Math 405: Numerical Methods for Differential Equations 2016 W1
Topic 4: 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 $x_k = x_0 + k \cdot h$, $k = 0, 1, \ldots, n$, where $h = (x_n - x_0)/n$. Suppose that $p_n(x)$ interpolates this data.

Idea: does

$$\int_{x_0}^{x_n} f(x)\,\mathrm{d}x \approx \int_{x_0}^{x_n} p_n(x)\,\mathrm{d}x? \tag{1}$$

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

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

where the coefficients

$$w_k = \int_{x_0}^{x_n} L_{n,k}(x)\,\mathrm{d}x \tag{3}$$

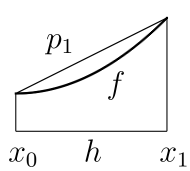
$k = 0, 1, \ldots, n$, are independent of f. A formula

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

with $x_k \in [a, b]$ and w_k independent of f for $k = 0, 1, \ldots, n$ 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):

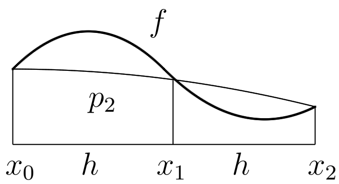


$$\int_{x_0}^{x_1} f(x)\,\mathrm{d}x \approx \frac{h}{2}[f(x_0) + f(x_1)]$$

Proof.

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

Simpson's Rule: $n = 2$:



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

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 $f \in \Pi_2 \implies p_2 = f$. (In fact it is better, see next page...) 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

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

so that

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

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

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

In fact, we can prove a tighter result using the Integral Mean-Value Theorem[1]:

Theorem. $\displaystyle\int_{x_0}^{x_1} f(x)\,\mathrm{d}x - \frac{(x_1 - x_0)}{2}[f(x_0) + f(x_1)] = -\frac{(x_1 - x_0)^3}{12} f''(\xi)$ 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

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

Proof. Recall $\displaystyle\int_{x_0}^{x_2} p_2(x)\,\mathrm{d}x = \tfrac{1}{3}h[f(x_0) + 4f(x_1) + f(x_2)]$, 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,

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

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

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

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

the last result following from the Intermediate-Value Theorem[2] 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

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

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

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

as required. □

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

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

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

Proof. See Süli and Mayers, Thm. 7.2. □

[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 $d \cdot f(a) + e \cdot f(b) = (d + e) \cdot f(\xi)$.