Numerical Integration

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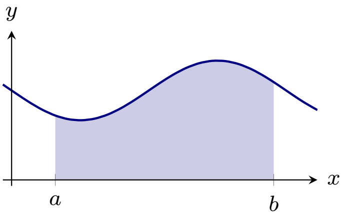
Introduction

Quadrature Problem

Consider the definite integral

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

which represents the *net area* of the region between the curve $y = f(x)$ and the x-axis on $[a, b]$.



We seek to approximate it numerically by a weighted sum

$$I\{f\} \approx \sum_{i=1}^{n} \omega_i f(x_i).$$

- ω_i's are called the *weights*;
- x_i's are called the *nodes* for the particular numerical method used.

Some Questions

Q1. Why do we care?

- An exact antiderivative of f is not accessible
- f may be known at limited points

Q2. How do we do?

- Replace $f(x)$ by an approximate function $p(x)$ and integrate it instead.

Q3. What are good candidates for $p(x)$?

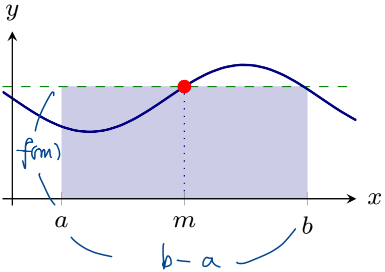
- In choosing $p(x)$, we require that (a) $f(x) - p(x)$ is not too large and (b) $p(x)$ can be exactly integrated (by hand).
  - (piecewise) constant $\longrightarrow$ (composite) midpoint rule
  - (piecewise) linear $\longrightarrow$ (composite) trapezoidal rule
  - (piecewise) quadratic $\longrightarrow$ (composite) Simpson's rule

Newton-Cotes Formulas

Newton-Cotes methods are a collection of numerical integration methods in which nodes are equally spaced in $[a, b]$. Let $m = (a + b)/2$.

- **Midpoint Method:**

$$I^{[\mathrm{m}]}\{f\} = f(m)(b - a)$$



Midpoint method: one node

Newton-Cotes Formulas

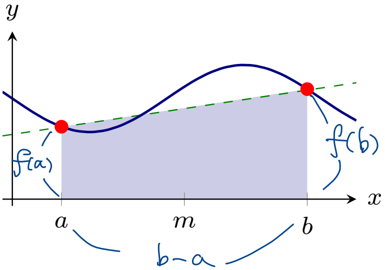
Newton-Cotes methods are a collection of numerical integration methods in which nodes are equally spaced in $[a, b]$. Let $m = (a + b)/2$.

- **Midpoint Method:**

$$I^{[\mathrm{m}]}\{f\} = f(m)(b - a)$$

- **Trapezoidal Method:**

$$I^{[\mathrm{t}]}\{f\} = \frac{1}{2}\left(f(a) + f(b)\right)(b - a)$$



Trapezoid method: two nodes

Newton-Cotes Formulas

Newton-Cotes methods are a collection of numerical integration methods in which nodes are equally spaced in $[a, b]$. Let $m = (a + b)/2$.

- **Midpoint Method:**

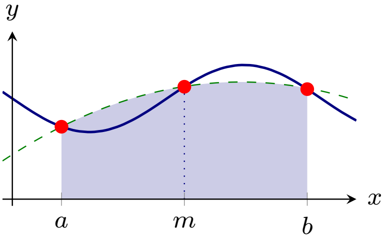
$$I^{[\mathrm{m}]}\{f\} = f(m)(b - a)$$

- **Trapezoidal Method:**

$$I^{[\mathrm{t}]}\{f\} = \frac{1}{2}\big(f(a) + f(b)\big)(b - a)$$

- **Simpson's Method:**

$$I^{[\mathrm{s}]}\{f\} = \frac{1}{6}\big(f(a) + 4f(m) + f(b)\big)(b-a)$$



Simpson's method: three node

Convergence of Midpoint and Trapezoidal Methods

Both of $I^{[\mathrm{m}]}\{f\}$ and $I^{[\mathrm{t}]}\{f\}$ are **third-order** accurate:

$$I^{[\mathrm{m}]}\{f\} - I\{f\} = \underbrace{-\frac{1}{24} f''(m)(b-a)^3}_{\text{leading error}} - \frac{1}{1920} f^{(4)}(m)(b-a)^5 + O\left((b-a)^7\right),$$

$$I^{[\mathrm{t}]}\{f\} - I\{f\} = \underbrace{\frac{1}{12} f''(m)(b-a)^3}_{\text{leading error}} + \frac{1}{480} f^{(4)}(m)(b-a)^5 + O\left((b-a)^7\right).$$

Convergence of Simpson's Methods

The Simpson's method is **fifth-order** accurate:

$$I^{[\mathrm{s}]}\{f\} - I\{f\} = \underbrace{\frac{1}{2880} f^{(4)}(m)(b-a)^5}_{\text{leading error}} + O\left((b-a)^7\right),$$

Derivation of Simpson's Method via Extrapolation

The Simpson's method can be derived by forming a suitable linear combination of two 3rd-order accurate methods, $I^{[\mathrm{m}]}\{f\}$ and $I^{[\mathrm{t}]}\{f\}$:

We know that

$$\begin{aligned} I^{[\mathrm{m}]}\{f\} &= I\{f\} - \frac{1}{24} f''(m)(b-a)^3 - \frac{1}{1920} f^{(4)}(m)(b-a)^5 + O\left((b-a)^7\right), \\ I^{[\mathrm{t}]}\{f\} &= I\{f\} + \frac{1}{12} f''(m)(b-a)^3 + \frac{1}{480} f^{(4)}(m)(b-a)^5 + O\left((b-a)^7\right). \end{aligned}$$

It follows that

$$\underbrace{\frac{2}{3} I^{[\mathrm{m}]}\{f\} + \frac{1}{3} I^{[\mathrm{t}]}\{f\}} = I\{f\} + \frac{1}{2880} f^{(4)}(m)(b-a)^5 + O\left((b-a)^7\right).$$

The underbraced left-hand side is the Simpson's method. (Confirm it.)

Composite Methods

Composite Trapezoidal and Midpoint Methods

For better accuracy, we can subdivide the interval $[a, b]$ into equispaced subintervals

$$a = x_1 < x_2 < \cdots < x_n = b \quad \text{with } x_i = a + (i-1)h \text{ and } h = \frac{b-a}{n-1}.$$

- **Composite Midpoint Method**:

$$I_h^{[\mathrm{m}]}\{f\} = \sum_{i=1}^{n-1} f(x_{i+1/2})h,$$

  where $x_{i+1/2} = (x_i + x_{i+1})/2$.

- **Composite Trapezoidal Method**:

$$I_h^{[\mathrm{t}]}\{f\} = \sum_{i=1}^{n-1} \frac{1}{2}\left(f(x_i) + f(x_{i+1})\right) h = \frac{1}{2}\left(f(x_1) + f(x_n)\right) h + \sum_{i=2}^{n-1} f(x_i)h.$$

Composite Simpson's Methods

- **Composite Simpson's Method:**

$$I_h^{[\mathrm{s}]}\{f\} = \sum_{i=1}^{n-1} \frac{1}{6} \Big(f(x_i) + 4f(x_{i+1/2}) + f(x_{i+1}) \Big)\, h.$$

Convergence of Composite Methods

The composite midpoint and trapezoidal methods are **second-order** accurate while the composite Simpson's method is **fourth-order** accurate:

$$
\begin{aligned}
I_h^{[\mathrm{m}]}\{f\} - I\{f\} &= -\frac{f''(\xi_m)}{24}(b-a)h^2, \\
I_h^{[\mathrm{t}]}\{f\} - I\{f\} &= \frac{f''(\xi_t)}{12}(b-a)h^2, \\
I_h^{[\mathrm{s}]}\{f\} - I\{f\} &= -\frac{f^{(4)}(\xi_s)}{2880}(b-a)h^4.
\end{aligned}
$$