Numerical Integration: Basic Rule

CS/SE 4X03

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Outline

The problem

- Approximate numerically the integral

$$I_f = \int_a^b f(x)dx$$

- Closed form may not exist, e.g. $\int_a^b e^{-x^2} dx$, or may be difficult to compute
- The integrand $f(x)$ may be known only at certain points obtained via sampling (e.g. embedded applications)

Derivation

$$I_f = \int_a^b f(x)dx \approx \sum_{j=0}^{n} a_j f(x_j)$$

- The sum is called a *quadrature rule*
- The a_j are weights
- How to find them?

Derivation cont.

- Let $x_0, \ldots, x_n$ be distinct points in $[a, b]$
- Let $p_n(x)$ be the interpolating polynomial for $f(x)$ through these points
- $\int_a^b f(x)dx \approx \int_a^b p_n(x)dx$
- From the Lagrange form $p_n(x) = \sum_{j=0}^n f(x_j)L_j(x)$,

$$
\begin{aligned}
\int_a^b f(x)dx \approx \int_a^b p_n(x)dx &= \int_a^b \sum_{j=0}^n f(x_j)L_j(x)dx \\
&= \sum_{j=0}^n f(x_j) \underbrace{\int_a^b L_j(x)dx}_{a_j}
\end{aligned}
$$

- $a_j = \int_a^b L_j(x)dx$

Trapezoidal rule

Let $n = 1$. Then $x_0 = a$ and $x_1 = b$ and

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} = \frac{x - b}{a - b}, \quad L_1(x) = \frac{x - x_0}{x_1 - x_0} = \frac{x - a}{b - a}$$

$$\begin{aligned} f(x) \approx p_1(x) &= f(x_0)L_0(x) + f(x_1)L_1(x) \\ &= f(a)L_0(x) + f(b)L_1(x) \end{aligned}$$

Integrating

$$\begin{aligned} I_f = \int_a^b f(x)dx &\approx f(a) \underbrace{\int_a^b L_0(x)dx}_{a_0} + f(b) \underbrace{\int_a^b L_1(x)dx}_{a_1} \\ &= f(a) \int_a^b \frac{x - b}{a - b} dx + f(b) \int_a^b \frac{x - a}{b - a} dx \\ &= \frac{b - a}{2} \left[f(a) + f(b) \right] \end{aligned}$$

Trapezoidal rule cont.

$$I_f \approx I_{\text{trap}} = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

Example 1.

- Approximate $\int_0^1 e^x dx = e - 1 = 1.7182\ldots$ using the trapezoidal rule:

$$I_{\text{trap}} = \frac{1}{2}[f(0) + f(1)] = 0.5(1 + e) = 1.8591\cdots$$

- Approximate $\int_0^{0.1} e^x dx = e^{0.1} - 1 = 0.10517\cdots$ using the trapezoidal rule:

$$I_{\text{trap}} = \frac{0.1}{2}[f(0) + f(0.1)] = 0.05\left(1 + e^{0.1}\right) = 0.10525\cdots$$

Errror of trapezoidal rule

In the trapezoidal rule, $f(x)$ is approximated by linear interpolation

$$p_1(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a}$$

The error is

$$f(x) - p_1(x) = \tfrac{1}{2} f''(\xi(x))(x-a)(x-b)$$

Then

$$\begin{aligned}\int_a^b (f(x) - p_1(x))dx &= \int_a^b f(x)dx - \frac{b-a}{2}[f(a) + f(b)] \\ &= \frac{1}{2}\int_a^b f''(\xi(x))(x-a)(x-b)dx\end{aligned}$$

Errror of trapezoidal rule cont.

$(x-a)(x-b) \leq 0$ does not change sign on $[a,b]$

From the Mean-Value Theorem for integrals, there exists $\eta \in (a,b)$ such that

$$\int_a^b f''(\xi(x))(x-a)(x-b)dx = f''(\eta)\int_a^b (x-a)(x-b)dx$$

Using $\int_a^b (x-a)(x-b)dx = -(b-a)^3/6$, the error in the trapezoidal rule is

$$I_f - I_{\text{trap}} = -\frac{f''(\eta)}{12}(b-a)^3$$

Midpoint rule

$$I_f \approx I_{\text{mid}} = (b-a) f\left(\frac{a+b}{2}\right)$$

Example 2.

- Approximate $\int_0^1 e^x dx = e - 1 \approx 1.7182\cdots$ using the midpoint rule:

$$I_{\text{mid}} = (1-0) f(0.5) = e^{0.5} = 1.6487\cdots$$

- Approximate $\int_0^{0.1} e^x dx = e^{0.1} - 1 \approx 0.10517\cdots$ using the midpoint rule:

$$I_{\text{mid}} = (0.1-0) f(0.05) = 0.1 e^{0.05} = 0.10512\cdots$$

Error of midpoint rule

Let $m = (a+b)/2$. Expand f in Taylor series

$$f(x) = f(m) + f'(m)(x-m) + \tfrac{1}{2} f''(\xi(x))(x-m)^2$$

Then

$$I_f = \int_a^b f(x) = \underbrace{(b-a)f(m)}_{I_{\text{mid}}} + \frac{1}{2}\int_a^b f''(\xi(x))(x-m)^2 dx$$

Since $(x-m)^2$ does not change sign, there exists $\eta \in (a,b)$ such that

$$\frac{1}{2}\int_a^b f''(\xi(x))(x-m)^2 dx = \frac{1}{2} f''(\eta)\int_a^b (x-m)^2 dx = \frac{f''(\eta)}{24}(b-a)^3$$

Then

$$I_f - I_{\text{mid}} = \frac{f''(\eta)}{24}(b-a)^3$$

Simpson's rule

Let $n = 2$, and $x_0 = a$, $x_1 = (a+b)/2$, $x_2 = b$

Simpson's rule is obtained from integrating the second order polynomial

$$\begin{aligned} p_2(x) &= f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x) \\ &= f(a)L_0(x) + f((a+b)/2)L_1(x) + f(b)L_2(x) \end{aligned}$$

$$I_f \approx I_{\mathsf{Simpson}} = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

The error is

$$I_f - I_{\mathsf{Simpson}} = -\frac{f^{(4)}(\xi)}{90}\left(\frac{b-a}{2}\right)^5, \quad \xi \in (a,b)$$

Simpson's rule cont.

Example 3. Approximate $\int_0^1 e^x dx = e - 1 \approx 1.71828\cdots$ using Simpson's rule:

$$
\begin{aligned}
I_{\mathsf{Simpson}} &= \frac{1}{6}\left[f(0) + 4f\,(0.5) + f(1)\right] = \frac{1}{6}(1 + 4e^{0.5} + e) \\
&= 1.71886\cdots
\end{aligned}
$$