Chapter 5: Numerical Differentiation and Integration

Liangda Fang

Dept. of Computer Science
Jinan University

Motivation

Given a function $f(x)$,

- Differentiation Problem: compute the derivative of $f(x)$ at a value x_0?

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- Differentiation Problem: compute the derivative of $f(x)$ at a value x_0?

- Integration Problem: compute the definite integral of $f(x)$ on an interval $[a, b]$?

Outline

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Finite difference formulas

Definition (Derivative)

The derivative of $f(x)$ at a value x is

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

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Theorem (Taylor's Theorem)

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(c),$$

where $x < c < x + h$.

Two-point forward-difference formula

From Taylor's Theorem, we obtain

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where $x < c < x + h$.

When h is small, we can approximate $f'(x)$ as follows:

$$f'(x) = \frac{f(x+h) - f(x)}{h},$$

where $|\frac{h}{2} f''(c)|$ is the error.

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- Use the two-point difference formula with $h = 0.1$ to approximate the derivative of $f(x) = \frac{1}{x}$ at $x = 2$.

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- The actual error is $|-0.2381-(-0.25)| = 0.0119$.
- The estimation error $\max\{\frac{hf''(c)}{2} \mid 2 \leq c \leq 2.1\}$ where $f''(x) = 2x^{-3}$.
- $\frac{0.1f''(c)}{2} = 0.0125 < 0.0119$ where $c = 2$.

Three-point centered-difference formula

Theorem (Taylor's Theorem)

Suppose that $f(x)$ is 3-times continuously differentiable.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f''(c_1),$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f''(c_2),$$

where $x-h < c_2 < x < c_1 < x+h$.

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Subtracting the above two equations gives the following

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6}f'''(c_1) - \frac{h^2}{6}f'''(c_2).$$

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Could we combine the last two terms into one? Yes!

Generalized intermediate value theorem

Theorem (Generalized intermediate value theorem)

Let f be a continuous function on the interval $[a, b]$.
Let $x_1, \cdots, x_n$ be points in $[a, b]$, and $a_1, \cdots, a_n > 0$.
Then, there exists a number c between a and b s.t.

$$(a_1 + \cdots + a_n)f(c) = a_1 f(x_1) + \cdots a_n f(x_n).$$

Generalized intermediate value theorem

Proof.

Let $f(x_i)$ and $f(x_j)$ be the minimum and maximum of $f(x_1), \cdots, f(x_n)$ respectively.

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It follows that
$a_1 f(x_i) + \cdots + a_n f(x_i) \leq a_1 f(x_1) + \cdots + a_n f(x_n) \leq a_1 f(x_j) + \cdots + a_n f(x_j)$.

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So $f(x_i) \leq \frac{a_1 f(x_1) + \cdots + a_n f(x_n)}{a_1 + \cdots + a_n} \leq f(x_j)$.

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So $f(x_i) \le \frac{a_1 f(x_1) + \cdots + a_n f(x_n)}{a_1 + \cdots + a_n} \le f(x_j)$.
By the Intermediate Value Theorem, there is a number c between x_i and x_j s.t.

$$f(c) = \frac{a_1 f(x_1) + \cdots + a_n f(x_n)}{a_1 + \cdots + a_n}.$$

Moreover, $a < c < b$.

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- Use the three-point centered difference formula with $h = 0.1$ to approximate the derivative of $f(x) = \frac{1}{x}$ at $x = 2$.

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- The actual error is $|-0.2506-(-0.25)| = 0.0006$.
- The estimation error $\max\{\frac{h^2 f'''(c)}{6} \mid 1.9 \leq c \leq 2.1\}$ where $f'''(x) = -6x^{-4}$.
- $\frac{(0.2)^2 f'''(c)}{6} = 0.0031 > 0.0006$ where $c = 1.9$.

Three-point centered-difference formula for second derivative

Theorem (Taylor's Theorem)

Suppose that $f(x)$ is 4-times continuously differentiable.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(c_1),$$

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Combing the last two terms leads to

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- The correct derivative $f''(x) = 2x^{-3} = 0.25$.
- The actual error is $|0.2506 - 0.25| = 0.0006$.
- The estimation error $\max\{\frac{h^2}{12}f^{(4)}(c) \mid 1.9 \le c \le 2.1\}$ where $f^{(4)}(x) = 24x^{-5}$.
- $\frac{(0.2)^2 f^{(iv)}(c)}{12} = 0.0025 > 0.0006$ where $c = 1.9$.

Outline

Extrapolation

Definition

$$Q = F(h) + K_n h^n + K_{n+1} h^{n+1} + \cdots ,$$

where $K_n, K_{n+1}, \cdots$ are constants.
We call $F(h)$ is an order n formula for approximating a given quantity Q.

- The truncation error for $F(h)$ is $O(h^n)$, in general $K_n h^n$, unless $K_{n+1}, K_{n+2}, \cdots$ is very large.
- $Q - F(0.1) \approx 0.1^n \cdot K_n$.
- $Q - F(0.01) \approx 0.01^n \cdot K_n$

Extrapolation

Example

Using Taylor expansion, we obtain that

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + \frac{h^5}{120}f^{(5)}(x) + \cdots,$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) - \frac{h^5}{120}f^{(5)}(x) + \cdots,$$

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Subtracting the two equations, we get that

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Hence, $\frac{f(x+h)-f(x-h)}{2h}$ is an order 2 formula for approximating $f'(x)$.

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Adding the two equations, we get that

$$f'(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{2h} - \frac{h^2}{12} f^{(4)}(x) - \cdots$$

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Extrapolation

- Provide an order $n+1$ formula via approximations with $O(h^n)$ truncation error.

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3. $2^n Q = 2^n F_n(\frac{h}{2}) + K_n h^n + \frac{K_{n+1}}{2} h^{n+1} + \cdots;$

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4. $Q = \frac{2^n F_n(\frac{h}{2}) - F_n(h)}{2^n - 1} - \frac{K_{n+1}}{2^{n+1} - 2} h^{n+1} + \cdots;$

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4. $Q = \frac{2^n F_n(\frac{h}{2}) - F_n(h)}{2^n - 1} - \frac{K_{n+1}}{2^{n+1} - 2} h^{n+1} + \cdots;$
5. $F_{n+1}(n) = \frac{2^n F_n(\frac{h}{2}) - F_n(h)}{2^n - 1}$ is an order $n+1$ formula for approximating Q.

Extrapolated formula for the derivative

Example

- $f'(x) = \frac{f(x+h)-f(x-h)}{2h} - \frac{h^2}{6}f'''(x) - \frac{h^4}{120}f^{(5)}(x)$;
- $F_2(x) = \frac{f(x+h)-f(x-h)}{2h}$;
- $F_4(x) = \frac{2^2 F_2(\frac{h}{2})-F_2(h)}{2^2-1} = \frac{f(x-h)-8f(x-\frac{h}{2})+8f(x+\frac{h}{2})-f(x+h)}{6h}$
- $F_4(x)$ is of order 4 since the order 3 error terms cancel out.

Extrapolated formula for the second derivative

Example

- $f''(x) = \frac{f(x+h)-2f(x)+f(x-h)}{2h} - \frac{h^2}{12} f^{(4)}(x) - \cdots;$
- $F_2(x) = \frac{f(x+h)-2f(x)+f(x-h)}{2h};$
- $F_4(x) = \frac{2^2 F_2(\frac{h}{2}) - F_2(h)}{2^2-1} = \frac{-f(x-h)+16f(x-\frac{h}{2})-30f(x)+16f(x+\frac{h}{2})-f(x+h)}{3h^2}$
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Outline

Trapezoid rule

- f: a function with a continuous second derivative on $[x_0, x_1]$.
- $y_0 = f(x_0)$ and $y_1 = f(x_1)$.

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- $f(x) = y_0 \frac{x-x_1}{x_0-x_1} + y_1 \frac{x-x_0}{x_1-x_0} + \frac{(x-x_0)(x-x_1)}{2!} f''(c) = P(x) + E(x)$
- $P(x)$: the Lagrange interpolating polynomial $y_0 \frac{x-x_1}{x_0-x_1} + y_1 \frac{x-x_0}{x_1-x_0}$;
- $E(x)$: the error formula $\frac{(x-x_0)(x-x_1)}{2!} f''(c)$ where $x_0 \le c \le x_1$.

Trapezoid rule

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- $\int_{x_0}^{x_1} f(x)\,dx = \int_{x_0}^{x_1} P(x)\,dx + \int_{x_0}^{x_1} E(x)\,dx$.

Trapezoid rule

$$\int_{x_0}^{x_1} P(x)\,dx = \int_{x_0}^{x_1} y_0 \frac{x - x_1}{x_0 - x_1}\,dx + \int_{x_0}^{x_1} y_1 \frac{x - x_0}{x_1 - x_0}\,dx$$

Trapezoid rule

$$\begin{aligned}\int_{x_0}^{x_1} P(x)\,dx &= \int_{x_0}^{x_1} y_0 \frac{x-x_1}{x_0-x_1}\,dx + \int_{x_0}^{x_1} y_1 \frac{x-x_0}{x_1-x_0}\,dx \\ &= y_0\frac{h}{2} + y_1\frac{h}{2} \qquad (h = x_1 - x_0)\end{aligned}$$

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Trapezoid rule

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$$\int_{x_0}^{x_1} E(x)\,dx = \frac{1}{2!}\int_{x_0}^{x_1} (x-x_0)(x-x_1)f''(c)\,dx$$

Trapezoid rule

$$\begin{aligned}
\int_{x_0}^{x_1} P(x)\,dx &= \int_{x_0}^{x_1} y_0 \frac{x-x_1}{x_0-x_1}\,dx + \int_{x_0}^{x_1} y_1 \frac{x-x_0}{x_1-x_0}\,dx \\
&= y_0 \frac{h}{2} + y_1 \frac{h}{2} \qquad (h = x_1 - x_0) \\
&= h \frac{y_0 + y_1}{2}
\end{aligned}$$

$$\begin{aligned}
\int_{x_0}^{x_1} E(x)\,dx &= \frac{1}{2!} \int_{x_0}^{x_1} (x-x_0)(x-x_1) f''(c)\,dx \\
&= \frac{f''(c)}{2} \int_{x_0}^{x_1} (x-x_0)(x-x_1)\,dx
\end{aligned}$$

Trapezoid rule

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$$\begin{aligned}\int_{x_0}^{x_1} E(x)\,dx &= \frac{1}{2!}\int_{x_0}^{x_1}(x-x_0)(x-x_1)f''(c)\,dx \\ &= \frac{f''(c)}{2}\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx \\ &= \frac{f''(c)}{2}\int_0^h u(u-h)\,du \qquad (h = x_1 - x_0 \text{ and } u = x - x_0)\end{aligned}$$

Trapezoid rule

$$
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\int_{x_0}^{x_1} P(x)\,dx &= \int_{x_0}^{x_1} y_0 \frac{x-x_1}{x_0-x_1}\,dx + \int_{x_0}^{x_1} y_1 \frac{x-x_0}{x_1-x_0}\,dx \\
&= y_0 \frac{h}{2} + y_1 \frac{h}{2} \qquad (h = x_1 - x_0) \\
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$$

$$
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\int_{x_0}^{x_1} E(x)\,dx &= \frac{1}{2!} \int_{x_0}^{x_1} (x-x_0)(x-x_1) f''(c)\,dx \\
&= \frac{f''(c)}{2} \int_{x_0}^{x_1} (x-x_0)(x-x_1)\,dx \\
&= \frac{f''(c)}{2} \int_{0}^{h} u(u-h)\,du \qquad (h = x_1 - x_0 \text{ and } u = x - x_0) \\
&= -\frac{h^3}{12} f''(c)
\end{aligned}
$$

Trapezoid rule

Definition (Trapezoid rule)

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}(y_0 + y_1) - \frac{h^3}{12} f''(c)$$

where $h = x_1 - x_0$ and $x_0 \leq c \leq x_1$.

Outline

Simpson's rule

- f: a function with a continuous fourth derivative on $[x_0, x_1]$.
- $y_0 = f(x_0)$ and $y_1 = f(x_1)$.

Simpson's rule

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- $y_0 = f(x_0)$ and $y_1 = f(x_1)$.
- $f(x) = y_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + y_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + y_2 \frac{(x-x_0)(x-x_1}{(x_2-x_0)(x_0-x_1)} + \frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f'''(c)$.
- $P(x)$: $y_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + y_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + y_2 \frac{(x-x_0)(x-x_1}{(x_2-x_0)(x_0-x_1)}$;
- $E(x)$: the error formula $\frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f'''(c)$ where $x_0 \leq c \leq x_2$.

Simpson's rule

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- $P(x)$: $y_0\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + y_1\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + y_2\frac{(x-x_0)(x-x_1}{(x_2-x_0)(x_0-x_1)}$;
- $E(x)$: the error formula $\frac{(x-x_0)(x-x_1)(x-x_2)}{3!}f''(c)$ where $x_0 \le c \le x_2$.
- $\int_{x_0}^{x_1} f(x)\,dx = \int_{x_0}^{x_1} P(x)\,dx + \int_{x_0}^{x_1} E(x)\,dx$.

Simpson's rule

$$\int_{x_0}^{x_2} P(x)\,dx = y_0 \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\,dx + y_1 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\,dx + y_2 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_0-x_1)}\,dx$$

Simpson's rule

$$
\begin{aligned}
\int_{x_0}^{x_2} P(x)\,dx &= y_0\int_{x_0}^{x_2}\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\,dx + y_1\int_{x_0}^{x_2}\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\,dx + \\
&\quad y_2\int_{x_0}^{x_2}\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_0-x_1)}\,dx \\
&= y_0\frac{h}{3} + y_1\frac{4h}{3} + y_2\frac{h}{3} \qquad (h = x_2 - x_1 = x_1 - x_0)
\end{aligned}
$$

$$
\int_{x_0}^{x_2} E(x)\,dx = -\frac{h^5}{90} f^{(iv)}(c)
$$

Simpson's rule

Definition (Simpson's rule)

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}(y_0 + 4y_1 + y_2) - \frac{h^5}{90} f^{(iv)}(c)$$

where $h = x_2 - x_1 = x_1 - x_0$ and $x_0 \leq c \leq x_2$.

Example

Example

Apply the Trapezoid rule and Simpson's rule to approximate $\int_1^2 \ln x dx$, and find an upper bound for the error in your approximations.

- $\int_1^2 \ln x dx = x \ln x|_1^2 - \int_1^2 dx = 2\ln 2 - 1\ln 1 - 1 \approx 0.3863.$

Example

Example (Trapezoid rule)

- $y_0 = 1$ and $y_1 = 2$.
- Approximation:
  $\int_1^2 \ln x dx \approx \frac{h}{2}(y_0 + y_1) = \frac{1}{2}(\ln 1 + \ln 2) = \frac{\ln 2}{2} \approx 0.3466.$
- Error: $-\frac{h^3}{12}f''(c) \leq = \frac{1^3}{12c^2} \leq \frac{1}{2} \approx 0.0834$ $(f''(x) = -\frac{1}{x^2})$.
- $\int_1^2 \ln x dx = 0.3466 \pm 0.0834.$

Example

Example (Simpson's rule)

- $y_0 = 1,\ y_1 = \frac{3}{2}$ and $y_2 = 2$.
- Approximation:
  $\int_1^2 \ln x dx \approx \frac{h}{3}(y_0 + 4y_1 + y_2) = \frac{0.5}{3}(\ln 1 + 4\ln\frac{3}{2}\ln 2) = \frac{\ln 2}{2} \approx 0.3858.$
- Error: $-\frac{h^5}{90}f^{(iv)}(c) \leq \frac{6(0.5)^5}{90c^4} \leq \frac{6(0.5)^5}{90} = \frac{1}{480} \approx 0.0021.$
- $\int_1^2 \ln x dx = 0.3858 \pm 0.0021.$

Outline

Composite Newton-Cotes formulas (Composite Trapezoid Rule)

- f: a function with a continuous second derivative on $[a, b]$.
- evenly spaced grid: $a = x_0 < x_1 < \cdots < x_{m-1} < x_m = b$.
- $y_0 = f(x_0) = f(a)$ and $y_m = f(x_m) = f(b)$.

Composite Trapezoid Rule

Apply the **Trapezoid Rule** separately on each subinterval $[x_i, x_{i+1}]$:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{h}{2}(f(x_i) + f(x_{i+1})) - \frac{h^3}{12}f''(c_i),$$

where $h = x_{i+1} - x_i$ and $x_i \leq c_i \leq x_{i+1}$.

Composite Trapezoid Rule

Apply the **Trapezoid Rule** separately on each subinterval $[x_i, x_{i+1}]$:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{h}{2}(f(x_i) + f(x_{i+1})) - \frac{h^3}{12}f''(c_i),$$

where $h = x_{i+1} - x_i$ and $x_i \le c_i \le x_{i+1}$.

Total up over all subintervals:

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{i=0}^{m-1} \int_{x_i}^{x_{i+1}} f(x)\,dx \\ &= \frac{h}{2}[f(a) + f(b) + 2\sum_{i=1}^{m-1} f(x_i)] - \sum_{i=0}^{m-1} \frac{h^3}{12}f''(c_i).\end{aligned}$$

Composite Trapezoid Rule

Apply the **Trapezoid Rule** separately on each subinterval $[x_i, x_{i+1}]$:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{h}{2}(f(x_i) + f(x_{i+1})) - \frac{h^3}{12}f''(c_i),$$

where $h = x_{i+1} - x_i$ and $x_i \le c_i \le x_{i+1}$.

Total up over all subintervals:

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{i=0}^{m-1}\int_{x_i}^{x_{i+1}} f(x)\,dx \\ &= \frac{h}{2}[f(a) + f(b) + 2\sum_{i=1}^{m-1} f(x_i)] - \sum_{i=0}^{m-1}\frac{h^3}{12}f''(c_i).\end{aligned}$$

According to **Generalized Intermediate Value Theorem**, the error term can be written:

$$\sum_{i=0}^{m-1}\frac{h^3}{12}f''(c_i) = \frac{h^3}{12}mf''(c), \text{ where } a < c < b.$$

Composite Trapezoid Rule

Definition (Composite Trapezoid Rule)

$$\int_a^b f(x)\,dx = \frac{h}{2}\left(y_0 + y_m + 2\sum_{i=1}^{m-1} y_i\right) - \frac{(b-a)h^2}{12} f''(c)$$

where $h = (b-a)/m$ and $a \le c \le b$.

Composite Newton-Cotes formulas (Composite Simpson's Rule)

- f: a function with a continuous fourth derivative on $[a, b]$.
- evenly spaced grid: $a = x_0 < x_1 < \cdots < x_{2m-1} < x_{2m} = b$.
- $y_0 = f(x_0) = f(a)$ and $y_{2m} = f(x_{2m}) = f(b)$.

Composite Simpson's Rule

Apply the **Simpson's Rule** separately on each subinterval $[x_{2i}, x_{2i+2}]$:

$$\int_{x_{2i}}^{x_{2i+2}} f(x)\,dx = \frac{h}{3}[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})] - \frac{h^5}{90}f^{(iv)}(c_i),$$

where $h = x_{i+1} - x_i$ and $x_{2i} \leq c_i \leq x_{2i+2}$.

Composite Simpson's Rule

Apply the **Simpson's Rule** separately on each subinterval $[x_{2i}, x_{2i+2}]$:

$$\int_{x_{2i}}^{x_{2i+2}} f(x)\,dx = \frac{h}{3}[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})] - \frac{h^5}{90}f^{(iv)}(c_i),$$

where $h = x_{i+1} - x_i$ and $x_{2i} \le c_i \le x_{2i+2}$.

Total up over all subintervals:

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{i=0}^{m-1} \int_{x_{2i}}^{x_{2i+2}} f(x)\,dx \\ &= \frac{h}{3}[f(a) + f(b) + 4\sum_{i=1}^{m} f(x_{2i-1}) + 2\sum_{i=1}^{m-1} f(x_{2i})] - \sum_{i=0}^{m-1} \frac{h^5}{90} f^{(iv)}(c_i)\end{aligned}$$

According to **Generalized Intermediate Value Theorem**, the error term can be written:

$$\sum_{i=0}^{m-1} \frac{h^5}{90} f^{(iv)}(c_i) = \frac{h^5}{90} m f^{(iv)}(c),$$ where $a < c < b$.

Composite Simpson's Rule

Definition (Composite Simpson's Rule)

$$\int_a^b f(x)\,dx = \frac{h}{3}[y_0 + y_{2m} + 4\sum_{i=1}^{m} y_{2i-1} + 2\sum_{i=1}^{m-1} y_{2i}] - \frac{(b-a)h^4}{180} f^{(iv)}(c)$$

where $h = (b-a)/2m$ and $a \le c \le b$.

Composite Newton-Cotes formulas (Example)

Example

Carry out **four-panel** approximations of $\int_1^2 \ln x dx$ using the composite Trapezoid Rule and composite Simpson's Rule.

- $\int_1^2 \ln x dx = x \ln x|_1^2 - \int_1^2 dx = 2\ln 2 - 1\ln 1 - 1 \approx 0.3863.$

Example

Example (composite Trapezoid rule)

- $h = 1/4,\ y_0 = \ln 1,\ y_1 = \ln\frac{5}{4},\ y_2 = \ln\frac{3}{2},\ y_3 = \ln\frac{7}{4}$ and $y_4 = \ln 2$.
- Approximation: $\int_1^2 \ln x dx \approx \frac{h}{2}(y_0 + y_4 + 2\sum_{i=1}^{3} y_i) =$ $\frac{1}{8}[\ln 1 + \ln 2 + 2(\ln\frac{5}{4} + \ln\frac{3}{2} + \ln\frac{7}{4})] \approx 0.3837.$
- Error: $-\frac{(b-a)h^2}{12} f''(c) \le \frac{1/16}{12c^2} \le \frac{1}{(16)(12)(1^2)} \approx 0.0052.$ $(f''(x) = -\frac{1}{x^2})$
- $\int_1^2 \ln x dx = 0.3837 \pm 0.0052.$

Example

Example (composite Simpson's rule)

- $h = 1/8,\ y_0 = \ln 1,\ y_1 = \ln\frac{9}{8},\ y_2 = \ln\frac{5}{4},\ y_3 = \ln\frac{11}{8},\ y_4 = \ln\frac{6}{4},$ $y_5 = \ln\frac{13}{8},\ y_6 = \ln\frac{7}{4},\ y_7 = \ln\frac{15}{8}$ and $y_8 = \ln 2$.
- Approximation:
  $\int_1^2 \ln x dx \approx \frac{1/8}{3}[y_0 + y_8 + 4\sum_{i=1}^{8} y_{2i-1} + 2\sum_{i=1}^{7} y_{2i}] = \frac{1}{24}[\ln 1 + \ln 2 + 4(\ln\frac{9}{8} + \ln\frac{11}{8} + \ln\frac{13}{8} + \ln\frac{15}{8}) + 2(\ln\frac{5}{4} + \ln\frac{6}{4} + \ln\frac{7}{4})] \approx 0.386292.$
- Error: $-\frac{(b-a)h^4}{180} f^{(iv)}(c) \leq \frac{6}{8^4 \cdot 180 \cdot 1^4} \approx 0.000008.$ $(f^{(iv)}(x) = -\frac{6}{x^4})$
- $\int_1^2 \ln x dx = 0.386292 \pm 0.000008.$

Outline

Open Newton-Cotes Methods (Midpoint Rule)

- f: a function with a continuous second derivative on $[x_0, x_1]$.
- $h = x_1 - x_0$ and $w = x_0 + \frac{h}{2}$.

Open Newton-Cotes Methods (Midpoint Rule)

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The degree 1 Taylor expansion of $f(x)$ about the midpoint w:

$f(x) = f(w) + (x - w)f'(w) + \frac{(x-w)^2}{2}f''(c_x)$, where $x_0 < c_x < x_1$.

Open Newton-Cotes Methods (Midpoint Rule)

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The degree 1 Taylor expansion of $f(x)$ about the midpoint w:
$f(x) = f(w) + (x-w)f'(w) + \frac{(x-w)^2}{2}f''(c_x)$, where $x_0 < c_x < x_1$.

Integrate both sides:

$$\begin{aligned}
\int_{x_0}^{x_1} f(x)\,dx &= hf(w) + f'(w)\int_{x_0}^{x_1}(x-w)\,dx + \frac{1}{2}\int_{x_0}^{x_1} f''(c_x)(x-w)^2\,dx \\
&= hf(w) + 0 + \frac{f''(c)}{2}\int_{x_0}^{x_1}(x-w)^2\,dx \ \textbf{(Mean Value Theorem)} \\
&= hf(w) + \frac{h^3}{24}f''(c) \text{ , where } x_0 < c < x_1
\end{aligned}$$

Midpoint Rule

Definition (Midpoint Rule)

$$\int_{x_0}^{x_1} f(x)\,dx = hf(w) + \frac{h^3}{24} f''(c)$$

where $h = x_1 - x_0$, $w = x_0 + \frac{h}{2}$ and $x_0 < c < x_1$.

- does not use values from the endpoints;
- cut the number of function evaluations needed;
- the error term is half the size of the Trapezoid Rule error term.

Open Newton-Cotes Methods (Composite Midpoint Rule)

- f: a function with a continuous second derivative on $[a, b]$.
- evenly spaced grid: $a = x_0 < x_1 < \cdots < x_{m-1} < x_m = b$.

Open Newton-Cotes Methods (Composite Midpoint Rule)

- f: a function with a continuous second derivative on $[a, b]$.
- evenly spaced grid: $a = x_0 < x_1 < \cdots < x_{m-1} < x_m = b$.

Definition (Composite Midpoint Rule)

$$\int_a^b f(x)\,dx = h\sum_{i=1}^{m} f(w_i) + \frac{(b-a)h^2}{24} f''(c)$$

where $h = (b-a)/m$, $w_i = \frac{(x_{i-1}+x_i)}{2}$ for $1 \le i \le m$ and $a < c < b$.

Open Newton-Cotes Methods (Example)

Example

Approximate $\int_0^1 \frac{\sin x}{x} dx$ by using the Composite Midpoint Rule with $m = 10$ panels.

- The correct answer to eight places of $\int_0^1 \frac{\sin x}{x} dx$ is 0.94608307.
- $h = 0.1, \{w_1, w_2, \ldots, w_{10}\} = \{0.05, 0.15, \ldots, 0.95\}$.
- Approximation: $\int_0^1 \frac{\sin x}{x} dx \approx 0.1 \sum_{i=1}^{10} f(w_i) \approx 0.94620858$.

Outline

Romberg Integration

A method to apply **extrapolation** to the **composite Trapezoid Rule**.

Definition (Extrapolation)

$$M = R(h) + K_n h^n + K_{n+1} h^{n+1} + \cdots ,$$

where $K_n, K_{n+1}, \cdots$ are constants.
We say $R(h)$ is a n**th-order approximation** of a given quantity M.

Romberg Integration

A method to apply **extrapolation** to the **composite Trapezoid Rule**.

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$$M = R(h) + K_n h^n + K_{n+1} h^{n+1} + \cdots ,$$

where $K_n, K_{n+1}, \cdots$ are constants.
We say $R(h)$ is a n**th-order approximation** of a given quantity M.

Definition (Composite Trapezoid Rule)

Let f be an infinitely differentiable function.

$$\int_a^b f(x)\,dx = \frac{h}{2}(y_0 + y_m + 2\sum_{i=1}^{m-1} y_i) + c_2 h^2 + c_4 h^4 + c_6 h^6 + \cdots$$

where $h = (b-a)/m$ and c_i is a constant that depends only on higher derivatives of f at a and b.

Romberg Integration

$$\boxed{\int_a^b f(x)\,dx = \frac{h}{2}\left(y_0 + y_m + 2\sum_{i=1}^{m-1} y_i\right) + c_2 h^2 + c_4 h^4 + c_6 h^6 + \cdots}$$

Example (Single extrapolation)

- $h_1 = b - a$, $h_2 = \frac{h_1}{2}$
- Approximation $R_{11}(h_1)$: $\frac{h_1}{2}[f(a) + f(b)]$
- Approximation $R_{21}(h_2)$: $\frac{h_2}{2}[f(a) + f(b) + 2f(\frac{a+b}{2})]$
- $\int_a^b f(x)\,dx = R_{11}(h_1) + c_2 h_1^2 + O(h_1^4)$
- $\int_a^b f(x)\,dx = R_{21}(h_2) + c_2 h_2^2 + O(h_2^4)$
- Combining the above equations gives the following:
  $\int_a^b f(x)\,dx = \frac{4}{3} R_{21}(h_2) - \frac{1}{3} R_{11}(h_1) + O(h_1^4)$

Romberg Integration

Table: The Romberg Table

Error	$O(h_1^2)$	$O(h_1^4)$	$O(h_1^6)$	$\cdots$	$O(h_1^{2j})$
h_1	R_{11}				
h_2	R_{21}	R_{22}			
h_3	R_{31}	R_{32}	R_{33}		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
h_j	R_{j1}	R_{j2}	R_{j3}	$\cdots$	R_{jj}

- The first column R_{j1} is the approximations using the composite Trapezoid Rule at step size h_j. (2th-order approximations)
- The second column R_{j2} is the extrapolations of the first column R_{j1}. (4th-order approximations)
- Similarly, the k-th column R_{jk} is the extrapolations of the $(k-1)$-th column column $R_{j,k-1}$. ($2k$th-order approximations)
- The best approximation for $\int_a^b f(x)\,dx$ is R_{jj}. ($2j$th-order approximations)

Romberg Integration (calculate composite Trapezoid Rule incrementally)

$$\boxed{\int_a^b f(x)\,dx = \frac{h}{2}\left(y_0 + y_m + 2\sum_{i=1}^{m-1} y_i\right) + c_2h^2 + c_4h^4 + c_6h^6 + \cdots}$$

- $h_j = \frac{(b-a)}{2^{j-1}}$ for $j = 2, 3, \ldots$
- Approximation using h_j : $R_{j1} = \frac{h_j}{2}\left(f(a) + f(b) + 2\sum_{i=1}^{2^{j-1}-1} y_i\right)$.

Romberg Integration (calculate composite Trapezoid Rule incrementally)

$$\boxed{\int_a^b f(x)\,dx = \frac{h}{2}(y_0 + y_m + 2\sum_{i=1}^{m-1} y_i) + c_2h^2 + c_4h^4 + c_6h^6 + \cdots}$$

- $h_j = \frac{(b-a)}{2^{j-1}}$ for $j = 2, 3, \ldots$
- Approximation using h_j : $R_{j1} = \frac{h_j}{2}(f(a) + f(b) + 2\sum_{i=1}^{2^{j-1}-1} y_i)$.

  e.g.

$$\begin{aligned} R_{11} &= \frac{h_1}{2}[f(a) + f(b)], \\ R_{21} &= \frac{h_2}{2}[f(a) + f(b) + 2f(\frac{a+b}{2})] \\ &= \frac{1}{2}R_{11} + h_2 f(\frac{a+b}{2}) \end{aligned}$$

Romberg Integration (calculate composite Trapezoid Rule incrementally)

$$\boxed{\int_a^b f(x)\,dx = \frac{h}{2}(y_0 + y_m + 2\sum_{i=1}^{m-1} y_i) + c_2h^2 + c_4h^4 + c_6h^6 + \cdots}$$

- $h_j = \frac{(b-a)}{2^{j-1}}$ for $j = 2, 3, \ldots$
- Approximation using h_j : $R_{j1} = \frac{h_j}{2}(f(a) + f(b) + 2\sum_{i=1}^{2^{j-1}-1} y_i)$.

  e.g.

$$\begin{aligned} R_{11} &= \frac{h_1}{2}[f(a) + f(b)], \\ R_{21} &= \frac{h_2}{2}[f(a) + f(b) + 2f(\frac{a+b}{2})] \\ &= \frac{1}{2}R_{11} + h_2 f(\frac{a+b}{2}) \end{aligned}$$

It can be written by induction as follows :

$$R_{j1} = \frac{1}{2}R_{j-1,1} + h_j\sum_{i=1}^{2^{j-2}} f(a + (2j-1)h_j)$$

, for each $j = 2, 3, \ldots$.

Romberg Integration (extrapolation)

Error	$O(h_1^2)$	$O(h_1^4)$	$O(h_1^6)$	$\cdots$	$O(h_1^{2j})$
h_1	R_{11}				
h_2	R_{21}	R_{22}			
h_3	R_{31}	R_{32}	R_{33}		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
h_j	R_{j1}	R_{j2}	R_{j3}	$\cdots$	R_{jj}

$$R_{22} = \frac{2^2 R_{21} - R_{11}}{3}, R_{33} = \frac{4^2 R_{32} - R_{22}}{4^2 - 1}, \cdots$$
$$R_{32} = \frac{2^2 R_{31} - R_{21}}{3}, R_{43} = \frac{4^2 R_{42} - R_{32}}{4^2 - 1}, \cdots$$
$$R_{42} = \frac{2^2 R_{41} - R_{31}}{3}, R_{53} = \frac{4^2 R_{52} - R_{42}}{4^2 - 1}, \cdots$$

Romberg Integration (extrapolation)

Error	$O(h_1^2)$	$O(h_1^4)$	$O(h_1^6)$	$\cdots$	$O(h_1^{2j})$
h_1	R_{11}				
h_2	R_{21}	R_{22}			
h_3	R_{31}	R_{32}	R_{33}		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
h_j	R_{j1}	R_{j2}	R_{j3}	$\cdots$	R_{jj}

$$R_{22} = \frac{2^2 R_{21} - R_{11}}{3}, R_{33} = \frac{4^2 R_{32} - R_{22}}{4^2 - 1}, \cdots$$
$$R_{32} = \frac{2^2 R_{31} - R_{21}}{3}, R_{43} = \frac{4^2 R_{42} - R_{32}}{4^2 - 1}, \cdots$$
$$R_{42} = \frac{2^2 R_{41} - R_{31}}{3}, R_{53} = \frac{4^2 R_{52} - R_{42}}{4^2 - 1}, \cdots$$

- Extrapolations of the approximations $R_{j,k-1}$ and $R_{j-1,k-1}$:

$$R_{jk} = \frac{1}{4^{k-1} - 1}(4^{k-1} R_{j,k-1} - R_{j-1,k-1})$$

, for each $j = 2, 3, \ldots$ and $k = j, j+1, \ldots$.

Romberg Integration

Example

Apply Romberg Integration to approximate $\int_1^2 \ln x dx$.

- $\int_1^2 \ln x dx = x \ln x|_1^2 - \int_1^2 dx = 2\ln 2 - 1\ln 1 - 1 \approx 0.38629436.$

j	h_j	R_{j1}	R_{j2}	R_{j3}	R_{jj}
1	1	0.34657359027997			
2	0.5	0.37601934919407	0.38583460216543		
3	0.25	0.38369950940944	0.38625956281457	0.38628789352451	
4	0.125	0.38564390995210	0.38629204346631	0.38629420884310	0.38629430908625

- R_{11}: Approximation using the Trapezoid Rule;
- R_{22}: Approximation using the Simpson's Rule;
- R_{31}: four-panel approximation using the composite Trapezoid Rule;
- R_{42}: four-panel approximation using the composite Simpson's Rule;

Outline

Adaptive Quadrature (Adaptive Trapezoid Rule Quadrature)

Adaptive Quadrature:

1. Variable step size.
2. The integration error is estimated by the integration approximations rather than by the error formulas directly.

- f: a function with a continuous second derivative on $[a, b]$.
- $h = b - a$.
- c: the midpoint of [a,b].
- $S_{[a,b]}$: the approximation for $\int_a^b f(x)\,dx$ using Trapezoid Rule on the interval $[a, b]$.
- $S_{[a,c]}$ (resp. $S_{[c,b]}$): the approximation for $\int_a^b f(x)\,dx$ using Trapezoid Rule on the interval $[a, c]$ (resp. $[c, b]$).

Adaptive Trapezoid Rule Quadrature

Apply Trapezoid Rule on interval $[a, b]$ and half-intervals $[a, c]$ and $[c, b]$:

$$\int_a^b f(x)\,dx \quad = \quad S_{[a,b]} - h^3 \frac{f''(c_0)}{12}, \text{ where } a < c_0 < b$$

Adaptive Trapezoid Rule Quadrature

Apply Trapezoid Rule on interval $[a, b]$ and half-intervals $[a, c]$ and $[c, b]$:

$$\begin{aligned}
\int_a^b f(x)\,dx &= S_{[a,b]} - h^3\frac{f''(c_0)}{12}, \text{ where } a < c_0 < b \\
\int_a^b f(x)\,dx &= S_{[a,c]} - \frac{h^3}{8}\frac{f''(c_1)}{12} + S_{[c,b]} - \frac{h^3}{8}\frac{f''(c_2)}{12} \\
&= S_{[a,c]} + S_{[c,b]} - \frac{h^3}{4}\frac{f''(c_3)}{12} \\
&\quad \text{where } a < c_1 < c, c < c_2 < b \text{ and } a < c_3 < b
\end{aligned}$$

Adaptive Trapezoid Rule Quadrature

Apply Trapezoid Rule on interval $[a, b]$ and half-intervals $[a, c]$ and $[c, b]$:

$$\begin{aligned}
\int_a^b f(x)\,dx &= S_{[a,b]} - h^3 \frac{f''(c_0)}{12}, \text{ where } a < c_0 < b \\
\int_a^b f(x)\,dx &= S_{[a,c]} - \frac{h^3}{8}\frac{f''(c_1)}{12} + S_{[c,b]} - \frac{h^3}{8}\frac{f''(c_2)}{12} \\
&= S_{[a,c]} + S_{[c,b]} - \frac{h^3}{4}\frac{f''(c_3)}{12} \\
&\quad \text{where } a < c_1 < c, c < c_2 < b \text{ and } a < c_3 < b
\end{aligned}$$

Subtracting the above two equations gives the following:

$$\begin{aligned}
S_{[a,b]} - (S_{[a,c]} + S_{[c,b]}) &= -\frac{h^3}{4}\frac{f''(c_3)}{12} + h^3 \frac{f''(c_0)}{12} \\
&\approx \frac{3}{4} h^3 \frac{f''(c_3)}{12}, \text{ where } f''(c_3) \approx f''(c_0)
\end{aligned}$$

It is **approximately three times** the size of the integration error of the approximation $S_{[a,c]} + S_{[c,b]}$.

Adaptive Trapezoid Rule Quadrature

Algorithm 1: Adaptive Trapezoid Rule Quadrature

`// To approximate` $\int_a^b f(x)\,dx$ `within tolerance` TOL:

1 $c = \frac{a+b}{2}$

2 $S_{[a,b]} = (b-a)\frac{f(a)+f(b)}{2}$

3 **if** $|S_{[a,b]} - (S_{[a,c]} + S_{[c,b]}| < 3 \cdot TOL \cdot \left(\frac{b-a}{b_{orig}-a_{orig}}\right)$ **then**

4 accept $S_{[a,c]} + S_{[c,b]}$ as approximation over $[a, b]$

5 **else**

6 repeat above recursively for $[a, c]$ and $[c, b]$

- Every time breaking intervals in half, the required error tolerance for the subinterval goes down by a factor of 2.
- Line 3 is to check whether $S_{[a,c]} + S_{[c,b]}$ approximates the unknown exact integral within $TOL \cdot (\frac{b-a}{b_{orig}-a_{orig}})$.

Adaptive Quadrature (Adaptive Simpson's Rule Quadrature)

- f: a function with a continuous fourth derivative on $[a, b]$.
- $h = b - a$.
- c: the midpoint of $[a, b]$.
- $S_{[a,b]}$ (resp. $S_{[a,c]}$, $S_{[c,b]}$): the approximation for $\int_a^b f(x)\,dx$ using Simpson's Rule on the interval $[a, b]$ (resp. $[a, c]$, $[c, b]$).

Adaptive Simpson's Rule Quadrature

Apply Simpson's Rule on interval $[a, b]$ and its two halves:

$$\int_a^b f(x)\,dx = S_{[a,b]} - h^5 \frac{f^{(iv)}(c_0)}{90}, \text{ where } a < c_0 < b$$

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Apply Simpson's Rule on interval $[a, b]$ and its two halves:

$$\int_a^b f(x)\,dx = S_{[a,b]} - h^5 \frac{f^{(iv)}(c_0)}{90}, \text{ where } a < c_0 < b$$

$$\begin{aligned}\int_a^b f(x)\,dx &= S_{[a,c]} - \frac{h^5}{32}\frac{f^{(iv)}(c_1)}{90} + S_{[c,b]} - \frac{h^5}{32}\frac{f^{(iv)}(c_2)}{90} \\ &= S_{[a,c]} + S_{[c,b]} - \frac{h^5}{16}\frac{f^{(iv)}(c_3)}{90}\end{aligned}$$

where $a < c_1 < c$, $c < c_2 < b$ and $a < c_3 < b$

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where $a < c_1 < c$, $c < c_2 < b$ and $a < c_3 < b$

Subtracting the above two equations gives the following:

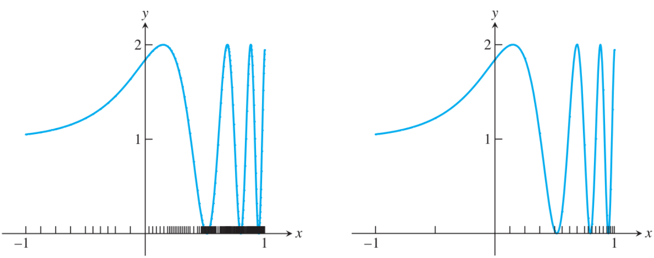
$$\begin{aligned}S_{[a,b]} - (S_{[a,c]} + S_{[c,b]}) &= h^5 \frac{f^{(iv)}(c_0)}{90} - \frac{h^5}{16}\frac{f^{(iv)}(c_3)}{90} \\ &\approx \frac{15}{16} h^5 \frac{f^{(iv)}(c_3)}{90}, \text{ where } f^{(iv)}(c_3) \approx f^{(iv)}(c_0)\end{aligned}$$

It is **approximately 15 times** the size of the integration error of the approximation $S_{[a,c]} + S_{[c,b]}$.

Adaptive Quadrature

Example

Use Adaptive Quadrature to approximate the integral $\int_{-1}^{1}(1+\sin e^{3x})\,dx$.



(a) (b)

- Tolerance $TOL = 0.005$.
- (a) Adaptive Trapezoid Rule requires 140 subintervals.
- (b) Adaptive Simpson's Rule requires 20 subintervals.

Outline

Gaussian Quadrature (Orthogonality)

Definition (Orthogonality)

The set of nonzero functions $\{p_0, p_1, \cdots, p_n\}$ on the interval $[a, b]$ is **orthogonal** on $[a, b]$ if

$$\int_a^b p_j(x)p_k(x)\,dx = \begin{cases} 0 & , j \neq k \\ \neq 0 & , j = k \end{cases}$$

Theorem

If $\{p_0, p_1, \cdots, p_n\}$ is an orthogonal set of polynomials on the interval $[a, b]$, where deg $p_i = i$, then:

- *$\{p_0, p_1, \cdots, p_n\}$ is a basis for the vector space of degree at most n polynomials on $[a, b]$.*
- *p_i has i distinct roots in the interval (a, b).*

Orthogonality

Example

Find a set of three orthogonal polynomials on the interval $[-1, 1]$.

- $p_0(x) = 1, p_1(x) = x, p_2(x) = x^2 + c$

Orthogonality

Example

Find a set of three orthogonal polynomials on the interval $[-1, 1]$.

- $p_0(x) = 1, p_1(x) = x, p_2(x) = x^2 + c$
- p_0 and p_1 are orthogonal:
$$\int_{-1}^{1} p_0(x)p_1(x)\,dx = \int_{-1}^{1} 1 \cdot x dx = \frac{1}{2}x^2|_{-1}^{1} = 0$$
- p_1 and p_2 are orthogonal:
$$\int_{-1}^{1} p_1(x)p_2(x)\,dx = \int_{-1}^{1} x \cdot (x^2 + c)\,dx = (\frac{1}{4}x^4 + \frac{c}{2}x^2)|_{-1}^{1} = 0$$

Orthogonality

Example

Find a set of three orthogonal polynomials on the interval $[-1, 1]$.

- $p_0(x) = 1, p_1(x) = x, p_2(x) = x^2 + c$
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- p_1 and p_2 are orthogonal:
$$\int_{-1}^{1} p_1(x)p_2(x)\,dx = \int_{-1}^{1} x \cdot (x^2 + c)\,dx = (\frac{1}{4}x^4 + \frac{c}{2}x^2)|_{-1}^{1} = 0$$
- when $c = \frac{-1}{3}$, p_0 and p_2 are orthogonal:
$$\int_{-1}^{1} p_0(x)p_2(x)\,dx = \int_{-1}^{1} 1 \cdot (x^2 + c)\,dx = \frac{2}{3} + 2c = 0$$
- the set $\{1, x, x^2 - 1/3\}$ is an orthogonal set on $[-1, 1]$.

Gaussian Quadrature (Legendre polynomials)

The set of **Legendre polynomials**

$$p_i(x) = \frac{1}{2^i i!}\frac{d^i}{dx^i}[(x^2-1)^i]$$

for $0 \leq i \leq n$ is orthogonal on $[-1, 1]$.

Gaussian Quadrature (Legendre polynomials)

The set of **Legendre polynomials**

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for $0 \leq i \leq n$ is orthogonal on $[-1, 1]$.

- $\int_{-1}^{1} p_i(x)p_i(x)dx = \frac{2}{2i+1} \neq 0$ for $0 \leq i \leq n$.
- $\int_{-1}^{1} p_i(x)p_j(x)dx = 0$ for $0 \leq i \neq j \leq n$.

Legendre polynomials

Proof of the second item.

We show that if $i < j$, then $\int_{-1}^{1} [(x^2-1)^i]^{(i)} [(x^2-1)^j]^{(j)}\, dx = 0$.

- Integrate by parts with $u = [(x^2-1)^i]^{(i)}$ and $dv = [(x^2-1)^j]^{(j)}\, dx$:

$$\begin{aligned} uv - \int_{-1}^{1} v du &= [(x^2-1)^i]^{(i)} [(x^2-1)^j]^{(j-1)} |_{-1}^{1} \\ &\quad - \int_{-1}^{1} [(x^2-1)^i]^{(i+1)} [(x^2-1)^j]^{(j-1)}\, dx \\ &= - \int_{-1}^{1} [(x^2-1)^i]^{(i+1)} [(x^2-1)^j]^{(j-1)}\, dx \end{aligned}$$

since $[(x^2-1)^j]^{(j-1)}$ is divisible by $x^2 - 1$.

Legendre polynomials

Proof of the second item.

We show that if $i < j$, then $\int_{-1}^{1}[(x^2-1)^i]^{(i)}[(x^2-1)^j]^{(j)}\,dx = 0$.

- Integrate by parts with $u = [(x^2-1)^i]^{(i)}$ and $dv = [(x^2-1)^j]^{(j)}\,dx$:

$$
\begin{aligned}
uv - \int_{-1}^{1} v du &= [(x^2-1)^i]^{(i)}[(x^2-1)^j]^{(j-1)}\Big|_{-1}^{1} \\
&\quad - \int_{-1}^{1}[(x^2-1)^i]^{(i+1)}[(x^2-1)^j]^{(j-1)}\,dx \\
&= -\int_{-1}^{1}[(x^2-1)^i]^{(i+1)}[(x^2-1)^j]^{(j-1)}\,dx
\end{aligned}
$$

  since $[(x^2-1)^j]^{(j-1)}$ is divisible by x^2-1.

- After $i+1$ repeated integration by parts, we get that:

$$
(-1)^{i+1}\int_{-1}^{1}[(x^2-1)^i]^{(2i+1)}[(x^2-1)^j]^{(j-i-1)}\,dx = 0
$$

  because the $(2i+1)$st derivative of $(x^2-1)^i$ is zero.

Gaussian Quadrature

Gaussian Quadrature of a function is simply a linear combination of function evaluations at the Legendre roots.

Gaussian Quadrature

Gaussian Quadrature of a function is simply a linear combination of function evaluations at the Legendre roots.

- $x_1, \cdots, x_n$: n distinct roots in $[-1, 1]$ of the nth Legendre polynomial $p_n(x)$.
- $Q(x)$: the Lagrange interpolating polynomial for the integrand $f(x)$ at the nodes $x_1, \cdots, x_n$.

Gaussian Quadrature

Using the Lagrange formulation, we can write:

$$Q(x) = \sum_{i=1}^{n} L_i(x) f(x_i), \text{ where } L_i(x) = \frac{(x - x_1)\cdots\overline{(x - x_i)}(x - x_n)}{(x_i - x_1)\cdots\overline{(x_i - x_i)}(x_i - x_n)}$$

Integrating both sides yields the following approximation for the integral:

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i), \text{ where } c_i = \int_{-1}^{1} L_i(x)\,dx,\ i = 1, \cdots, n$$

.

n	roots x_i	coefficients c_i
2	$-\sqrt{1/3} = -0.57735026918963$	$1 = 1.00000000000000$
	$\sqrt{1/3} = 0.57735026918963$	$1 = 1.00000000000000$
3	$-\sqrt{3/5} = -0.77459666924148$	$5/9 = 0.55555555555555$
	$0 = 0.00000000000000$	$8/9 = 0.88888888888888$
	$\sqrt{3/5} = 0.77459666924148$	$5/9 = 0.55555555555555$
4	$-\sqrt{\frac{15+2\sqrt{30}}{35}} = -0.86113631159405$	$\frac{90-5\sqrt{30}}{180} = 0.34785484513745$
	$-\sqrt{\frac{15-2\sqrt{30}}{35}} = -0.33998104358486$	$\frac{90+5\sqrt{30}}{180} = 0.65214515486255$
	$\sqrt{\frac{15-2\sqrt{30}}{35}} = 0.33998104358486$	$\frac{90+5\sqrt{30}}{180} = 0.65214515486255$
	$\sqrt{\frac{15+2\sqrt{30}}{35}} = 0.86113631159405$	$\frac{90-5\sqrt{30}}{180} = 0.34785484513745$

Gaussian Quadrature

Example

Approximate $\int_{-1}^{1} e^{-\frac{x^2}{2}}\,dx$, using Gaussian Quadrature.

- $f(x) = e^{-\frac{x^2}{2}}$.
- The correct answer to 14 digits is 1.71124878378430.
- The $n = 2$ approximation:

$$\begin{aligned}\int_{-1}^{1} e^{-\frac{x^2}{2}}\,dx &\approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)\\ &= 1\cdot f(-\sqrt{1/3}) + 1\cdot f(\sqrt{1/3})\\ &\approx 1.69296344978123\end{aligned}$$

Gaussian Quadrature

Example

Approximate $\int_{-1}^{1} e^{-\frac{x^2}{2}}\,dx$, using Gaussian Quadrature.

- The $n = 3$ approximation:

$$\begin{aligned}\int_{-1}^{1} e^{-\frac{x^2}{2}}\,dx &\approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)\\ &= \frac{5}{9}\cdot f(-\sqrt{3/5}) + \frac{8}{9}\cdot f(0) + \frac{5}{9}\cdot f(\sqrt{3/5})\\ &\approx 1.71202024520191\end{aligned}$$

- The $n = 4$ approximation:

$$\begin{aligned}\int_{-1}^{1} e^{-\frac{x^2}{2}}\,dx &\approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3) + c_4 f(x_4)\\ &\approx 1.71122450459949\end{aligned}$$

Gaussian Quadrature (Degree of precision)

Definition (Degree of precision)

The **degree of precision** of a numerical integration method is the greatest integer k for which all degree k or less polynomials are integrated exactly by the method.

Gaussian Quadrature (Degree of precision)

Example (The degree of precision of the Trapezoid Rule)

$$\int_a^b f(x)\,dx = \frac{h}{2}[f(a)+f(b)] - \frac{h^3}{12}f''(c)$$

where $h = b - a$ and $a \leq c \leq b$.

- $f_1(x)$: a polynomial of degree 1 or less;
- $f_2(x) = x^2$.
- $P_i = \frac{h}{2}(f_i(a)+f_i(b))$, $E_i = -\frac{h^3}{12}f_i''(c)$ for $i = 1, 2$;
- $I_i = \int_a^b f_i(x)\,dx$ for $i = 1, 2$.

i	$f_i''(c)$	E_i	
1	0	0	$P_i = I_i$
2	$\neq 0$	$\neq 0$	$P_i \neq I_i$

Gaussian Quadrature (Degree of precision)

Newton-Cotes Methods of degree n have degree of precision n (for n odd) and $n+1$ (for n even).

- The Trapezoid Rule $(n = 1)$ has degree of precision one.
- The Simpson's Rule $(n = 2)$ has degree of precision three.

Gaussian Quadrature

Theorem (Degree of precision of Gaussian Quadrature Method)

The Gaussian Quadrature Method, using the degree n Legendre polynomial on $[-1, 1]$, has degree of precision $2n - 1$.

- $P(x)$: the integrand, a polynomial of degree at most $2n - 1$.
- $p_n(x)$: the nth Legendre polynomial.
- $x_1, \cdots, x_n$: n distinct roots in $[-1, 1]$ of $p_n(x)$.

Proof of Theorem

Proof.

We proof that $P(x)$ is integrated exactly by Gaussian Quadrature.

- Using **long division of polynomials**, we can express:

$$P(x) = S(x)p_n(x) + R(x)$$

  , where $S(x)$ and $R(x)$ are polynomials of degree less than n.

Proof of Theorem

Proof.

We proof that $P(x)$ is integrated exactly by Gaussian Quadrature.

- Using **long division of polynomials**, we can express:

$$P(x) = S(x)p_n(x) + R(x)$$

, where $S(x)$ and $R(x)$ are polynomials of degree less than n.

- Gaussian Quadrature approximation for $P(x)$ is identical with the integration of $R(x)$ on $[-1, 1]$.
    - Gaussian Quadrature is exact on the polynomial $R(x)$:

$$\int_{-1}^{1} R(x)\,dx = \sum_{i=1}^{n} c_i R(x_i), \text{ where } c_i = \int_{-1}^{1} L_i(x)\,dx, i = 1, \cdots, n$$

Proof of Theorem

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  - As $p_n(x_i) = 0$ for all i, we get that $P(x_i) = R(x_i)$. So,

$$\sum_{i=1}^{n} c_i P(x_i) = \sum_{i=1}^{n} c_i R(x_i) = \int_{-1}^{1} R(x)\,dx$$

Proof of Theorem

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- The integration for $P(x)$ and $R(x)$ on $[-1,1]$ are identical. By the fact that $S(x)$ is **orthogonal** to $p_n(x)$, we get that:

$$\int_{-1}^{1} P(x)\,dx = \int_{-1}^{1} S(x)p_n(x)\,dx + \int_{-1}^{1} R(x)\,dx = 0 + \int_{-1}^{1} R(x)\,dx$$

Therefore, it holds that $\int_{-1}^{1} P(x)\,dx = \sum_{i=1}^{n} c_i P(x_i)$.

Gaussian Quadrature approximations on a general interval

- $p_n(t)$: the nth Legendre polynomial.
- $t_1, \cdots, t_n$: n distinct roots in $[-1, 1]$ of $p_n(t)$.

Using the substitution $t = \frac{(2x-a-b)}{(b-a)}$, we obtain that:

$$\begin{aligned} \int_a^b f(x)\,dx &= \int_{-1}^{1} f\Big(\frac{(b-a)t+b+a}{2}\Big)\frac{b-a}{2}\,dt \\ &\approx \frac{b-a}{2}\sum_{i=1}^{n} c_i f\Big(\frac{(b-a)t_i+b+a}{2}\Big) \end{aligned}$$

, where $c_i = \int_{-1}^{1} \frac{(t-t_1)\cdots\overline{(t-t_i)}(t-t_n)}{(t_i-t_1)\cdots\overline{(t_i-t_i)}(t_i-t_n)}\,dt,\ i = 1, \cdots, n.$

Gaussian Quadrature approximations on a general interval

Example

Approximate the integral $\int_1^2 \ln x dx$, using Gaussian Quadrature.

- Exact value: $\int_1^2 \ln x dx = 2\ln 2 - 1\ln 1 - 1 \approx 0.38629436111989$.
- Using the substitution $t = \frac{(2x-1-2)}{(2-1)} = 2x - 3$, we obtain that: $\int_1^2 \ln x dx = \int_{-1}^1 \ln(\frac{t+3}{2})\frac{1}{2}dt$.
- The $n = 4$ approximation:

$$\begin{aligned} \int_{-1}^{1} \ln(\frac{t+3}{2})\frac{1}{2}dt &\approx c_1 f(t_1) + c_2 f(t_2) + c_3 f(t_3) + c_4 f(t_4) \\ &\approx \color{blue}{0.386294}\color{black}{49693871} \end{aligned}$$

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&\approx 0.38629449693871
\end{aligned}
$$

- 4-panel composite Trapezoid Rule approximation:
  ≈ 0.38369950940944;
- 4-panel Romberg Integration: $R_{33} \approx 0.38628789352451$.

Outline

Conclusions

Two methods for Numerical Differentiation

1. Finite difference formulas
   - Two-point forward-difference formula
   - Three-point centered-difference formula
   - Three-point centered-difference formula for second derivative
2. Extrapolation

Conclusions

Four methods for Numerical Integration

1. Newton–Cotes Formulas for Numerical Integration
    - Closed Newton–Cotes Method: Trapezoid and Simpson's Rules
    - Open Newton–Cotes Method: Midpoint Rule
    - Composite Newton–Cotes Method: Composite Trapezoid (resp. Simpson's / Midpoint) Rule
2. Romberg Integration
3. Adaptive Quadrature: Adaptive Trapezoid and Simpson's) Rule Quadrature
4. Gaussian Quadrature: Gauss-Legendre Quadrature formula

Thank you!