
Numerical Analysis Hilary Term 2018

Lecture 2: Newton–Cotes Quadrature

See Chapter 7 of Süli and Mayers.

Terminology: Quadrature \equiv numerical integration

Setup: given $f(x_k)$ at $n + 1$ equally spaced points $x_k = x_0 + k \cdot h$, $k = 0, 1, \dots, n$, where $h = (x_n - x_0)/n$. Suppose that $p_n(x)$ interpolates this data.

Idea: does

$$\int_{x_0}^{x_n} f(x) \, dx \approx \int_{x_0}^{x_n} p_n(x) \, dx \quad (1)$$

We investigate the error in such an approximation below, but note that

$$\begin{aligned} \int_{x_0}^{x_n} p_n(x) \, dx &= \int_{x_0}^{x_n} \sum_{k=0}^n f(x_k) \cdot L_{n,k}(x) \, dx \\ &= \sum_{k=0}^n f(x_k) \cdot \int_{x_0}^{x_n} L_{n,k}(x) \, dx \\ &= \sum_{k=0}^n w_k f(x_k), \end{aligned} \quad (2)$$

where the coefficients

$$w_k = \int_{x_0}^{x_n} L_{n,k}(x) \, dx \quad (3)$$

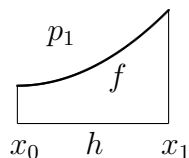
$k = 0, 1, \dots, n$, are independent of f . A formula

$$\int_a^b f(x) \, dx \approx \sum_{k=0}^n w_k f(x_k)$$

with $x_k \in [a, b]$ and w_k independent of f for $k = 0, 1, \dots, n$ is called a **quadrature formula**; the coefficients w_k are known as **weights**. The specific form (1)–(3), based on equally spaced points, is called a **Newton–Cotes formula** of order n .

Examples:

Trapezium Rule: $n = 1$ (also known as the trapezoid or trapezoidal rule):

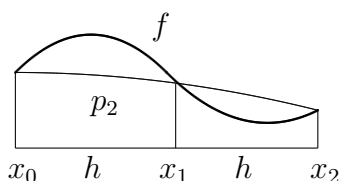


$$\int_{x_0}^{x_1} f(x) \, dx \approx \frac{h}{2} [f(x_0) + f(x_1)]$$

Proof.

$$\begin{aligned} \int_{x_0}^{x_1} p_1(x) \, dx &= f(x_0) \int_{x_0}^{x_1} \overbrace{\frac{x - x_1}{x_0 - x_1}}^{L_{1,0}(x)} \, dx + f(x_1) \int_{x_0}^{x_1} \overbrace{\frac{x - x_0}{x_1 - x_0}}^{L_{1,1}(x)} \, dx \\ &= f(x_0) \frac{(x_1 - x_0)}{2} + f(x_1) \frac{(x_1 - x_0)}{2} \end{aligned}$$

Simpson's Rule: $n = 2$:



$$\int_{x_0}^{x_2} f(x) dx \approx \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$

Note: The trapezium rule is exact if $f \in \Pi_1$, since if $f \in \Pi_1 \implies p_1 = f$. Similarly, Simpson's Rule is exact if $f \in \Pi_2$, since if $f \in \Pi_2 \implies p_2 = f$. The highest degree of polynomial exactly integrated by a quadrature rule is called the **(polynomial) degree of accuracy** (or degree of exactness).

Error: we can use the error in interpolation directly to obtain

$$\int_{x_0}^{x_n} [f(x) - p_n(x)] dx = \int_{x_0}^{x_n} \frac{\pi(x)}{(n+1)!} f^{(n+1)}(\xi(x)) dx$$

so that

$$\left| \int_{x_0}^{x_n} [f(x) - p_n(x)] dx \right| \leq \frac{1}{(n+1)!} \max_{\xi \in [x_0, x_n]} |f^{(n+1)}(\xi)| \int_{x_0}^{x_n} |\pi(x)| dx, \quad (4)$$

which, e.g., for the trapezium rule, $n = 1$, gives

$$\left| \int_{x_0}^{x_1} f(x) dx - \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)] \right| \leq \frac{(x_1 - x_0)^3}{12} \max_{\xi \in [x_0, x_1]} |f''(\xi)|.$$

In fact, we can prove a tighter result using the Integral Mean-Value Theorem¹:

Theorem. $\int_{x_0}^{x_1} f(x) dx - \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)] = -\frac{(x_1 - x_0)^3}{12} f''(\xi)$ for some $\xi \in (x_0, x_1)$.

Proof. See problem sheet. □

For $n > 1$, (4) gives pessimistic bounds. But one can prove better results such as:

Theorem. Error in Simpson's Rule: if f'''' is continuous on (x_0, x_2) , then

$$\left| \int_{x_0}^{x_2} f(x) dx - \frac{(x_2 - x_0)}{6} [f(x_0) + 4f(x_1) + f(x_2)] \right| \leq \frac{(x_2 - x_0)^5}{720} \max_{\xi \in [x_0, x_2]} |f''''(\xi)|.$$

Proof. Recall $\int_{x_0}^{x_2} p_2(x) dx = \frac{1}{3} h [f(x_0) + 4f(x_1) + f(x_2)]$, where $h = x_2 - x_1 = x_1 - x_0$. Consider $f(x_0) - 2f(x_1) + f(x_2) = f(x_1 - h) - 2f(x_1) + f(x_1 + h)$. Then, by Taylor's Theorem,

$$\begin{aligned} f(x_1 - h) &= f(x_1) - hf'(x_1) + \frac{1}{2} h^2 f''(x_1) - \frac{1}{6} h^3 f'''(x_1) + \frac{1}{24} h^4 f''''(\xi_1) \\ -2f(x_1) &= -2f(x_1) \\ +f(x_1 + h) &= f(x_1) + hf'(x_1) + \frac{1}{2} h^2 f''(x_1) + \frac{1}{6} h^3 f'''(x_1) + \frac{1}{24} h^4 f''''(\xi_2) \end{aligned}$$

¹**Integral Mean-Value Theorem:** if f and g are continuous on $[a, b]$ and $g(x) \geq 0$ on this interval, then there exists an $\eta \in (a, b)$ for which $\int_a^b f(x)g(x) dx = f(\eta) \int_a^b g(x) dx$ (see problem sheet).

for some $\xi_1 \in (x_0, x_1)$ and $\xi_2 \in (x_1, x_2)$, and hence

$$\begin{aligned} f(x_0) - 2f(x_1) + f(x_2) &= h^2 f''(x_1) + \frac{1}{24} h^4 [f''''(\xi_1) + f''''(\xi_2)] \\ &= h^2 f''(x_1) + \frac{1}{12} h^4 f''''(\xi_3), \end{aligned} \quad (5)$$

the last result following from the Intermediate-Value Theorem² for some $\xi_3 \in (\xi_1, \xi_2) \subset (x_0, x_2)$. Now for any $x \in [x_0, x_2]$, we may use Taylor's Theorem again to deduce

$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &= f(x_1) \int_{x_1-h}^{x_1+h} dx + f'(x_1) \int_{x_1-h}^{x_1+h} (x - x_1) dx \\ &\quad + \frac{1}{2} f''(x_1) \int_{x_1-h}^{x_1+h} (x - x_1)^2 dx + \frac{1}{6} f'''(x_1) \int_{x_1-h}^{x_1+h} (x - x_1)^3 dx \\ &\quad + \frac{1}{24} \int_{x_1-h}^{x_1+h} f''''(\eta_1(x)) (x - x_1)^4 dx \\ &= 2hf(x_1) + \frac{1}{3} h^3 f''(x_1) + \frac{1}{60} h^5 f''''(\eta_2) \\ &= \frac{1}{3} h [f(x_0) + 4f(x_1) + f(x_2)] + \frac{1}{60} h^5 f''''(\eta_2) - \frac{1}{36} h^5 f''''(\xi_3) \\ &= \int_{x_0}^{x_2} p_2(x) dx + \frac{1}{180} \left(\frac{x_2 - x_0}{2} \right)^5 (3f''''(\eta_2) - 5f''''(\xi_3)) \end{aligned}$$

where $\eta_1(x)$ and $\eta_2 \in (x_0, x_2)$, using the Integral Mean-Value Theorem and (5). Thus, taking moduli,

$$\left| \int_{x_0}^{x_2} [f(x) - p_2(x)] dx \right| \leq \frac{8}{2^5 \cdot 180} (x_2 - x_0)^5 \max_{\xi \in [x_0, x_2]} |f''''(\xi)|$$

as required. \square

Note: Simpson's Rule is exact if $f \in \Pi_3$ since then $f'''' \equiv 0$.

In fact, it is possible to compute a slightly stronger bound.

Theorem. Error in Simpson's Rule II: if f'''' is continuous on (x_0, x_2) , then

$$\int_{x_0}^{x_2} f(x) dx = \frac{x_2 - x_0}{6} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{(x_2 - x_0)^5}{2880} f''''(\xi)$$

for some $\xi \in (x_0, x_2)$.

Proof. See Süli and Mayers, Thm. 7.2. \square

²**Intermediate-Value Theorem:** if f is continuous on a closed interval $[a, b]$, and c is any number between $f(a)$ and $f(b)$ inclusive, then there is at least one number ξ in the closed interval such that $f(\xi) = c$. In particular, since $c = (df(a) + ef(b))/(d + e)$ lies between $f(a)$ and $f(b)$ for any positive d and e , there is a value ξ in the closed interval for which $d \cdot f(a) + e \cdot f(b) = (d + e) \cdot f(\xi)$.