CS 3331 Numerical Methods

Lecture 10: Numerical Differentiation and Integration

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Outline

- Differentiation
  - Finite difference methods
  - Richardson extrapolation
- Integration
  - Newton-Cotes methods
  - Gaussian quadrature

Differentiation

Two points formula LVF pp.426

- Given function values $\ldots, f(x_{i-1}), f(x_i), f(x_{i+1}), \ldots$

- Forward difference

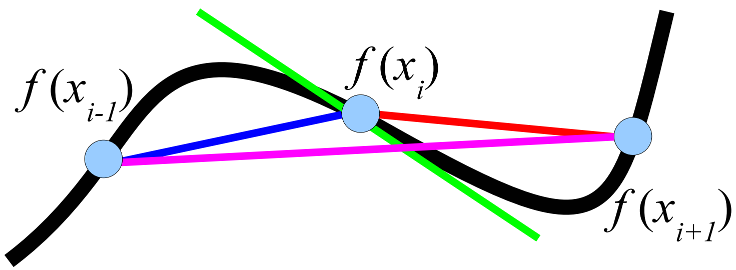
$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

- Backward difference

$$f'(x_i) \approx \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}$$

- Central difference

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$



Measure the accuracy LVF pp.428

- Suppose $x_{i+1} = x_i + h$ and $x_{i-1} = x_i - h$.
- Taylor expansion $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\eta)$
  - Forward difference $f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2}f''(\eta)$

$$\Rightarrow f'(x) = [f(x_{i+1}) - f(x_i)]/h - \frac{h}{2}f''(\eta)$$

  - Backward difference $f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2}f''(\eta)$

$$\Rightarrow f'(x) \approx [f(x_{i-1}) - f(x_i)]/(-h) + \frac{h}{2}f''(\eta)$$

  - Suppose $|f''(x)|$ is bounded, then the error of forward and backward difference is $O(h)$.

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

$$\begin{cases} f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2}f''(x_i) + \frac{h^3}{6}f'''(\eta_1), & (1); \\ f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2}f''(x_i) - \frac{h^3}{6}f'''(\eta_2), & (2). \end{cases}$$

  – Central difference : (1)-(2)

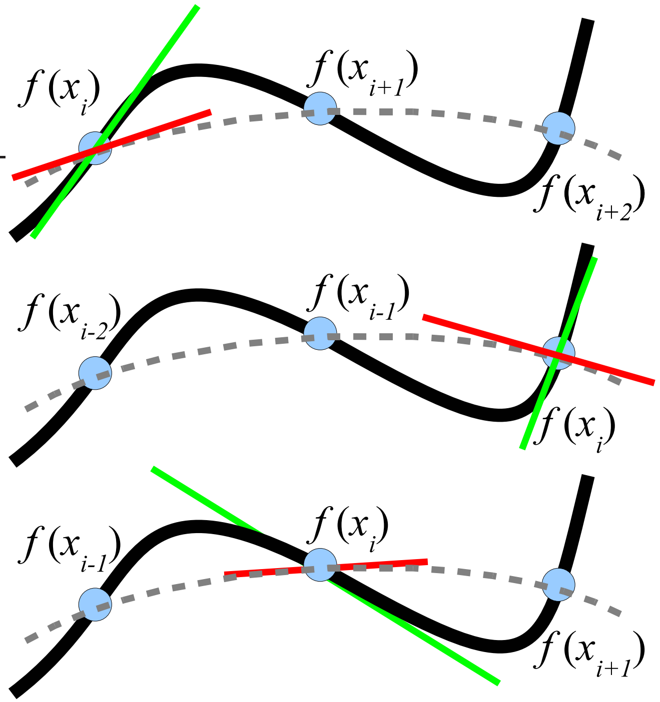
$$f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + \frac{h^3}{6}(f'''(\eta_1) - f'''(\eta_2))$$

$$f'(x) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + \frac{h^2}{12}(f'''(\eta_1) - f'''(\eta_2))$$

  – If $|f'''|$ is bounded, the error of central difference is $O(h^2)$

Three points formula LVF pp.426,429

- Given $f(x_{i-1}), f(x_i), f(x_{i+1})$. The three point formula uses quadratic polynomial to approximate the derivative.
  - Forward:
  $$f'(x_i) \approx \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{x_{i+2} - x_i}$$
  - Backward:
  $$f'(x_i) \approx \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{x_i - x_{i-2}}$$
  - Central:
  $$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$



Suppose $h = x_{i+2} - x_{i+1} = x_{i+1} - x_i = x_i - x_{i-1} = x_{i-1} - x_{i-2}$

$$p(x) = \frac{(x-x_2)(x-x_3)f(x_1)}{(x_1-x_2)(x_1-x_3)} + \frac{(x-x_1)(x-x_3)f(x_2)}{(x_2-x_1)(x_2-x_3)} + \frac{(x-x_1)(x-x_2)f(x_3)}{(x_3-x_1)(x_3-x_2)}$$

$$p'(x) = \frac{(2x-x_2-x_3)f(x_1)}{(x_1-x_2)(x_1-x_3)} + \frac{(2x-x_1-x_3)f(x_2)}{(x_2-x_1)(x_2-x_3)} + \frac{(2x-x_1-x_2)f(x_3)}{(x_3-x_1)(x_3-x_2)}$$

Forward formula $x_1 = x_i, x_2 = x_{i+1}, x_3 = x_{i+2}$

$$\begin{aligned} p'(x_1) &= \frac{(2x_1-x_2-x_3)f(x_1)}{(x_1-x_2)(x_1-x_3)} + \frac{(x_1-x_3)f(x_2)}{(x_2-x_1)(x_2-x_3)} + \frac{(x_1-x_2)f(x_3)}{(x_3-x_1)(x_3-x_2)} \\ &= \frac{-3f(x_1)}{2h} + \frac{2f(x_2)}{h} + \frac{-f(x_3)}{2h} = \frac{-3f(x_1) + 4f(x_2) - f(x_3)}{2h} \end{aligned}$$

Backward formula $x_1 = x_{i-2}, x_2 = x_{i-1}, x_3 = x_i$

$$\begin{aligned} p'(x_3) &= \frac{(x_3-x_2)f(x_1)}{(x_1-x_2)(x_1-x_3)} + \frac{(x_3-x_1)f(x_2)}{(x_2-x_1)(x_2-x_3)} + \frac{(2x_3-x_1-x_2)f(x_3)}{(x_3-x_1)(x_3-x_2)} \\ &= \frac{f(x_1)}{2h} + \frac{2f(x_2)}{-h} + \frac{3f(x_3)}{2h} = \frac{f(x_1) - 4f(x_2) + 3f(x_3)}{2h} \end{aligned}$$

Central formula $x_1 = x_{i-1}, x_2 = x_i, x_3 = x_{i+1}$

$$
\begin{aligned}
p'(x_2) &= \frac{(x_2 - x_3) f(x_1)}{(x_1 - x_2)(x_1 - x_3)} + \frac{(2x_2 - x_1 - x_3) f(x_2)}{(x_2 - x_1)(x_2 - x_3)} + \frac{(x_2 - x_1) f(x_3)}{(x_3 - x_1)(x_3 - x_2)} \\
&= \frac{-f(x_1)}{2h} + \frac{f(x_3)}{2h} = \frac{f(x_3) - f(x_1)}{2h}
\end{aligned}
$$

Second derivative

$$
\begin{cases}
f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2} f''(x_i) + \frac{h^3}{6} f'''(x) + O(h^4 f^{(4)}), & (1); \\
f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2} f''(x_i) - \frac{h^3}{6} f'''(x) + O(h^4 f^{(4)}), & (2).
\end{cases}
$$

- From (1)+(2), $f(x_{i+1}) + f(x_{i-1}) = 2f(x) + h^2 f''(x) + O(h^4 f^{(4)})$

$$
f''(x) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2 f^{(4)})
$$

Richardson extrapolation LVF pp.432

- Example, the central difference

$$f'(x) = D(h) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) + O(h^4)$$

- Half the step,

$$f'(x) = D(h/2) = \frac{f(x+h/2) - f(x-h/2)}{h} - \frac{h^2}{24} f'''(x) + O(h^4)$$

- Richardson extrapolation

$$\begin{aligned} f'(x) &= [4D(h/2) - D(h)]/3 \\ &= \frac{8[f(x+\frac{h}{2}) - f(x-\frac{h}{2})] - [f(x+h) - f(x-h)]}{12h} + O(h^4) \end{aligned}$$

Numerical Integration

Newton–Cote formula LVF pp.434

- Use polynomials to approximate functions by interpolating function values at equidistant points.
- Closed formula: interpolate end points
  - Linear polynomial: Trapezoid rule
  - Quadratic polynomial: Simpson's rule
- Open formula: interpolate mid points (no end points)
  - Constant polynomial: midpoint rule
  - Linear polynomial: two point formula
  - Quadratic polynomial: three point formula

Error of interpolation LVF pp.295

- What is the error when using a polynomial to approximate a function $f(x)$ by interpolating n points $(x_1, f(x_1)), \cdots, (x_n, f(x_n))$?
  - $f(x)$ has n continuous derivatives.
  - For some η in the interval containing $x_1, x_2, \cdots, x_n$

$$|f(t) - p(t)| \leq \frac{(t - x_1)\cdots(t - x_n)}{n!} f^{(n)}(\eta)$$

- If $f(x)$ is a polynomial of degree less than n, the interpolation will be exact, so is the integration $\int_a^b f(x)dx = \int_a^b p(x)dx$.

Trapezoid rule LVF pp.434

$$\int_a^b f(x)dx \approx \frac{b-a}{2}[f(a)+f(b)]$$

- Approximate $f(x)$ by $p(x) = \dfrac{x-b}{a-b}f(a) + \dfrac{x-a}{b-a}f(b)$

$$\begin{aligned}
\int_a^b \frac{x-b}{a-b}f(a)dx &= \frac{f(a)}{a-b}\int_a^b (x-b)dx = \frac{f(a)}{a-b}\left[\frac{x^2}{2} - bx\right]\Big|_a^b \\
&= \frac{f(a)}{2(a-b)}\left[b^2 - 2b^2 - a^2 - 2ab\right] = \frac{b-a}{2}f(a) \\
\int_a^b \frac{x-a}{b-a}f(b)dx &= \frac{f(b)}{b-a}\int_a^b (x-a)dx = \frac{f(b)}{b-a}\left[\frac{x^2}{2} - ax\right]\Big|_a^b \\
&= \frac{f(b)}{2(b-a)}\left[b^2 - 2ab - a^2 + 2a^2\right] = \frac{b-a}{2}f(b)
\end{aligned}$$

- Error of trapezoid rule

$$\int_a^b (f(x)-p(x))dx = 1/2\int_a^b f''(\eta)(x-a)(x-b)dx$$
$$= \frac{f''(\eta)}{2}\left[\frac{x^3}{3}-(a+b)\frac{x^2}{2}+abx\right]\Bigg|_a^b = -\frac{(b-a)^3}{12}f''(\eta)$$

- Composite integration: equally divide $b-a$ into n subintervals. Let $h=\frac{b-a}{n}$, $a=x_0, b=x_n$, $x_k=a+kh$ for $k=1,\cdots,n-1$.

$$\int_a^b f(x)dx = \int_a^{x_1} f(x)dx+\cdots+\int_{x_{n-1}}^b f(x)dx$$
$$\approx \frac{h}{2}[f(a)+f(x_1)]+\cdots+\frac{h}{2}[f(x_{n-1})+f(b)]$$
$$= \frac{h}{2}[f(a)+2f(x_1)+\cdots+2f(x_{n-1})+f(b)]$$

Error of composite trapezoid: $-\frac{(b-a)h^2}{12}f''(\eta)$

Simpson's rule LVF pp.438

$$\int_a^b f(x)dx \approx \frac{b-a}{6}[f(a) + 4f(\frac{a+b}{2}) + f(b)]$$

- Let $c = (a+b)/2$, and approximate $f(x)$ by

$$p(x) = \frac{(x-b)(x-c)}{(a-b)(a-c)}f(a) + \frac{(x-a)(x-b)}{(c-a)(c-b)}f(c) + \frac{(x-a)(x-c)}{(b-a)(b-c)}f(b)$$

$$\begin{aligned}
\int_a^b \frac{(x-b)(x-c)}{(a-b)(a-c)}f(a)dx &= (b-a)\frac{f(a)}{6} \\
\int_a^b \frac{(x-a)(x-b)}{(c-a)(c-b)}f(c)dx &= (b-a)\frac{4f(c)}{6} \\
\int_a^b \frac{(x-a)(x-c)}{(b-a)(b-c)}f(b)dx &= (b-a)\frac{f(b)}{6}
\end{aligned}$$

Error of Simpson's rule

$$\begin{aligned}\int_a^b (f(x)-p(x))dx &= \frac{1}{4!}\int_a^b f^{(4)}(\eta)(x-a)(x-c)(x-b)dx \\ &= \frac{f^{(4)}(\eta)}{24}\left[\frac{x^4}{4}-(a+c+b)\frac{x^3}{3}+(ab+bc+ac)\frac{x^2}{2}-abcx\right]\Big|_a^b \\ &= -\frac{(b-a)^5}{2880}f^{(4)}(\eta)\end{aligned}$$

Composite rule: The same setting as trapezoid rule

$$\begin{aligned}\int_a^b f(x)dx &= \int_a^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{b} f(x)dx \\ &\approx \frac{h}{3}[f(a)+4f(x_1)+f(x_2)]+\cdots+\frac{h}{3}[f(x_{n-2})+4f(x_{n-1})+f(b)] \\ &= \frac{h}{3}[f(a)+4f(x_1)+2f(x_2)+\cdots+2f(x_{n-2})+4f(x_{n-1})+f(b)]\end{aligned}$$

Error of composite rule: $-\dfrac{(b-a)h^4}{180}f^{(4)}(\eta)$

Midpoint rule LVF pp.444

$$\int_a^b f(x)dx \approx (b-a)f(\frac{a+b}{2})$$

Error of midpoint rule $\int_a^b f(x)dx - (b-a)f(\frac{a+b}{2}) = \frac{(b-a)^3}{24} f''(\eta)$

- Let $c = \frac{a+b}{2}$, $p(x) = f'(c)(x-c) + f(c) \Rightarrow \int_a^b p(x)dx = (b-a)f(c)$

$$\begin{aligned} \int_a^b f(x)dx - (b-a)f(c) &= \int_a^b (f(x) - p(x))dx \\ &= \int_a^b \frac{(x-c)^2}{2} f''(\eta)dx \\ &= \frac{f''(\eta)}{2} \left.\frac{(x-c)^3}{3}\right|_a^b = \frac{(b-a)^3}{24} f''(\eta) \end{aligned}$$

Other formulas LVF pp.445

- Two point formula: $x_1 = \frac{2a+b}{3}, x_2 = \frac{a+2b}{3}$

$$\int_a^b f(x)dx \approx \frac{b-a}{2}[f(x_1) + f(x_2)]$$

  - Error: $\frac{(b-a)^3}{36} f''(\eta)$

- Three point formula: $x_1 = \frac{3a+b}{4}, x_2 = \frac{2a+2b}{4}, x_3 = \frac{a+3b}{4}$

$$\int_a^b f(x)dx \approx \frac{b-a}{3}[2f(x_1) + f(x_2) + 2f(x_3)]$$

  - Error: $\frac{14(b-a)^5}{46080} f^{(4)}(\eta)$

Extrapolation acceleration LVF pp.446

- Trapezoid rule: $I_T = \frac{b-a}{2}[f(a)+f(b)] = \int_a^b f(x)dx + \frac{(b-a)^3}{12} f''(a) + O((b-a)^4)$
- Midpoint rule : $I_M = (b-a)f(\frac{a+b}{2}) = \int_a^b f(x)dx - \frac{(b-a)^3}{24} f''(a) + O((b-a)^4)$
- The method $(2I_M + I_T)/3 = \int_a^b f(x)dx + O((b-a)^4)$.
  - which is the Simpson's rule:

$$\frac{2I_M + I_T}{3} = \frac{1}{6}[f(a) + 4f(\frac{a+b}{2}) + f(b)]$$

Romberg integration LVF pp.446

- Let $b - a = h$
  - 1 interval: $I_1 = \int_a^b f(x)dx + \frac{h^3}{12} f''(a) + O(h^5)$
  - 2 intervals: $I_2 = \int_a^b f(x)dx + \frac{h^3}{4*12} f''(a) + O(h^5)$
  - 4 intervals: $I_4 = \int_a^b f(x)dx + \frac{h^3}{16*12} f''(a) + O(h^5)$
- Romberg integral $R_{11} = (4I_2 - I_1)/3$, which has error $O(h^5)$
  - $R_{12} = (4I_4 - I_2)/3$ also has error $O(h^5)$
  - $R_{21} = (16R_{12} - R_{11})/15$ has error $O(h^7)$
- In general, $R_{k1} = \frac{2^{k+2} R_{k-1,2} - R_{k-1,1}}{2^{k+2} - 1}$ has error $O(h^{2k+1})$

Gaussian Quadrature

Idea of Gaussian quadrature LVF pp.452

- Usually $\int_a^b f(x)dx \approx c_1 f(x_1) \cdots + c_n f(x_n)$ gives n degrees of freedom, if $x_0, x_1, \ldots, x_n$ are fixed.

- If $x_1, \ldots, x_n$ are allowed to change, they add another n degrees of freedom.

- For example, $\int_a^b f(x)dx \approx c_1 f(a) + c_2 f(b)$ can only approximate $f(x) = \alpha_1 x + \alpha_0$ exactly. But

$$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

can approximate $f(x) = \alpha_3 x^3 + \alpha_2 x^2 + \alpha_1 x + \alpha_0$ exactly.

- Let $[a,b]=[-1,1]$. $$\begin{aligned}\int_{-1}^{1} 1dx &= 2 = c_1 + c_2\\ \int_{-1}^{1} xdx &= 0 = c_1x_1 + c_2x_2\\ \int_{-1}^{1} x^2dx &= 2/3 = c_1x_1^2 + c_2x_2^2\\ \int_{-1}^{1} x^3dx &= 0 = c_1x_1^3 + c_2x_2^3\end{aligned}$$
  Solution is $c_1 = c_2 = 1, x_1 = -1/\sqrt{3}, x_2 = 1/\sqrt{3}$
- $f(-1/\sqrt{3}) + f(1/\sqrt{3})$ can exactly approximate
$$\int_{-1}^{1}[\alpha_3x^3 + \alpha_2x^2 + \alpha_1x + \alpha_0]dx$$
- $\int_a^b f(x)dx - \sum_{i=1}^{n} f(x_i) = O((b-a)^{2n+1})$

Change intervals LVF pp.452

- If the integration is over $[a, b]$, then use changing variable

$$x = \frac{b-a}{2}z + \frac{a+b}{2} \text{ and } dx = \frac{b-a}{2}dz$$

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}z + \frac{a+b}{2}\right) dz$$

- Gaussian quadrature rule becomes

$$\frac{b-a}{2}\sum_{i=1}^{n} f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

Gauss-Legendre quadrature LVF pp.452

- For any polynomial $f(x)$ of degree equal or less than $2n-1$, find $x_1, x_2, \cdots, x_n$ and $c_1, c_2, \cdots, c_n$ such that

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

- It is a difficult problem to solve x_i and c_i directly (nonlinear).

- The solution of x_i "happens" to be the zeros of the nth degree Legendre polynomial, P_n, and choose c_i such that the integration of polynomials of degree $< n$ are exact,

$$c_i = \int_{-1}^{1} \prod_{j=1, j\neq i}^{n} \frac{(x - x_j)}{(x_i - x_j)} dx$$

- Why? Any polynomial $f(x)$ of degree $2n-1$ can be represented as $f(x) = p_n(x)q(x) + r(x)$, where $q(x)$ and $r(x)$ are of degree less than n.

$$
\begin{aligned}
\sum_{i=1}^{n} c_i f(x_i) &= \sum_{i=1}^{n} c_i [p_n(x_i)q(x_i) + r(x_i)] && \text{// direct subsitution.} \\
&= \sum_{i=1}^{n} c_i r(x_i) && \text{// } p_n(x_i) = 0 \\
&= \int_{-1}^{1} r(x)dx && \text{// degree of } r(x) < n \\
&= \int_{-1}^{1} [p_n(x)q(x) + r(x)]dx && \text{// } p_n \text{ orthogonal to } q \\
&= \int_{-1}^{1} f(x)dx && \text{// direct subsitution.}
\end{aligned}
$$

- Error is $\dfrac{< p_n, p_n >}{(2n)!} f^{(2n)}(\eta)$