University at Albany
State University of New York

CSI 401 (Fall 2025)

Numerical Methods

Lecture 17: Numerical Differentiation

Chong Liu

Department of Computer Science

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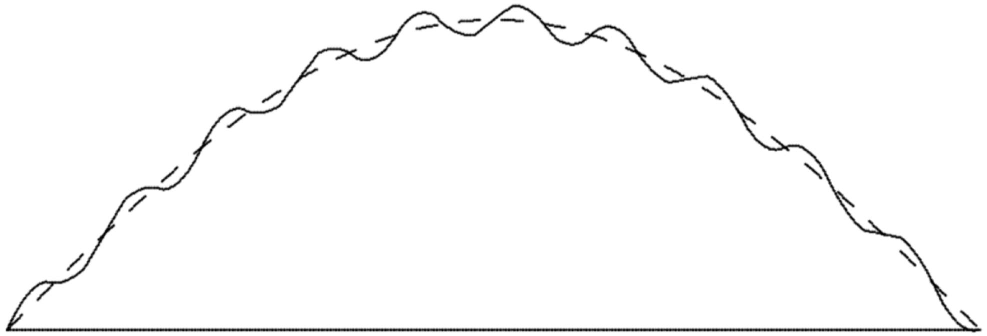
Agenda

- Problem setup of numerical differentiation
- Methods of numerical differentiation
- Richardson Extrapolation
  - A method used to improve accuracy of numerical integration and differentiation

Numerical differentiation vs. integration

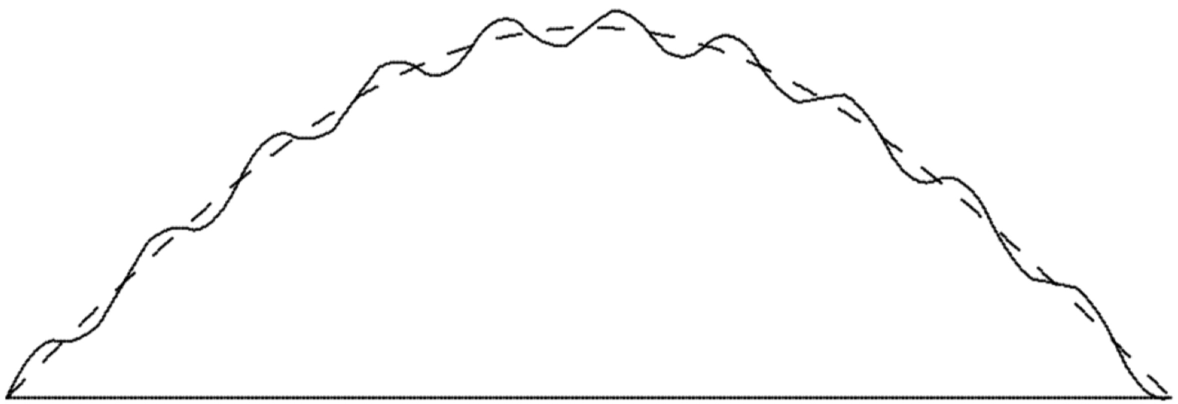
- Discussion: What’s the relationship between differentiation and integration?
  - Differentiation is inverse of integration.
- Suppose we have two functions shown below



- Discussion:
  - Suppose you do differentiation and integration for these two functions. Which results will be similar?

Numerical differentiation

- Differentiation is inherently sensitive, as small perturbations in data can cause large changes in result
- Integration is inherently stable because of its smoothing effect
  - For example, two functions shown below have very similar definite integrals but very different derivatives



Problem setup of numerical differentiation

- Given smooth function $f\colon R \to R$, we wish to approximate its first and second derivatives at point x
- Key question today: How can we use computers to calculate the differentiation by querying f only?
  - Discussion: what is your idea?
- Consider Taylor series expansions

$$
\begin{aligned}
f(x+h) &= f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \cdots \\
f(x-h) &= f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \cdots
\end{aligned}
$$

Finite Difference Approximations

- Solving for $f'(x)$ in first series, obtain forward difference approximation

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

  - which is first-order accurate since dominant term in remainder of series is O(h)

Finite Difference Approximations

- Similarly , from second series derive backward difference approximation

$$
\begin{aligned}
f'(x) &= \frac{f(x) - f(x-h)}{h} + \frac{f''(x)}{2}h + \cdots \\
&\approx \frac{f(x) - f(x-h)}{h}
\end{aligned}
$$

  - which is also first-order accurate

- Subtracting second series from first series gives centered difference approximation

$$
\begin{aligned}
f'(x) &= \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(x)}{6}h^2 + \cdots \\
&\approx \frac{f(x+h) - f(x-h)}{2h}
\end{aligned}
$$

  - which is second-order accurate

Finite Difference Approximations

- Adding both series together gives centered difference approximation for second derivative

$$
\begin{aligned}
f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{f^{(4)}(x)}{12}h^2 + \cdots \\
&\approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}
\end{aligned}
$$

  - which is also second-order accurate

In-class exercise

- Consider $f(x) = e^x$, and we want to approximate $f'(1)$
  - Derive the forward difference approximation
  - Derive the central difference approximation
  - For step size $h = 0.1$, compute:
    - forward and centered difference approximations
    - the exact derivative
- Solutions:

Forward difference:

$$D_f = \frac{f(1.1) - f(1)}{0.1} = \frac{3.004166023 - 2.718281828}{0.1} \approx \frac{0.285884195}{0.1} \approx 2.85884195$$

Central difference:

$$D_c = \frac{f(1.1) - f(0.9)}{2 \cdot 0.1} = \frac{3.004166023 - 2.459603111}{0.2} = \frac{0.544562912}{0.2} \approx 2.72281456.$$

$$f'(x) = e^x, \quad f'(1) = e \approx 2.718281828.$$

Numerical differentiation in practice

- Computer program expressing function is composed of basic arithmetic operations and elementary functions, each of whose derivatives is easily computed

- Derivatives can be propagated through program by repeated use of chain rule, computing derivative of function step by step along with function itself

Checkpoint – Numerical Differentiation

- Differentiation is inherently sensitive to perturbations
- For continuously defined smooth function, finite difference approximations to derivatives can be derived by Taylor series or polynomial interpolation
- Another option is that computer program expressing given function is differentiated step by step to compute derivative

Richardson Extrapolation - Motivation

- In many problems, such as numerical integration or differentiation, approximate value for some quantity is computed based on some step sizes
  - Discussion: What happens if step size is very large or small?
- Ideally , we would like to obtain limiting value as step size approaches zero, but we cannot take step size arbitrarily small because of excessive cost or rounding error
- Based on values for nonzero step sizes, however, we may be able to estimate value for step size of zero

Richardson Extrapolation

- Let $F(h)$ denote value obtained with step size h
  - This is NOT a function of weights or nodes!
- Key idea:
  - If we compute value of F for some nonzero step sizes, and if we know theoretical behavior of $F(h)$ as $h \to 0$, then we can extrapolate from known values to obtain approximate value for $F(0)$
- How?
  - Suppose that
    $$F(h) = a_0 + a_1 h^p + \mathcal{O}(h^r)$$
  - as $h \to 0$ for some p and r, with $r > p$
  - Assume we know values of p and r, but not a_0 or a_1 (indeed, $\mathrm{F}(0) = a_0$ is what we seek)

Richardson Extrapolation

- Suppose we have computed F for two step sizes, say h and h/q for some positive integer q

- Then we

$$
\begin{aligned}
F(h) &= a_0 + a_1 h^p + \mathcal{O}(h^r) \\
F(h/q) &= a_0 + a_1 (h/q)^p + \mathcal{O}(h^r) = a_0 + a_1 q^{-p} h^p + \mathcal{O}(h^r)
\end{aligned}
$$

- This system of two linear equations in two unknowns a_0 and a_1 is easily solved to obtain

$$
a_0 = F(h) + \frac{F(h) - F(h/q)}{q^{-p} - 1} + \mathcal{O}(h^r)
$$

Example of Richardson Extrapolation

- Use Richardson extrapolation to improve accuracy of finite difference approximation to derivative of function sin(x) at x=1
    - Discussion: what's the result of forward difference approximation with step size 0.5?
- Using first-order accurate forward difference approximation, we have $F(h) = a_0 + a_1 h + \mathcal{O}(h^2)$
    - so $p = 1$ and $r = 2$ in this instance
- Using step sizes of $h = 0.5$ and $h/2 = 0.25$ i.e., $q = 2$, we obtain

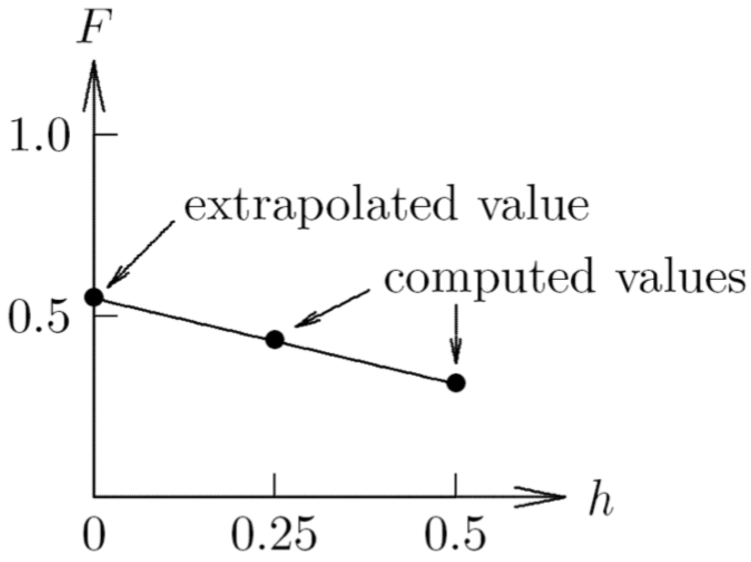
$$
\begin{aligned}
F(h) &= \frac{\sin(1.5) - \sin(1)}{0.5} = 0.312048 \\
F(h/2) &= \frac{\sin(1.25) - \sin(1)}{0.25} = 0.430055
\end{aligned}
$$

Example of Richardson Extrapolation

- Extrapolated value is then given by

$$F(0) = a_0 = F(h) + \frac{F(h) - F(h/2)}{(1/2) - 1} = 2F(h/2) - F(h) = 0.548061$$

- For comparison, correctly rounded result is $\cos(1) = 0.540302$



Announcements

- Week 14:
  - Lecture 18: Advanced Topic: Differential Equations
    - A very interesting topic, foundational tool of many engineering applications
    - Not part of the final exam
  - Lecture 19: Course Review
    - Very important, covering all topics in Lectures 1-17 *for your final exam*
- Week 15:
  - Final Exam Practice and Review
- Week 16:
  - Last instructor's office hours
  - HW 3 and 4 Review *for your final exam*
  - Final project presentation (15')
    - Soundness (3'), organization (3'), clarity (3'), performance (3'), novelty (3')
- Week 17:
  - Monday Dec 15, 2025, Final Exam (5:45-7:15 pm, 30')