Math 405: Numerical Methods for Differential Equations 2017 W1
Topic 4: Newton–Cotes Quadrature

"Quadrature" means numerical integration. Main idea: find a polynomial interpolant as proxy/model for $f(x)$ and integrate that instead. A reference is Chapter 7 of Süli and Mayers book.

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

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

where the coefficients

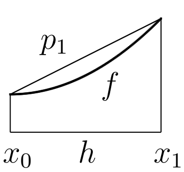
$$w_k = \int_{x_0}^{x_n} L_{n,k}(x)\,\mathrm{d}x \tag{3}$$

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

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

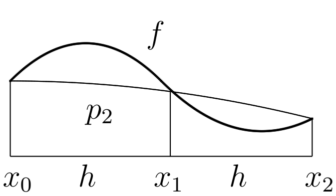
with $x_k \in [a, b]$ and w_k independent of f for $k = 0, 1, \ldots, n$ is called a **quadrature formula**; the coefficients w_k are known as **weights**. The specific form (1)–(3), based on equally spaced points, is called a **Newton–Cotes formula** of order n.

Trapezoidal Rule: $n = 1$ (also known as the trapezium rule):



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

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 trapezoidal 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

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

which, e.g., for the trapezoidal 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. $\int_{x_0}^{x_1} f(x) \, \mathrm{d}x - \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)] = -\frac{(x_1 - x_0)^3}{12} f''(\xi)$ for some $\xi \in (x_0, x_1)$.

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

Theorem. Error in Simpson's Rule I: 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. First a more general lemma:

Lemma. Let $x_0 = x_1 - h$ and $x_2 = x_1 + h$. Suppose f'''' is continuous on (x_0, x_2). Then

$$\frac{f(x_0) - 2f(x_1) + f(x_2)}{h^2} = f''(x_1) + \tfrac{1}{12} h^2 f''''(\eta), \tag{5}$$

Proof uses Taylor expansions and Intermediate-Value Theorem[2] for some $\eta \in (x_0, x_2)$. □

Back to the main proof: now for any $x \in [x_0, x_2]$, we may use Taylor's Theorem again

[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 $\int_a^b f(x)g(x) \, \mathrm{d}x = f(\eta) \int_a^b g(x) \, \mathrm{d}x$.

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

to deduce

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

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

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

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. □