MA 322: Scientific Computing

Lecture - 11

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

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

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

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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Combining the two expansions, the desired result follows.

Degree of exactness

The error $E_2(f) = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\theta)$ shows that Simpson's rule $S(f)$ is exact for polynomials of degree ≤ 3, which is one degree more than a 3-points Newton-Cotes quadrature formula can guarantee.

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Thus, the degree of exactness of an $(n+1)$-point Newton-Cotes rule is n if n is odd, but the degree of exactness is $n+1$ if n is even.

Example

Consider the integral

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

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

$$M(f) \quad = \quad (1-0)e^{-0.25} \approx 0.778801$$

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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.

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This shows that the degree of exactness of $M(f)$ is 1.

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

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

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$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx \\ &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx\end{aligned}$$

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Thus the composite Simpson's rule is given by

$$S_n(f) := \frac{h}{3}[f(x_0) + 2\sum_{j=2}^{n/2} f(x_{2j-2}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)]$$

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with error $E_n^S(f) = -\frac{1}{90}h^5 \sum_{j=1}^{n/2} f^{(4)}(\theta_j) = -\frac{(b-a)}{180}h^4 f^{(4)}(\theta)$ for some $\theta \in [a, b]$.