Numerical Methods :: Numerical integration

Numerical integration

The goal of numerical integration is to obtain approximate values of the definite integral

$$I = \int_a^b f(x)\,\mathrm{d}x.$$

Numerical integration is needed when:

- It is impossible to calculate the integral analytically. For example, try evaluating

$$I = \int_0^2 \exp(\sin x)\,\mathrm{d}x.$$

- The function is given empirically as a table of values.

Numerical integration

One way to derive numerical integration formulae is to approximate the function $f(x)$ using an interpolant, and then integrate the interpolant.

This is accomplished by sampling the function on a discrete set of points, and finding the interpolant that passes through those points. Piecewise polynomials are ideal for this — they are easily integrated!

Midpoint rule

Example 1.1

Consider the integral

$$I = \int_0^{\pi} \sin x \, \mathrm{d}x = 2.$$

Approximate $f(x) = \sin x$ using piecewise constant interpolation through three equispaced data points. We have

$$y(x) = \begin{cases} \frac{1}{2}, & 0 \leq x \leq \frac{\pi}{3}, \\ 1, & \frac{\pi}{3} \leq x \leq \frac{2\pi}{3}, \\ \frac{1}{2}, & \frac{2\pi}{3} \leq x \leq \pi. \end{cases}$$

The area under the interpolant is $I \approx \frac{2\pi}{3} = 2.0944$.

Midpoint rule

More generally, divide the interval $[a, b]$ into n equispaced subintervals of width $h = (b - a)/n$. Let $f_j = f(x_j)$, where x_j is the midpoint of the j-th interval and use piecewise constant interpolation.

The integral over the j-th subinterval is

$$\int_{x_j - \frac{h}{2}}^{x_j + \frac{h}{2}} f(x)\,\mathrm{d}x \approx \int_{x_j - \frac{h}{2}}^{x_j + \frac{h}{2}} f_j\,\mathrm{d}x = hf_j,$$

hence the total integral is

$$\int_a^b f(x)\,\mathrm{d}x = \sum_{j=1}^{n} \int_{x_j - \frac{h}{2}}^{x_j + \frac{h}{2}} f(x)\,\mathrm{d}x \approx h \sum_{j=1}^{n} f_j.$$

Midpoint rule

Example 1.2

Evaluate

$$I = \int_0^{\pi} \sin x \, \mathrm{d}x = 2$$

using the midpoint rule.

```
n     I       error
------------------
 3 2.0944 0.094395
 6 2.0230 0.023030
12 2.0057 0.005723
24 2.0014 0.001429
48 2.0004 0.000357
------------------
```

Midpoint rule

Theorem 1.3

For a smooth function $f(x)$ with bounded second derivative $|f''(x)| < M$ for $a \leq x \leq b$, the error of the midpoint integration rule is

$$|\varepsilon_{mid}| \leq \frac{1}{24}(b-a)Mh^2,$$

where h is the grid spacing.

Proof.

We will establish this result using Taylor's theorem. $\square$

Taylor's theorem

Theorem 1.4

If a function $f(x)$ *has* $(n+1)$ *derivatives in the neighbourhood of a point* $x = a$*, then*

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots \\ + \frac{f^{(n)}}{n!}(x-a)^n + \underbrace{\frac{f^{(n+1)}(t)}{(n+1)!}(x-a)^{n+1}}_{\textit{remainder}},$$

for some t *between* a *and* x.

Error scaling

Definition 1.5

For any quantity q (such as the error) and any parameter h (such as the size of the subintervals) we write "q is of the order h^p" as

$$q = O(h^p) \text{ as } h \to 0,$$

which means that

$$\lim_{h \to 0} \frac{q}{h^p} = C$$

for some finite constant C.

Example 1.6

For midpoint integration, $|\varepsilon_{\text{mid}}| = O(h^2)$ as $h \to 0$.

Trapezoidal rule

Divide the interval $[a, b]$ into $(n-1)$ equispaced subintervals of width $h = (b-a)/(n-1)$. Let $f_j = f(x_j)$, where $x_j = a + (j-1)h$ for $j = 1, \ldots, n$, and use piecewise linear interpolation.

The integral over the j-th subinterval is

$$\int_{x_j}^{x_{j+1}} f(x)\,\mathrm{d}x \approx \int_{x_j}^{x_{j+1}} f_j \frac{x - x_{j+1}}{x_j - x_{j+1}} + f_{j+1} \frac{x - x_j}{x_{j+1} - x_j}\,\mathrm{d}x$$
$$= \frac{h}{2}(f_j + f_{j+1}),$$

hence the total integral is

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{j=1}^{n-1} \frac{1}{2} h(f_j + f_{j+1}) = h\left(\frac{f_1}{2} + \sum_{j=2}^{n-1} f_j + \frac{f_n}{2}\right).$$

Trapezoidal rule

Theorem 1.7

For a smooth function $f(x)$ with bounded second derivative $|f''(x)| < M$ for $a \leq x \leq b$, the error of the trapezoidal integration rule is

$$|\varepsilon_{trap}| \leq \frac{1}{12}(b-a)Mh^2,$$

where h is the grid spacing.

Proof.

We will establish this result using the polynomial interpolation error theorem. □

Simpson's rule

Divide the interval $[a, b]$ into $(n-1)$ equispaced subintervals of width $h = (b-a)/(n-1)$, where n is odd. Let $f_j = f(x_j)$, where $x_j = a + (j-1)h$ for $j = 1, \ldots, n$, and consider the area under the piecewise quadratic interpolant.

The integral over each piecewise quadratic is

$$\int_{x_{j-1}}^{x_{j+1}} f(x)\,\mathrm{d}x \approx \frac{h}{3}(f_{j-1} + 4f_j + f_{j+1}).$$

Simpson's rule

The total integral is

$$\int_a^b f(x)\,\mathrm{d}x = \sum_{\substack{j=2\\ j\text{ even}}}^{n-1} \int_{x_{j-1}}^{x_{j+1}} f(x)\,\mathrm{d}x$$

$$\approx \frac{h}{3} \sum_{\substack{j=2\\ j\text{ even}}}^{n-1} f_{j-1} + 4f_j + f_{j+1}$$

$$= \frac{h}{3}\left(f_1 + 4 \sum_{\substack{j=2\\ j\text{ even}}}^{n-1} f_j + 2 \sum_{\substack{j=3\\ j\text{ odd}}}^{n-2} f_j + f_n \right)$$

Simpson's rule

Theorem 1.8

For a smooth function $f(x)$ *with bounded fourth derivative* $|f^{(iv)}(x)| < M$ *for* $a \le x \le b$*, the error of Simpson's integration rule is*

$$|\varepsilon_{Simp}| \le \frac{1}{180}(b-a)Mh^4,$$

where h *is the grid spacing.*

Proof.

If we use the same approach as used for the trapezoidal rule, we obtain the weaker result $|\varepsilon_{\mathrm{Simp}}| \le \frac{1}{24}(b-a)Nh^3$, where $|f'''(x)| < N$. □

Numerical Methods :: Numerical differentiation

Numerical differentiation

The goal of numerical differentiation is to obtain approximate values of the derivatives $f'(x), f''(x), \ldots, f^{(n)}(x)$ of a given function $f(x)$.

Numerical derivatives are needed when:

- the function is given empirically as a table of values.
- numerically solving ordinary and partial differential equations.

Numerical differentiation

One way to derive numerical differentiation formulae is to approximate the function $f(x)$ using an interpolant, and then differentiate the interpolant.

As with integration, this is facilitated by sampling the function on a discrete set of points (or grid), and finding the interpolant that passes through those points.

Taylor series can also be used to derive and analyse numerical differentiation formulae.

Differentiation using linear interpolation

Example 1.9

Let $f_j = f(x_j)$. Find the linear polynomial that passes through (x_j, f_j) and (x_{j+1}, f_{j+1}) and differentiate it to obtain an approximation of $f'(x)$.

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The linear polynomial is

$$p_1(x) = f_j \frac{x - x_{j+1}}{x_j - x_{j+1}} + f_{j+1} \frac{x - x_j}{x_{j+1} - x_j}.$$

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$$p_1(x) = f_j \frac{x - x_{j+1}}{x_j - x_{j+1}} + f_{j+1} \frac{x - x_j}{x_{j+1} - x_j}.$$

The derivative is

$$f'(x) \approx p_1'(x) = \frac{f_{j+1} - f_j}{x_{j+1} - x_j}, \quad x_j \leq x \leq x_{j+1}.$$

Error analysis

Example 1.10

What is the error of the first-derivative approximation for $f'_j = f'(x_j)$ and $f'_{j+1} = f'(x_{j+1})$ from example 1.9.

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The error is

$$\varepsilon(x) = f'(x) - p'_1(x) = \epsilon'_1(x),$$

where $\epsilon_1(x)$ is the error given by the polynomial interpolation error theorem.

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What is the error of the first-derivative approximation for $f'_j = f'(x_j)$ and $f'_{j+1} = f'(x_{j+1})$ from example 1.9.

The error is

$$\varepsilon(x) = f'(x) - p'_1(x) = \epsilon'_1(x),$$

where $\epsilon_1(x)$ is the error given by the polynomial interpolation error theorem. The error at the grid points is

$$|\varepsilon(x_j)|, |\varepsilon(x_{j+1})| = \frac{1}{2}|f''(t)|h \leq \frac{1}{2}Mh = O(h) \text{ as } h \to 0,$$

where $h = x_{j+1} - x_j$ and $|f''(t)| \leq M$.

Differentiation using Taylor's theorem

Example 1.11

Let $f_j = f(x_j)$, where x_j are equally spaced with grid spacing h. Use Taylor's theorem to find an expression for $f'_j = f'(x_j)$ in terms of discrete data (x_{j-1}, f_{j-1}) (x_j, f_j) and (x_{j+1}, f_{j+1}).

Differentiation using Taylor's theorem

Example 1.11

Let $f_j = f(x_j)$, where x_j are equally spaced with grid spacing h. Use Taylor's theorem to find an expression for $f'_j = f'(x_j)$ in terms of discrete data (x_{j-1}, f_{j-1}) (x_j, f_j) and (x_{j+1}, f_{j+1}).

Neglecting terms of $O(h^2)$, the approximate derivative is

$$f'_j \approx \frac{f_{j+1} - f_{j-1}}{2h}$$

Error analysis

Example 1.12

What is the error of the approximate derivative in example 1.11?

Error analysis

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The error is

$$\varepsilon_j = f'_j - \frac{f_{j+1} - f_{j-1}}{2h}$$

Error analysis

Example 1.12

What is the error of the approximate derivative in example 1.11?

The error is

$$\varepsilon_j = f'_j - \frac{f_{j+1} - f_{j-1}}{2h}$$

Using Taylor's theorem, the error is

$$|\varepsilon_j| = \frac{1}{6}|f'''(v)|h^2 \leq \frac{1}{6}Mh^2 = O(h^2) \text{ as } h \to 0,$$

where $h = x_{j+1} - x_j$ and $|f'''(v)| \leq M$.

Differentiation using quadratic interpolation

Example 1.13

Let $f_j = f(x_j)$, where x_j are equally spaced with constant grid spacing h. Find the quadratic polynomial that passes through (x_{j-1}, f_{j-1}), (x_j, f_j) and (x_{j+1}, f_{j+1}) and differentiate it to obtain approximations for $f'(x)$ and $f''(x)$.

Differentiation using quadratic interpolation

Example 1.13

Let $f_j = f(x_j)$, where x_j are equally spaced with constant grid spacing h. Find the quadratic polynomial that passes through (x_{j-1}, f_{j-1}), (x_j, f_j) and (x_{j+1}, f_{j+1}) and differentiate it to obtain approximations for $f'(x)$ and $f''(x)$.

The derivatives are

$$\begin{aligned} f'(x) \approx p_2'(x) = {} & f_{j-1}\frac{2x - x_j - x_{j+1}}{2h^2} \\ & - f_j\frac{2x - x_{j-1} - x_{j+1}}{h^2} + f_{j+1}\frac{2x - x_{j-1} - x_j}{2h^2}. \\ f''(x) \approx p_2''(x) = {} & \frac{f_{j-1} - 2f_j + f_{j+1}}{h^2} \end{aligned}$$

Finite difference formulae

Evaluating the derivative of the quadratic interpolant at the data points yields the finite difference formulae

$$
\begin{aligned}
f'_{j-1} \approx p'_2(x_{j-1}) &= \frac{-f_{j+1} + 4f_j - 3f_{j-1}}{2h} \\
f'_j \approx p'_2(x_j) &= \frac{f_{j+1} - f_{j-1}}{2h} \\
f'_{j+1} \approx p'_2(x_{j+1}) &= \frac{3f_{j+1} - 4f_j + f_{j-1}}{2h} \\
f''_j \approx p''_2(x_j) &= \frac{f_{j-1} - 2f_j + f_{j+1}}{h^2}
\end{aligned}
$$

These formulae can also be derived using Taylor's theorem.