at least n.

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Gaussian quadrature rules are based on polynomial interpolation, but nodes as well as weights are chosen to maximize the degree of exactness.

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$$w_0 = G_0(1) = \int_a^b 1 \cdot dx = b - a.$$

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$$\int_a^b x^2 dx = \frac{b^3 - a^3}{3} \neq (b-a)\left(\frac{a+b}{2}\right)^2.$$

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Thus the degree of exactness of 1-point Gaussian quadrature rule is 1.

Two-point Gaussian quadrature rule

Now consider the case $n = 1$ so that $G_1(f) = w_0 f(x_0) + w_1 f(x_1)$. Then the exactness of $G_1(f)$ for polynomial of degree ≤ 2 yields

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Thus we have 3 nonlinear equations in 4 unknowns x_0, x_1, w_0, w_1.

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We shall see that a Gaussian quadrature rule of order m is exact for polynomials of degree $\leq 2m + 1$.

Orthogonal functions

Definition: Let f and g be integrable functions on an interval $[a, b]$. Then f and g are said to be orthogonal on $[a, b]$ if

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Example: $(x^2 - \frac{1}{3}) \perp \mathrm{span}\{1, x\}$ on $[-1, 1]$.

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If, in addition, $\int_a^b (f_k(x))^2 dx = 1$ for all $k = 1, \ldots, n$, then $\{f_0, \ldots, f_n\}$ is said to be an orthonormal set on $[a, b]$.

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Example: The Legendre polynomials $\{1, x, \frac{3x^2-1}{2}, \frac{5x^3-3x}{2}, \ldots, p_n(x)\}$ generated by

$$p_i(x) := \frac{1}{2^i i!} \frac{d^i}{dx^i} [(x^2 - 1)]^i, \ i = 0, 1, \ldots \text{ [Rodrigues Formula]}$$

form an orthonormal set of polynomials on $[-1, 1]$.

Orthonormal functions

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Orthonormal functions

Let $\mu \in C[a, b]$ such that $\mu(x) > 0$ for all $x \in [a, b]$.

A set of functions $\{f_0, \ldots, f_n\}$ on $[a, b]$ is said to be an orthogonal set on $[a, b]$ with respect to the *weight function* μ if

$$\int_a^b f_j(x) f_k(x) \mu(x) dx = 0 \text{ for } j \neq k.$$

If, in addition, $\int_a^b (f_k(x))^2 \mu(x) dx = 1$ for all $k = 1, \ldots, n$, then $\{f_0, \ldots, f_n\}$ is said to be an orthonormal set on $[a, b]$ with respect to μ.

Example: For $\mu(x) := 1/\sqrt{1 - x^2}$, the Chebyshev polynomials $T_n(x) := \cos(n \cos^{-1} x)$, $n = 0, 1, \ldots, k$ are a set of orthogonal polynomials on $[-1, 1]$.

Roots of orthogonal polynomials

Theorem An orthonormal set of polynomials $\{p_0, \ldots, p_n\}$ on an interval $[a, b]$ (with or without weight function) satisfying $\deg p_i = i$ is a basis of $\mathcal{P}_n$ on $[a, b]$.

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In particular, if $\{p_0(x), \ldots, p_n(x)\}$ is an orthonormal set of polynomials on $[a, b]$ with $\deg(p_\ell(x)) = \ell$ then $p_\ell(x)$ has ℓ distinct roots on $[a, b]$.

Nodes for Gaussian quadrature rules

Suppose that $G_n(f) = w_0 f(x_0) + \cdots + w_n f(x_n)$ is interpolatory. Then

$$G_n(f) = \int_a^b p_n(x)dx \;\text{ and }\; w_j = \int_a^b \ell_j(x)dx,\; j = 0 : n,$$

where $p_n(x)$ is the interpolating polynomial of degree n that interpolates the data $(x_0, f(x_0)), \ldots, (x_n, f(x_n))$.

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$$\int_a^b f(x)dx - \int_a^b p_n(x)dx = \int_a^b \frac{f^{(n+1)}(\theta_x)}{(n+1)!} w(x)dx = 0$$

when $f \in \mathcal{P}_{2n+1} \iff w(x) \perp \mathcal{P}_n$. [Note that $f(x) - p_n(x) = q(x)w(x)$ for some $q \in \mathcal{P}_n$ when $f \in \mathcal{P}_{2n+1}$.]

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Theorem: Consider the $(n+1)$-point quadrature rule

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Let $p(x)$ be a polynomial of degree $n+1$ such that $p \perp \mathcal{P}_n$ on $[a, b]$. If $x_0, \ldots, x_n$ are the zeros of p and $w_j = \int_a^b \ell_j(x)dx, j = 0 : n,$ then $G_n(f)$ is exact for polynomials of degree $\leq 2n+1$.

Proof: Let $f \in \mathcal{P}_{2n+1}$. Then $f = qp + r$ for some $q, r \in \mathcal{P}_n$.

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Note: Having determined the nodes x_j, the weights w_j can be determined by method of undetermined coefficients.

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Consider the Gaussian quadrature $\int_{-1}^{1} f(x)dx \approx w_0 f(x_0) + w_1 f(x_1)$.

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\int_{-1}^{1} x^4 dx &= \frac{2}{5} \neq \left(-\frac{1}{\sqrt{3}}\right)^4 + \left(\frac{1}{\sqrt{3}}\right)^4.
\end{aligned}$$

Example of Gauss quadrature with Legendre points

The Legendre nodes in $[-1, 1]$ can be used to approximate an integral over $[a, b]$ by change of interval:

$$\int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{b+a}{2} + \frac{(b-a)}{2}t\right)\frac{(b-a)}{2}dt.$$

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$$\int_1^2 \log(x)dx = \int_{-1}^1 \log\left(\frac{t+3}{2}\right)\frac{1}{2}dt.$$

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For $n = 4$ and $f(x) := \log(x)$, we have $G_n(f) = 0.38629449693871$ whereas $\int_1^2 \log(x)dx = 2\log(2) - 1 \approx 0.38629436111989.$

Summary of Gauss quadrature with Legendre nodes

To compute $\int_a^b f(x)dx$ via Gauss quadrature:

Step 1. Convert $\int_a^b f(x)dx \to \int_{-1}^1 g(t)dt$.

Step 2. Compute the nodes $x_0, \ldots, x_n$ as the roots of the Legendre polynomial $p_{n+1}(x) \perp \mathcal{P}_n$ on $[-1, 1]$.

Step 3. Compute the weights $w_0, \ldots, w_n$ by the method of undetermined coefficients on the interval $[-1, 1]$.

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Remark: Steps 2 and 3 are independent of f and hence can be performed in advance and stored.

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Note that

$$w_0 + w_1 = \int_{-1}^{1} (1-x^2)^{-1/2}dx = \pi$$

and

$$(-w_0 + w_1)/\sqrt{2} = \int_{-1}^{1} x(1-x^2)^{-1/2}dx = 0$$

yield $w_0 = w_1 = \pi/2$.

Example of weighted Gaussian quadrature

Now

$$\int_{-1}^{1} x^2(1-x^2)^{-1/2}dx \;=\; \frac{\pi}{2} = \frac{\pi}{2}\left[\left(-\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2\right]$$

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$$\begin{aligned}\int_{-1}^{1} x^2(1-x^2)^{-1/2}dx &= \frac{\pi}{2} = \frac{\pi}{2}\left[\left(-\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2\right]\\ \int_{-1}^{1} x^3(1-x^2)^{-1/2}dx &= 0 = \frac{\pi}{2}\left[\left(-\frac{1}{\sqrt{2}}\right)^3 + \left(\frac{1}{\sqrt{2}}\right)^3\right]\end{aligned}$$

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\int_{-1}^{1} x^4(1-x^2)^{-1/2}dx &= \frac{3\pi}{8} \neq \frac{\pi}{2}\left[\left(-\frac{1}{\sqrt{2}}\right)^4 + \left(\frac{1}{\sqrt{2}}\right)^4\right].
\end{aligned}
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Properties of Gaussian quadrature

Consider the Gaussian quadrature

$$G_n(f) = w_0 f(x_0) + \cdots + w_n f(x_n) \approx \int_a^b f(x)dx.$$

Then:

- All the nodes x_j are real, distinct, and contained in (a, b).
- All the weights w_j are positive. Indeed, for $j = 0 : n$, we have

$$0 < \int_a^b \ell_j(x)^2 dx = \sum_{k=0}^{n} w_k \ell_j(x_k)^2 = w_j.$$

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Theorem: Let $f \in C[a, b]$ and

$$E_n(f) := \|f - \widehat{p}\|_\infty = \min\{\|f - p\|_\infty : p \in \mathcal{P}_{2n+1}\}.$$

Then

$$\left| \int_a^b f(x)dx - G_n(f) \right| \le 2(b - a)E_n(f) \longrightarrow 0 \text{ as } n \to \infty.$$

Properties of Gaussian quadrature

Proof:

$$\begin{aligned}\left|\int_a^b f(x)dx - G_n(f)\right| &= \left|\int_a^b f(x)dx - G_n(\widehat{p}) + G_n(\widehat{p}) - G_n(f)\right| \\ &\leq \left|\int_a^b f(x)dx - G_n(\widehat{p})\right| + |G_n(\widehat{p}) - G_n(f)|\end{aligned}$$

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&\leq \left|\int_a^b f(x)dx - G_n(\widehat{p})\right| + |G_n(\widehat{p}) - G_n(f)| \\
&\leq \left|\int_a^b (f(x) - \widehat{p}(x))dx\right| + \sum_{j=0}^{n} w_j |f(x_j) - \widehat{p}(x_j)| \\
&\leq \max_{x\in[a,b]} |f(x) - \widehat{p}_n(x)| \left(\int_a^b dx + \sum_{j=0}^{n} w_j\right) \\
&\leq E_n(f)\left((b-a) + \sum_{j=0}^{n} w_j\right) = 2(b-a)E_n(f).
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&\leq \left|\int_a^b f(x)dx - G_n(\widehat{p})\right| + |G_n(\widehat{p}) - G_n(f)| \\
&\leq \left|\int_a^b (f(x) - \widehat{p}(x))dx\right| + \sum_{j=0}^{n} w_j |f(x_j) - \widehat{p}(x_j)| \\
&\leq \max_{x\in[a,b]} |f(x) - \widehat{p}_n(x)| \left(\int_a^b dx + \sum_{j=0}^{n} w_j\right) \\
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\end{aligned}$$

By Weierstrass theorem, $E_n(f) \to 0$ as $n \to \infty$. ■

Adaptive quadrature

Adaptive Trapezoid: Let $T(a,b) := \frac{b-a}{2}[f(a)+f(b)] \approx \int_a^b f(x)dx$. Then

$$\int_a^b f(x)dx = T(a,b) - \frac{h^3}{12} f''(c_0)$$

where $h := b-a$ and $a < c_0 < b$. Let $c = (a+b)/2$.

Adaptive quadrature

Adaptive Trapezoid: Let $T(a,b) := \frac{b-a}{2}[f(a)+f(b)] \approx \int_a^b f(x)dx$. Then

$$\int_a^b f(x)dx = T(a,b) - \frac{h^3}{12} f''(c_0)$$

where $h := b-a$ and $a < c_0 < b$. Let $c = (a+b)/2$. Then $T(a,c) + T(c,b) \approx \int_a^b f(x)dx$ and

$$\begin{aligned} \int_a^b f(x)dx &= T(a,c) - \frac{h^3}{8}\frac{f''(c_1)}{12} + T(c,b) - \frac{h^3}{8}\frac{f''(c_2)}{12} \\ &= T(a,c) + T(c,b) - \frac{h^3}{4}\frac{f''(c_3)}{12} \end{aligned}$$

where $c_1, c_2, c_3 \in (a,b)$ and the last equality follows from intermediate value theorem.

Adaptive quadrature

Assuming $f''(c_0) \approx f''(c_3)$, we have

$$T(a,b) - T(a,c) - T(c,b) = \frac{h^3}{12} f''(c_3) - \frac{h^3}{4} \frac{f''(c_0)}{12} \approx \frac{3}{4} \frac{h^3}{12} f''(c_3).$$

Adaptive quadrature

Assuming $f''(c_0) \approx f''(c_3)$, we have

$$T(a,b) - T(a,c) - T(c,b) = \frac{h^3}{12} f''(c_3) - \frac{h^3}{4}\frac{f''(c_0)}{12} \approx \frac{3}{4}\frac{h^3}{12} f''(c_3).$$

Thus

$$\left| \int_a^b f(x)dx - T(a,c) - T(c,b) \right| \approx \left| T(a,b) - T(a,c) - T(c,b) \right| / 3.$$

Adaptive quadrature

Assuming $f''(c_0) \approx f''(c_3)$, we have

$$T(a,b) - T(a,c) - T(c,b) = \frac{h^3}{12} f''(c_3) - \frac{h^3}{4}\frac{f''(c_0)}{12} \approx \frac{3}{4}\frac{h^3}{12} f''(c_3).$$

Thus

$$\left| \int_a^b f(x)dx - T(a,c) - T(c,b) \right| \approx |T(a,b) - T(a,c) - T(c,b)| /3.$$

This shows that if $|T(a,b) - T(a,c) - T(c,b)| < 3 * \mathrm{TOL}$ then

$$\left| \int_a^b f(x)dx - T(a,c) - T(c,b) \right| < \mathrm{TOL}.$$

Adaptive quadrature

Assuming $f''(c_0) \approx f''(c_3)$, we have

$$T(a,b) - T(a,c) - T(c,b) = \frac{h^3}{12} f''(c_3) - \frac{h^3}{4}\frac{f''(c_0)}{12} \approx \frac{3}{4}\frac{h^3}{12} f''(c_3).$$

Thus

$$\left| \int_a^b f(x)dx - T(a,c) - T(c,b) \right| \approx |T(a,b) - T(a,c) - T(c,b)| /3.$$

This shows that if $|T(a,b) - T(a,c) - T(c,b)| < 3 * \text{TOL}$ then

$$\left| \int_a^b f(x)dx - T(a,c) - T(c,b) \right| < \text{TOL}.$$

If this is not satisfied, then intervals $[a,c]$ and $[c,b]$ are further broken in halves and the above check for the error is applied to each of the halves and the process is repeated till the tolerance is met.

Adaptive quadrature

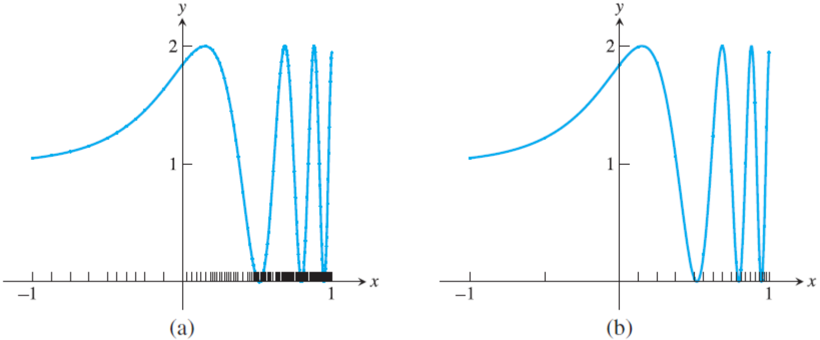

Figure : Adaptive quadrature for $\int_{-1}^{1}(1+\sin e^{3x})dx$ with TOL $= 0.0012$ via (a) Trapezoid rule (needing 140 subintervals) and (b) Simpson's rule (needing 15 subintervals)