Numerical integration

Quadratures

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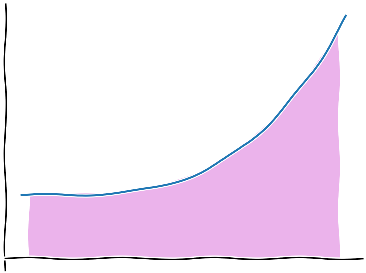
$$I = \int_a^b f(x)\,dx$$



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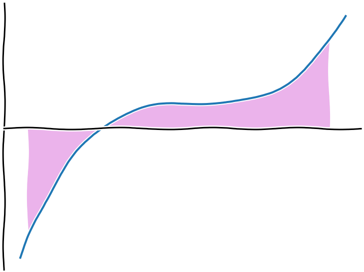

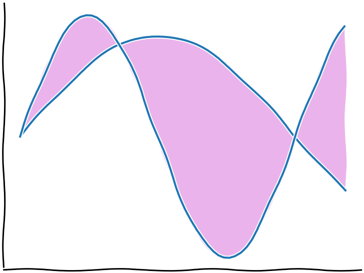

Quadratures

A *quadrature rule*

$$Q^{(N)} = \sum_{k=1}^{N} w_k f(x_k),$$

defined by its *nodes* and *weights*, approximates an integral

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Residual

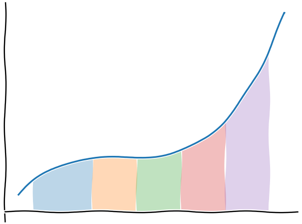
$$R^{(N)} = I - Q^{(N)} \to 0, \qquad N \to \infty$$

Want to maximize the convergence rate of $R^{(N)} \to 0$ as $N \to \infty$

Geometric construction of simple quadratures

Define a *mesh*

$$a = x_0 < x_1 < \cdots < x_N = b$$



Split the integral

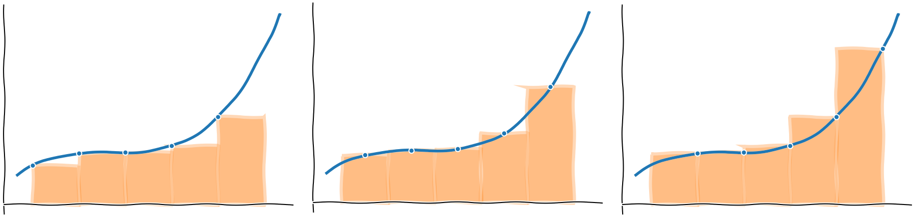
$$I = \int_a^b f(x)\,dx = \sum_{k=1}^{N} I_k$$

$$I_k = \int_{x_{k-1}}^{x_k} f(x)\,dx$$

Approximate each I_k by Q_k (an *elementary rule*), and then the *composite rule* is

$$Q^{(N)} = \sum_{k=1}^{N} Q_k$$

Geometric construction of simple quadratures



$Q_k = h_k f(x_{k-1})$ $\qquad$ $Q_k = h_k f(x_{k-1/2})$ $\qquad$ $Q_k = h_k f(x_k)$

Here $h_k = x_k - x_{k-1}$ and $x_{k-1/2} = (x_{k-1} + x_k)/2$

$Q^{(N)}$ becomes a Riemann sum for I:

$$Q^{(N)} = \sum_{k=1}^{N} Q_k \to I, \qquad N \to \infty$$

Convergence rates of simple quadratures

Rate of convergence: left-point rectangles

The residual for the elementary rule

$$
\begin{aligned}
R_k &= \int_{x_{k-1}}^{x_k} f(x)\,dx - hf(x_{k-1}) \\
&= \int_{x_{k-1}}^{x_k} \big[f(x) - f(x_{k-1})\big]\,dx
\end{aligned}
$$

Use the Taylor series

$$
f(x) = f(x_{k-1}) + f'(\xi)(x - x_{k-1}), \qquad \xi \in [x_{k-1}, x_k]
$$

Rate of convergence: left-point rectangles

$$\begin{aligned} R_k &= f'(\xi) \int_{x_{k-1}}^{x_k} (x - x_{k-1})\, dx \\ &= f'(\xi) \int_0^h y\, dy = \frac{1}{2} f'(\xi) h^2 \end{aligned}$$

Let $M_1 = \max\limits_{x \in [a,b]} |f'(x)|$

$$\begin{aligned} \left| R^{(N)} \right| = \left| \sum_{k=1}^{N} R_k \right| &\leqslant \frac{1}{2} M_1 h^2 N \qquad\qquad h_k = h = \text{const} \\ &= \frac{1}{2} M_1 (b-a) h \qquad\qquad hN = b - a \end{aligned}$$

Rate of convergence: mid-point rectangles

The residual for the elementary rule

$$\begin{aligned} R_k &= \int_{x_{k-1}}^{x_k} f(x)\,dx - hf(x_{k-1/2}) \\ &= \int_{x_{k-1}}^{x_k} \left[f(x) - f(x_{k-1/2})\right] dx \end{aligned}$$

Use the Taylor series

$$f(x) = f(x_{k-1/2}) + f'(x_{k-1/2})(x - x_{k-1/2}) + \frac{1}{2} f''(\xi)(x - x_{k-1/2})^2$$

$\xi \in [x_{k-1}, x_k]$

Rate of convergence: mid-point rectangles

$$R_k = f'(x_{k-1/2}) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})\, dx \quad + \frac{1}{2} f''(\xi) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})^2\, dx$$

Rate of convergence: mid-point rectangles

$$
\begin{aligned}
R_k &= f'(x_{k-1/2}) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})\, dx &&+ \frac{1}{2} f''(\xi) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})^2\, dx \\
&= f'(x_{k-1/2}) \int_{-h/2}^{h/2} y\, dy &&+ \frac{1}{2} f''(\xi) \int_{-h/2}^{h/2} y^2\, dy
\end{aligned}
$$

Rate of convergence: mid-point rectangles

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\begin{aligned}
R_k &= f'(x_{k-1/2}) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})\, dx \quad &&+ \frac{1}{2} f''(\xi) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})^2\, dx \\
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&= && \frac{1}{2} f''(\xi)\, \left. \frac{y^3}{3} \right|_{-h/2}^{h/2}
\end{aligned}
$$

Rate of convergence: mid-point rectangles

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R_k &= f'(x_{k-1/2}) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})\, dx && + \frac{1}{2} f''(\xi) \int_{x_{k-1}}^{x_k} (x - x_{k-1/2})^2\, dx \\
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&= && \frac{1}{2} f''(\xi) \left. \frac{y^3}{3} \right|_{-h/2}^{h/2} \\
&= && \frac{1}{24} f''(\xi) h^3
\end{aligned}$$

Rate of convergence: mid-point rectangles

Let

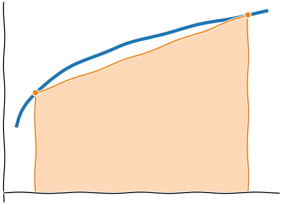
$$M_2 = \max_{x\in[a,b]} |f''(x)|$$

Then the residual

$$\begin{aligned}\left|R^{(N)}\right| = \left|\sum_{k=1}^{N} R_k\right| &\leqslant \frac{1}{24}M_2 h^3 N \qquad\qquad h_k = h = \text{const} \\ &= \frac{1}{24}M_2 (b-a) h^2 \qquad\qquad hN = b-a\end{aligned}$$

Simple geometric quadratures

Trapezoid rule



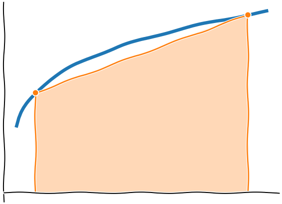
The elementary rule

$$Q_k = \frac{h}{2}\left(f_{k-1} + f_k\right)$$

The composite rule:

$$Q^{(N)} = \sum_{k=1}^{N} Q_k = \left(\frac{1}{2} f_0 + f_1 + \cdots + f_{N-1} + \frac{1}{2} f_N\right) h$$

Trapezoid rule



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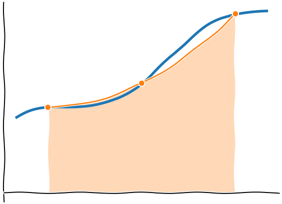
The error bound:

$$\left| R^{(N)} \right| \leqslant \frac{1}{12} M_2 (b-a) h^2$$

Simpson's rule



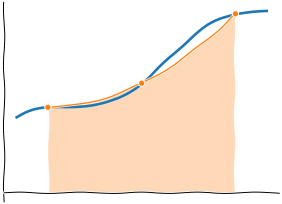
The elementary rule

$$Q_k = \frac{h}{6}\left(f_{k-1} + 4f_{k-1/2} + f_k\right)$$

The composite rule:

$$Q^{(N)} = (f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + f_N)\,\frac{h}{3}$$

Simpson's rule



The elementary rule

$$Q_k = \frac{h}{6}\left(f_{k-1} + 4f_{k-1/2} + f_k\right)$$

The composite rule:

$$Q^{(N)} = (f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + f_N)\,\frac{h}{3}$$

The error bound:

$$\left|R^{(N)}\right| \leqslant \frac{1}{2880} M_4 (b-a) h^4$$

Error bounds for quadratures

Practical matters

Error bounds

Have *a priori* error bounds. E.g., for midpoint rectangles

$$\left|R^{(N)}\right| \propto 1/N^2$$

A posteriori error bounds?

Error bounds

Have *a priori* error bounds. E.g., for midpoint rectangles

$$\left|R^{(N)}\right| \propto 1/N^2$$

A posteriori error bounds?

Compute $Q^{(N)}$ and $Q^{(2N)}$, check

$$\left|Q^{(2N)} - Q^{(N)}\right| < \epsilon$$

Romberg method

Consider the midpoint rule:

$$Q^{(N)} = I + \gamma N^{-2} + \cdots$$

Then an improved estimate

$$I_1 = \frac{4Q^{(2N)} - Q^{(N)}}{4 - 1}$$

c.f. Richardson extrapolation.

Integrals with singularities

Does this integral exist?

Before doing anything numerically, need to check if an integral exists.

$$\int_0^1 \frac{1}{\sin x}\, dx$$

Integrable singularities

$$\int_0^1 \frac{1}{\sin\sqrt{x}}\,dx$$

Integrable singularities

$$\int_0^1 \frac{1}{\sin\sqrt{x}}\,dx$$

- Change variables
- Subtract the singularity

Integrable singularities

Add and subtract the singular part:

$$
\begin{aligned}
I &= \int_0^1 \frac{1}{\sin\sqrt{x}}\,dx \\
&= \int_0^1 \left(\frac{1}{\sin\sqrt{x}} - \frac{1}{\sqrt{x}} + \frac{1}{\sqrt{x}} \right)\,dx
\end{aligned}
$$