

# Numerical Analysis

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with thanks to Endre Süli

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

Then,

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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

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

## 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.

# Generalisation



## Generalisation

Given data  $f_i, g_i$  at distinct  $x_i, i = 0, 1, \dots, n$ , with  $x_0 < x_1 < \dots < x_n$ , can we find a polynomial  $p$  such that  $p(x_i) = f_i$  and  $p'(x_i) = g_i$ ?

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*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

$$H_{n,k}(x) = [L_{n,k}(x)]^2(1 - 2(x - x_k)L'_{n,k}(x_k))$$

and  $K_{n,k}(x) = [L_{n,k}(x)]^2(x - x_k).$

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  $f$ .

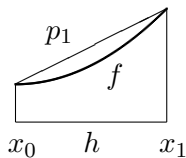
A formula

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

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  $n$ .

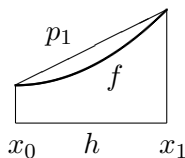


Trapezium Rule:  $n = 1$ :



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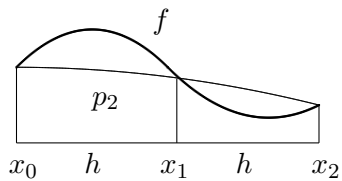


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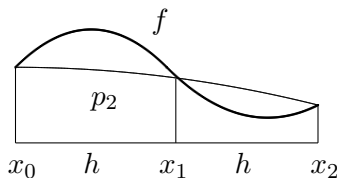
Proof.

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

Simpson's Rule:  $n = 2$ :

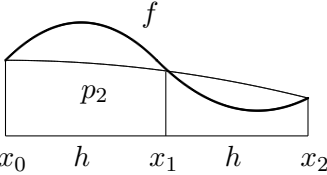


Simpson's Rule:  $n = 2$ :



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

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**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  $\xi$  in the closed interval such that  $f(\xi) = c$ .*

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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  $\xi$  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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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,

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

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

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

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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$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &= f(x_1) \int_{x_1-h}^{x_1+h} dx + f'(x_1) \int_{x_1-h}^{x_1+h} (x - x_1) dx \\ &\quad + \frac{1}{2} f''(x_1) \int_{x_1-h}^{x_1+h} (x - x_1)^2 dx + \frac{1}{6} f'''(x_1) \int_{x_1-h}^{x_1+h} (x - x_1)^3 dx \\ &\quad + \frac{1}{24} \int_{x_1-h}^{x_1+h} f''''(\eta_1(x))(x - x_1)^4 dx \quad \text{where } \eta_1(x) \in (x_0, x_2), \\ &\stackrel{\text{IMVT}}{=} 2hf(x_1) + \frac{1}{3}h^3 f''(x_1) + \frac{1}{60}h^5 f''''(\eta_2), \\ &\quad \text{where } \eta_2 \in (x_0, x_2) \text{ by the Integral Mean Value Theorem,} \\ &\stackrel{(2.7)}{=} \frac{1}{3}h[f(x_0) + 4f(x_1) + f(x_2)] + \frac{1}{60}h^5 f''''(\eta_2) - \frac{1}{36}h^5 f''''(\xi_3) \end{aligned}$$

Now for any  $x \in [x_0, x_2]$ , we may use Taylor's Theorem again to deduce

$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &= f(x_1) \int_{x_1-h}^{x_1+h} dx + f'(x_1) \int_{x_1-h}^{x_1+h} (x - x_1) dx \\ &\quad + \frac{1}{2} f''(x_1) \int_{x_1-h}^{x_1+h} (x - x_1)^2 dx + \frac{1}{6} f'''(x_1) \int_{x_1-h}^{x_1+h} (x - x_1)^3 dx \\ &\quad + \frac{1}{24} \int_{x_1-h}^{x_1+h} f''''(\eta_1(x))(x - x_1)^4 dx \quad \text{where } \eta_1(x) \in (x_0, x_2), \\ &\stackrel{\text{IMVT}}{=} 2hf(x_1) + \frac{1}{3}h^3 f''(x_1) + \frac{1}{60}h^5 f''''(\eta_2), \\ &\quad \text{where } \eta_2 \in (x_0, x_2) \text{ by the Integral Mean Value Theorem,} \\ &\stackrel{(2.7)}{=} \frac{1}{3}h[f(x_0) + 4f(x_1) + f(x_2)] + \frac{1}{60}h^5 f''''(\eta_2) - \frac{1}{36}h^5 f''''(\xi_3) \end{aligned}$$

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  $x \in [x_0, x_2]$ ,

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

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.