MA579H Scientific Computing

Numerical Integration I

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Lecture outline

- Quadrature formula
- Newton-Cotes formula
- Midpoint and composite midpoint rules
- Trapezoid and composite trapezoid rules
- Simpson's and composite Simpson's rule

Quadrature

Integrals such as

$$\int_0^2 e^{-x^2}dx, \ , \int_0^\pi \cos(3\sin(\log(1+x)))dx, \ \int_0^1 x^2 e^{\tan(sin(x))}dx$$

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Strategy: Integration via polynomial interpolation.

- Approximate f using an interpolating polynomial $p_n(x)$.
- Evaluate $Q_n(f) := \int_a^b p_n(x)dx$, since it is easy to evaluate integral of a polynomial. We expect that $Q_n(f) \approx I(f)$.

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$$\ell_j(x) := \frac{w(x)}{(x - x_j)w'(x_j)} = \prod_{i \neq j} \frac{(x - x_i)}{(x_j - x_i)}, \quad j = 0 : n,$$

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where $w_j := \int_a^b \ell_j(x)dx$ is called the j-th quadrature weight and

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Note that the quadrature weights do not depend on the function $f(x)$ and hence can be computed independently of $f(x)$ and stored.

Error estimate

Set $E_n(f) := I(f) - Q_n(f)$. If $f \in C^{n+1}[a,b]$ then

$$
\begin{aligned}
|E_n(f)| &\leq \int_a^b |f(x) - p_n(x)| dx = \frac{1}{(n+1)!} \int_a^b |f^{(n+1)}(\xi_x) w(x)| dx \\
&\leq \frac{\|f^{(n+1)}\|_\infty}{(n+1)!} \int_a^b |(x - x_0)(x - x_1) \cdots (x - x_n)| dx.
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The quadrature rule $Q_n(f) = \int_a^b p_n(x) dx$ has degree of exactness $\geq n$.

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$$|E_n(f)| \leq \frac{\|f^{(n+1)}\|_\infty}{(n+1)!} \int_a^b |(x - x_0)(x - x_1) \cdots (x - x_n)| dx$$

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Newton-Cotes is not useful for large n. There are two natural ways to ensure $Q_n(f) \longrightarrow I(f)$ as $n \to \infty$:

- Don't use equally spaced nodes.
- Integrate piecewise polynomial interpolant.

Midpoint rule

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Note, however, that

$$M(x) = \frac{b^2 - a^2}{2} = \int_a^b x dx,$$

which shows that it is exact for polynomials of degree 1. Thus, the midpoint rule is exact for polynomials of degree 1.

Midpoint rule

Theorem: If $f \in C^2[a,b]$ then there exists $\theta \in [a,b]$ such that

$$\int_a^b f(x)dx = M(f) + \frac{f''(\theta)}{24}(b-a)^3.$$

Hence $E(f) := I(f) - M(f) = \dfrac{f''(\theta)}{24}(b-a)^3.$

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Proof: Set $w := (a+b)/2$. Then by Taylor's theorem

$$f(x) = f(w) + f'(w)(x-w) + f''(\theta_x)(x-w)^2/2.$$

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$$\begin{aligned}\int_a^b f(x)dx &= (b-a)f(w) + 0 + \frac{f''(\theta)}{2}\int_a^b (x-w)^2 dx \\ &= M(f) + \frac{f''(\theta)}{24}(b-a)^3.\end{aligned}$$

Composite midpoint rule

Consider the equally spaced nodes $[x_0, \ldots, x_n]$, where $x_j = a + jh$, $j = 0 : n$, and $h := (b-a)/n$. Set $w_j := (x_j + x_{j+1})/2$ for $j = 0 : n-1$. Then

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By midpoint rule, $\int_{x_{j-1}}^{x_j} f(x)dx \approx hf(w_{j-1})$. Hence

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This yields the composite midpoint rule

$$\begin{aligned} M_n(f) &:= \sum_{j=1}^{n} hf(w_{j-1}) \\ &= h\left[f(w_0) + f(w_2) + \cdots + f(w_{n-1})\right]. \end{aligned}$$

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Consequently, there exists $\theta \in [a, b]$ such that

$$\begin{aligned} E_n(f) &:= I(f) - M_n(f) = \sum_{j=1}^{n} \frac{f''(\theta_j)}{24} h^3 \\ &= n\frac{f''(\theta)}{24}h^3 = \frac{h^2}{24}(b-a)f''(\theta). \end{aligned}$$

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Hence we have $|E_n(f)| \leq \frac{h^2}{24}(b-a)\|f''\|_\infty.$

Trapezoid rule

The quadrature $Q_n(f)$ is called Trapezoid rule when $n = 1$. Then nodes are $x_0 = a$ and $x_1 = b$, and $\ell_0(x) = \frac{x-b}{a-b}$ and $\ell_1(x) = \frac{x-a}{b-a}$.

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Hence the Trapezoid rule is given by

$$T(f) = \frac{(b-a)}{2}[f(a) + f(b)].$$

Trapezoid rule

Theorem: If $f \in C^2[a,b]$ then there exists $\theta \in [a,b]$ such that

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

Hence $E(f) := I(f) - T(f) = -\dfrac{f''(\theta)}{12}(b-a)^3.$

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Proof: By mean value theorem (MVT) of integral, we have

$$\begin{aligned}
E(f) &= \int_a^b (f(x) - p(x))dx \\
&= \int_a^b \frac{f''(\xi_x)}{2}(x-a)(x-b)dx \\
&= \frac{f''(\theta)}{2}\int_a^b (x-a)(x-b)dx \quad \text{for some } \theta \in (a,b) \\
&= -\frac{f''(\theta)}{12}(b-a)^3.
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By trapezoid rule, $\int_{x_{j-1}}^{x_j} f(x)dx \approx \frac{h}{2}[f(x_{j-1}) + f(x_j)]$. Hence

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This yields the composite trapezoid rule

$$\begin{aligned} T_n(f) &:= \sum_{j=1}^{n} \frac{h}{2}[f(x_{j-1}) + f(x_j)] \\ &= h\left[\frac{f(x_0)}{2} + f(x_2) + \cdots + f(x_{n-1}) + \frac{f(x_n)}{2}\right]. \end{aligned}$$

Error in composite trapezoid rule

By trapezoid rule, $\displaystyle\int_{x_{j-1}}^{x_j} f(x)dx - \frac{h}{2}[f(x_{j-1}) + f(x_j)] = -\frac{f''(\theta_j)}{12}h^3.$

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By intermediate value theorem (IVT), there exists $\theta \in [a, b]$ such that

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Hence $|E_n(f)| \le \frac{h^2}{12}(b-a)\|f''\|_\infty.$

Example

Consider the integral

$$I(f) := \int_0^1 e^{-x^2} dx.$$

The two Newton-Cotes (midpoint and trapezoid) formula yield

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The error from the trapezoid rule is about twice that of the midpoint rule, which validates the error estimate.

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

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Observe that $S(f) = \frac{1}{3}T(f) + \frac{2}{3}M(f),$ where $T(f)$ is the trapezoid rule and $M(f) = (b-a)f\left(\frac{a+b}{2}\right)$ is the midpoint rule.

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Observe that $S(x^j) = \int_0^1 x^j dx$ for $j = 0, 1, 2, 3$. Hence $S(f)$ is exact for polynomial of degree ≤ 3. As per the error analysis of quadrature rule, $S(f)$ is expected to be exact for polynomials of degree ≤ 2.

Error estimation of Simpson's rule

Theorem: Suppose that $f \in C^4[a, b]$. Then

$$\int_a^b f(x)dx = \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] + E_2(f),$$

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Composite Simpson's rule

Suppose that n is even. Set $h := (b-a)/n$ and consider the nodes $x_j = a + jh$ for $j = 0 : n$. Then

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx$$

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with error $E_n^S(f) = -\frac{1}{90}h^5 \sum_{j=1}^{n/2} f^{(4)}(\theta_j)$ for some $\theta_j \in (x_{2j-2}, x_{2j})$, $j = 1 : (n/2)$.

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By IVT (intermediate value theorem), there exists $\theta \in (a, b)$ such that

$$\sum_{j=1}^{n/2} f^{(4)}(\theta_j) = \frac{n}{2} f^{(4)}(\theta)$$

As $nh = b - a$,

$$E_n^S(f) = -\frac{b-a}{180} h^4 f^{(4)}(\theta).$$

Example

Consider the integral

$$I(f) := \int_0^1 e^{-x^2}\,dx.$$

The three Newton-Cotes (midpoint, trapezoid, and Simpson's rule) formula yield

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$|I(f)-M(f)| = 0.031977, |I(f)-T(f)| = 0.062884, |I(f)-S(f)| = 0.000356.$

The Simpson's rule, with an error of only 0.000356, seems remarkably accurate considering the size of the interval over which it is applied.