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 $x_k = x_0 + k \cdot h$, $k = 0, 1, \ldots, n$, where $h = (x_n - x_0)/n$. Suppose that $p_n(x)$ interpolates this data.

Idea:

$$\int_{x_0}^{x_n} f(x)dx \approx \int_{x_0}^{x_n} p_n(x)dx?$$

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

$$\int_{x_0}^{x_n} p_n(x)dx = \int_{x_0}^{x_n} \sum_{k=0}^{n} f(x_k) \cdot L_{n,k}(x)dx \tag{1}$$

$$= \sum_{k=0}^{n} f(x_k) \cdot \int_{x_0}^{x_n} L_{n,k}(x)dx \tag{2}$$

$$= \sum_{k=0}^{n} w_k f(x_k), \tag{3}$$

where the coefficients

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

$k = 0, 1, ..., n$, are independent of f. That is, can be precomputed.

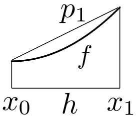
A formula

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

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):

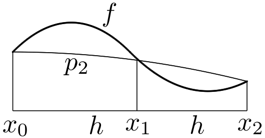


$$\int_{x_0}^{x_1} f(x)dx \approx \frac{h}{2}[f(x_0) + f(x_1)]$$

Proof

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

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 $f \in \Pi_1$, therefore $p_1 = f$. Similarly, Simpson's Rule is exact if $f \in \Pi_2$, since if $f \in \Pi_2$, therefore $p_2 = f$. 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

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

so that

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

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

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

In fact, we can prove a tighter result:

Theorem. Error in Trapezoidal Rule:

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

for some $\xi \in (x_0, x_1)$. (And note equality)

Proof. Omitted (uses Integral Mean-Value Theorem).

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

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

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

Proof. See, e.g., Süli and Mayers, Thm. 7.2.

Note: Simpson's Rule is exact if $f \in \Pi_2$ since then $f''' \equiv 0$. (c.f. earlier statement viz. $f \in \Pi_1$).

Composite Quadrature

Motivation:
we've seen oscillations in polynomial interpolation (the Runge phenomenon) for high-degree polynomials on equispaced grids

Idea:
split a required integration interval $[a, b] = [x_0, x_n]$ into n equal intervals $[x_{i-1}, x_i]$ for $i = 1, ..., n$. Then use a composite rule:

$$\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx = \sum_{i=0}^{n} \int_{x_{i-1}}^{x_i} f(x)dx$$

in which each $\int_{x_{i-1}}^{x_i} f(x)dx$ is approximated by quadrature.

Example: Composite Trapezium Rule

$$\int_{x_0}^{x_n} f(x)dx \approx \sum_{i=0}^{n} \frac{h}{2}[f(x_{i-1}) + f(x_i)]$$
$$\approx h[f(x_0)/2 + f(x_1) + f(x_2) + \ldots + f(x_{n-1}) + f(x_n)/2]$$

Error

$$\text{Error} = \frac{h^3}{12}\sum_{i=0}^{n} f''(\xi) \leq \frac{h^3 n}{12} f''(\xi)$$
$$= \frac{(x_n - x_0)h^2}{12} f''(\xi)$$