

Numerical Analysis

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with thanks to Endre Süli

Oxford Mathematical Institute

HT 2020

Building Lagrange interpolating polynomials from lower degree ones

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Let $Q_{i,j}$ be the Lagrange interpolating polynomial at x_k , $k = i, \dots, j$.

Then,

$$Q_{i,j}(x) = \frac{(x - x_i)Q_{i+1,j}(x) - (x - x_j)Q_{i,j-1}(x)}{x_j - x_i} \quad (0.1)$$

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$Q_{i+1,j}(x_k) = f_k = Q_{i,j-1}(x_k)$, and hence

$$s(x_k) = \frac{(x_k - x_i)Q_{i+1,j}(x_k) - (x_k - x_j)Q_{i,j-1}(x_k)}{x_j - x_i} = f_k.$$

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We also have that $Q_{i+1,j}(x_j) = f_j$ and $Q_{i,j-1}(x_i) = f_i$, and hence

$$s(x_i) = Q_{i,j-1}(x_i) = f_i \quad \text{and} \quad s(x_j) = Q_{i+1,j}(x_j) = f_j.$$

□

Comment

This result can be used as the basis for constructing interpolating polynomials. In books: may find topics such as the Newton form and divided differences.

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Given data f_i, g_i at distinct $x_i, i = 0, 1, \dots, n$, with $x_0 < x_1 < \dots < x_n$,
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Theorem

There is a unique polynomial $p \in \Pi_{2n+1}$ such that $p(x_i) = f_i$ and $p'(x_i) = g_i$ for $i = 0, 1, \dots, n$.

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Construction: given $L_{n,k}(x) = \frac{(x-x_0)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)}{(x_k-x_0)\cdots(x_k-x_{k-1})(x_k-x_{k+1})\cdots(x_k-x_n)}$, let

$$\begin{aligned} H_{n,k}(x) &= [L_{n,k}(x)]^2(1 - 2(x - x_k)L'_{n,k}(x_k)) \\ \text{and } K_{n,k}(x) &= [L_{n,k}(x)]^2(x - x_k). \end{aligned}$$

Then **Hermite interpolating polynomial**

$$p_{2n+1}(x) = \sum_{k=0}^n [f_k H_{n,k}(x) + g_k K_{n,k}(x)] \quad (0.2)$$

interpolates the data as required.

Theorem

Let h_{2n+1} be the Hermite interpolating polynomial in the case where $f_i = f(x_i)$ and $g_i = f'(x_i)$ and f has at least $2n+2$ smooth derivatives. Then, for every $x \in [x_0, x_n]$,

$$f(x) - h_{2n+1}(x) = [(x - x_0)(x - x_{k-1}) \cdots (x - x_n)]^2 \frac{f^{(2n+2)}(\xi)}{(2n+2)!},$$

where $\xi \in (x_0, x_n)$ and $f^{(2n+2)}$ is the $2n+2$ -nd derivative of f .

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Compare with the error formula we obtained for Lagrange interpolation:

Theorem

For every $x \in [x_0, x_n]$ there exists $\xi = \xi(x) \in (x_0, x_n)$ such that

$$f(x) - p_n(x) = (x - x_0)(x - x_1) \cdots (x - x_n) \frac{f^{(n+1)}(\xi)}{(n+1)!},$$

where $f^{(n+1)}$ is the $n+1$ -st derivative of f .

Newton–Cotes Quadrature

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 $p_n \in \Pi_n$ interpolates this data.

Idea: does

$$\int_{x_0}^{x_n} f(x) \, dx \approx \int_{x_0}^{x_n} p_n(x) \, dx? \quad (2.3)$$

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

$$\begin{aligned}\int_{x_0}^{x_n} p_n(x) \, dx &= \int_{x_0}^{x_n} \sum_{k=0}^n f(x_k) \cdot L_{n,k}(x) \, dx \\ &= \sum_{k=0}^n f(x_k) \cdot \int_{x_0}^{x_n} L_{n,k}(x) \, dx \\ &= \sum_{k=0}^n w_k f(x_k),\end{aligned}\tag{2.4}$$

where the coefficients

$$w_k = \int_{x_0}^{x_n} L_{n,k}(x) \, dx\tag{2.5}$$

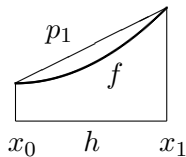
$k = 0, 1, \dots, n$, are independent of f .

A formula

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

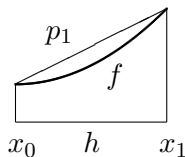
with $x_k \in [a, b]$ and w_k independent of f for $k = 0, 1, \dots, n$ is called a **quadrature formula**; the coefficients w_k are known as **weights**; the points x_k are called the **quadrature points**. The specific form (2.3)–(2.5) is called a **Newton–Cotes formula** of order n .

Trapezium Rule: $n = 1$:



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

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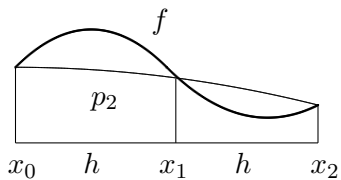


$$\int_{x_0}^{x_1} f(x) \, dx \approx \frac{h}{2} [f(x_0) + f(x_1)]$$

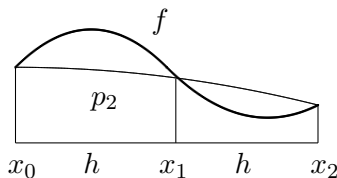
Proof.

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

Simpson's Rule: $n = 2$:

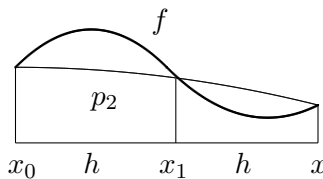


Simpson's Rule: $n = 2$:



$$\begin{aligned} \int_{x_0}^{x_2} f(x) \, dx &\approx \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] \\ &= \int_{x_0}^{x_2} p_2(x) \, dx \\ &= \sum_{k=0}^2 f(x_k) \cdot \int_{x_0}^{x_2} L_{2,k}(x) \, dx. \end{aligned}$$

Simpson's Rule: $n = 2$:



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

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$$= \sum_{k=0}^2 f(x_k) \cdot \int_{x_0}^{x_2} L_{2,k}(x) \, dx.$$

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 **degree of accuracy**.

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

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

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so that

$$\left| \int_{x_0}^{x_n} [f(x) - p_n(x)] \, dx \right| \leq \frac{1}{(n+1)!} \max_{\xi \in [x_0, x_n]} |f^{(n+1)}(\xi)| \int_{x_0}^{x_n} |\pi(x)| \, dx, \quad (2.6)$$

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which, e.g., for the Trapezium Rule, $n = 1$, gives

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

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In fact, we can prove a tighter result using the Integral Mean-Value Theorem.

Theorem (Integral Mean-Value Theorem)

Suppose that 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

$$\int_a^b f(x)g(x) \, dx = f(\eta) \int_a^b g(x) \, dx.$$

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Theorem

Suppose f'' is continuous on (x_0, x_1) . Then, there exists $\xi \in (x_0, x_1)$ such that

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

Proof. See problem sheet. □

For $n > 1$, (2.6) gives pessimistic bounds. For example, in the case $n = 2$, corresponding to Simpson's Rule, the bound becomes

$$\left| \int_{x_0}^{x_2} [f(x) - p_2(x)] dx \right| \leq \frac{(x_2 - x_0)^4}{192} \max_{\xi \in [x_0, x_2]} |f'''(\xi)|.$$

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We can prove a better result:

Theorem (Error in Simpson's Rule)

Suppose that f'''' is continuous on $[x_0, x_2]$. Then,

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

The proof relies on the following result.

Theorem (Intermediate-Value Theorem)

Suppose that 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 $f(\xi) = c$.

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

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 $h = x_2 - x_1 = x_1 - x_0$.

Proof. Recall

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where $h = x_2 - x_1 = x_1 - x_0$.

Consider $f(x_0) - 2f(x_1) + f(x_2) = f(x_1 - h) - 2f(x_1) + f(x_1 + h)$.

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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,

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

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

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

$$\begin{aligned} f(x_0) - 2f(x_1) + f(x_2) &= h^2f''(x_1) + \frac{1}{24}h^4[f''''(\xi_1) + f''''(\xi_2)] \\ &= h^2f''(x_1) + \frac{1}{12}h^4f''''(\xi_3), \end{aligned} \tag{2.7}$$

the last result following from the Intermediate-Value Theorem for some $\xi_3 \in (\xi_1, \xi_2) \subset (x_0, x_2)$.

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 &\stackrel{\text{IMVT}}{=} 2h f(x_1) + \frac{1}{3} h^3 f''(x_1) + \frac{1}{60} h^5 f''''(\eta_2), \\
 &\quad \text{where } \eta_2 \in (x_0, x_2) \text{ by the Integral Mean Value Theorem,}
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 \end{aligned}$$

for some $\xi_3 \in (\xi_1, \xi_2) \subset (x_0, x_2)$, having replaced $h^2 f''(x_1)$ from (2.7).

In summary, for any $x \in [x_0, x_2]$,

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

In summary, for any $x \in [x_0, x_2]$,

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Thus, taking moduli, and using the Intermediate-Value Theorem,

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

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)

Suppose that 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.