Math 405: Numerical Methods for Differential Equations 2015 W1
Topic 4: Newton–Cotes Quadrature

See Chapter 7 of Süli and Mayers.

**Terminology:** Quadrature ≡ 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 \( \int_{x_0}^{x_n} f(x) \, dx \approx \int_{x_0}^{x_n} p_n(x) \, dx \) ? (1)

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

\[
\int_{x_0}^{x_n} p_n(x) \, dx = \int_{x_0}^{x_n} \sum_{k=0}^{n} f(x_k) \cdot L_{n,k}(x) \, dx
\]

\[
= \sum_{k=0}^{n} f(x_k) \cdot \int_{x_0}^{x_n} L_{n,k}(x) \, dx
\]

\[
= \sum_{k=0}^{n} w_k f(x_k),
\]

where the coefficients

\[
w_k = \int_{x_0}^{x_n} L_{n,k}(x) \, dx
\]

\( k = 0, 1, \ldots, n, \) 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 \( k = 0, 1, \ldots, n \) 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):

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

**Proof.**

\[
\int_{x_0}^{x_1} p_1(x) \, dx = f(x_0) \int_{x_0}^{x_1} \frac{x - x_1}{x_0 - x_1} \, dx + f(x_1) \int_{x_0}^{x_1} \frac{x - x_0}{x_1 - x_0} \, dx
\]

\[
= f(x_0) \frac{(x_1 - x_0)}{2} + f(x_1) \frac{(x_1 - x_0)}{2}
\]
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 \( f \in \Pi_2 \implies p_2 = f \). (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

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

so that

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

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 Theorem\(^1\):

**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 \( \int_{x_0}^{x_2} p_2(x) \, dx = \frac{1}{2} h[f(x_0) + 4f(x_1) + f(x_2)] \), 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,

\[
\begin{align*}
 f(x_1 - h) &= f(x_1) - hf'(x_1) + \frac{1}{2} h^2 f''(x_1) - \frac{1}{6} h^3 f'''(x_1) + \frac{1}{12} h^4 f''''(\xi_1) \\
 -2f(x_1) &= -2f(x_1) + \ldots \\
 f(x_1 + h) &= f(x_1) + hf'(x_1) + \frac{1}{2} h^2 f''(x_1) + \frac{1}{6} h^3 f'''(x_1) + \frac{1}{12} h^4 f''''(\xi_2)
\end{align*}
\]

\(^1\)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).

Topic 4 pg 2 of 3
for some $\xi_1 \in (x_0, x_1)$ and $\xi_2 \in (x_1, x_2)$, and hence
\[ f(x_0) - 2f(x_1) + f(x_2) = h^2 f''(x_1) + \frac{1}{4} h^4 [f'''(\xi_1) + f'''(\xi_2)] = h^2 f''(x_1) + \frac{1}{4} h^4 f'''(\xi_3), \] (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
\[
\int_{x_0}^{x_2} f(x) \, dx = f(x_0) \int_{x_1}^{x_1 + h} \, dx + f'(x_0) \int_{x_1}^{x_1 + h} (x - x_1) \, dx \\
+ \frac{1}{2} f''(x_1) \int_{x_1}^{x_1 + h} (x - x_1)^2 \, dx + \frac{1}{6} f'''(x_1) \int_{x_1}^{x_1 + h} (x - x_1)^3 \, dx \\
+ \frac{1}{4} \int_{x_1}^{x_1 + h} f'''(\eta_1(x))(x - x_1)^4 \, dx
\]

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 Suli 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 $\xi$ in the closed interval such that $f(\xi) = c$. In particular, since $c = (df(a) + e f(b))/(d + e)$ lies between $f(a)$ and $f(b)$ for any positive $d$ and $e$, there is a value $\xi$ in the closed interval for which $d \cdot f(a) + e \cdot f(b) = (d + e) \cdot f(\xi)$. 