

Lecture 03 - A

§4.3 Numerical Differentiation

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We will answer these questions:

- What is the Taylor expansion of $f(x \pm h)$?
- How is the Taylor expansion used to develop finite difference schemes?
- How can we compare the performance of various finite difference algorithms?
- What is the central difference scheme and what makes it different from the forward or backward difference schemes?



Problem Statement

Given

- Some function $y = f(x)$
- A point x_0
- You may evaluate f at discrete locations e.g. $f(x_0 + h)$, $f(x_0)$ and $f(x_0 - h)$

Objective

- Approximate numerical value of $f'(x_0)$

Think of $f(x)$ as a black box. You cannot visualize f but you can input numbers and get an output.



Taylor Series



Taylor Expansion

- Recall the Taylor series expansion of $f(x)$ around x_0

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2!}f''(x_0) + \cdots + \frac{(x - x_0)^n}{n!}f^{(n)}(x_0) + \cdots$$

- Let $x = x_0 + h$

$$f(x_0 + h) = f(x_0) + (x_0 + h - x_0)f'(x_0) + \frac{(x_0 + h - x_0)^2}{2!}f''(x_0) + \cdots + \frac{(x_0 + h - x_0)^n}{n!}f^{(n)}(x_0) + \cdots$$

Alternate Taylor Expansion Formula

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \cdots + \frac{h^n}{n!}f^{(n)}(x_0) + \cdots$$

Expansion with $-h$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \cdots + (-1)^n \frac{h^n}{n!}f^{(n)}(x_0) + \cdots$$



Compare Taylor Expansion Formulas

Regular Taylor Series

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2!}f''(x_0) + \cdots + \frac{(x - x_0)^n}{n!}f^{(n)}(x_0) + \cdots$$

- Interested in approximating $f(x)$
- Approximation centered around x_0

v.s.

Alternate Taylor Series

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \cdots + \frac{h^n}{n!}f^{(n)}(x_0) + \cdots$$

- Interested in a small perturbation away from $f(x_0)$
- Approximation centered around x_0

- Use Taylor Series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\xi), \quad \text{for } \xi \in [x, x+h]$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(\xi), \quad \text{for } \xi \in [x-h, x]$$

- Don't worry about ξ , some unknown point in the interval
- Manipulate, add, and then subtract the above Taylor Series to obtain a formula for $f'(x)$



Forward Difference



First attempt: Taylor

Let's find an approximate formula for $f'(x)$

- Taylor series:

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

- Slight rearrangement

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



First attempt: Taylor

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- Slight rearrangement

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \cancel{\frac{h}{2}f''(\xi)}$$

- If we ignore the last term, we have our approximation

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



Approximation and Error

$$\underbrace{f'(x)}_{\text{true value}} = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{approximation}} - \underbrace{\frac{h}{2}f''(\xi)}_{\text{error}}$$

- We have a method to approximate the derivative
- Notice that we have a *formula for the error*
- Absolute error

$$\begin{aligned} E &= |\text{true} - \text{approx}| \\ &= \left| f'(x) - \frac{f(x+h) - f(x)}{h} \right| \\ &= \left| -\frac{h}{2}f''(\xi) \right| \end{aligned}$$



Forward Difference

Approximation

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

with an absolute error of

$$E = \frac{h}{2} |f''(\xi)|$$

Method: Forward Difference

- **Given:** function $f(x)$, step parameter h
- **Output:** approximation to $f'(x)$
- **Idea:** Obtain a parameterized value for $f'(x_0)$ mechanically.



Evaluating Performance



Evaluating Performance

Algorithm

- Goal: approximate $f'(x_0)$
- Given: $f(x)$, h , and x_0
- Method: $f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h}$

Question

- What happens if we decrease h ?
- Does the error decrease slowly?
- Does the error decrease quickly?
- How do you quantify such a thing?



Evaluating Performance

Algorithm

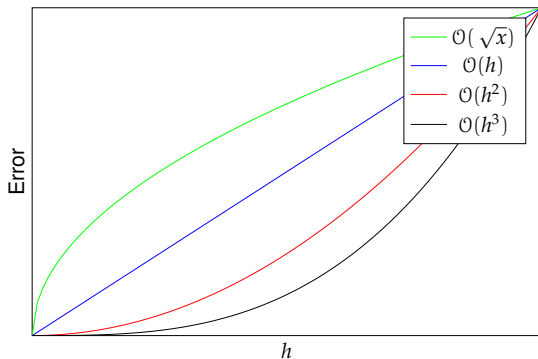
- Goal: approximate $f'(x_0)$
- Given: $f(x)$, h , and x_0
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Question

- What happens if we decrease h ?
- Does the error decrease slowly?
- Does the error decrease quickly?
- How do you quantify such a thing?
- **How do we describe the algorithm's perform?**



Convergence Rate



- We know error decreases with respect $h \rightarrow 0$.
- For the time being let's assume that error is algebraic

$$E = \mathcal{O}(h^p)$$

- Bigger $p \implies$ better algorithm



Testing Order of Convergence

Assumption

Assume error decreases like $E = \mathcal{O}(h^p)$.

Numerical Experiment

- 1 Implement your algorithm as a function of h
- 2 Choose a test function $y = f(x)$ whose true derivative $f'(x)$ is known
- 3 Choose two values for h e.g. $h_1 = 0.01$, $h_2 = 0.00001$
- 4 For each h , use your code to approximate $f'(x)$ and compute the error
- 5 Calculate

$$p = \frac{\log(E_1/E_2)}{\log(h_1/h_2)}$$



Derivation

Let $E = \mathcal{O}(h^p)$.

- Calculate the error for two different values of h

$$E_1 \approx ch_1^p \quad E_2 \approx ch_2^p$$

- Compute ratio

$$\frac{E_1}{E_2} \approx \frac{ch_1^p}{ch_2^p} = \left(\frac{h_1}{h_2}\right)^p$$

- Take the log

$$\log\left(\frac{E_1}{E_2}\right) \approx p \log\left(\frac{h_1}{h_2}\right)$$

- Thus

$$p = \frac{\log(E_1/E_2)}{\log(h_1/h_2)}$$



- Consider

$$f(x) = \sin(\pi x) \text{ on } [-1, 1]$$

- Approximate $f'(x) = \pi \cos(\pi x)$ with

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

- Compute

$$p = \frac{\log(\text{err}_k / \text{err}_j)}{\log(h_k / h_j)}$$

- Results:

See `diff_fwd.m`



Plotting Convergence

How to display experimental rate of convergence:

- 1 Implement your algorithm as a function of h
- 2 Choose a test function $y = f(x)$ whose true derivative $f'(x)$ is known
- 3 Choose a range of values for h e.g. $h = 1/2, 1/4, 1/8, 1/16, \dots$
- 4 For each h , use your code to approximate $f'(x)$ and compute the error
- 5 Tabulate the results

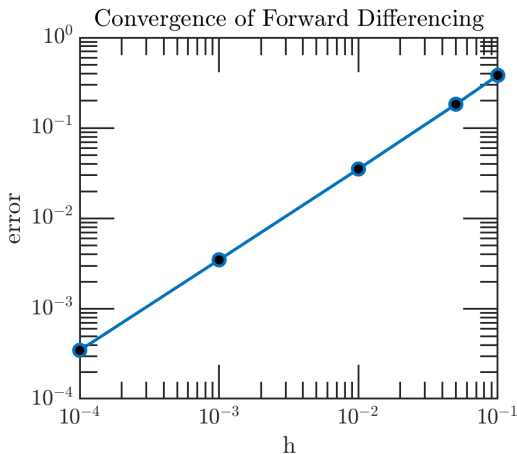
h	1/2	1/4	1/8	1/16
Error				

- 6 Plot Error versus h on a log-log plot or a log-linear plot

See `diff_fwd_plot.m`



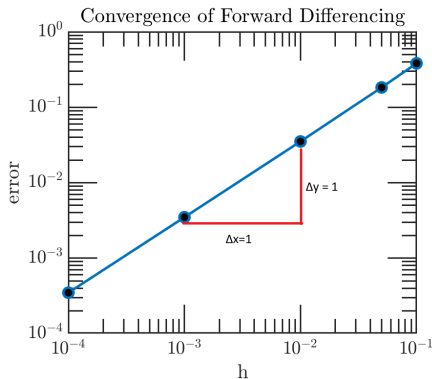
Plotting Convergence



- This is a log-log plot
- h decreases going from right to left
- As h decreases, the error decreases



Assessing Convergence Rate



- If $E = Ch^p$, then $\log(E) = p \log(h) + K$ so the slope must be p

Key Idea

Count the slope on the log-log plot to find p . Forward difference plot shows $p = 1$.

- Experimentally, we have found that the forward difference has an error

$$E = \mathcal{O}(h^p), \quad p = 1$$

Definition: Order of Accuracy

The integer p in $E = \mathcal{O}(h^p)$ is called the **order of accuracy**.

- We say that forward difference scheme is

"first-order accurate"



Truncation Error

- The term ignored in the Taylor expansion *is* the error term

$$\underbrace{f'(x)}_{\text{true value}} = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{approximation}} - \underbrace{\frac{h}{2}f''(\xi)}_{\text{ignore}}$$

- The error depends on f'' , ξ , and h but $f''(\xi)$ is roughly constant if f is smooth so we write

$$\text{error} = \frac{h}{2} |f''(\xi)| \approx Ch = \mathcal{O}(h)$$

Key Idea

The theoretical error terms is called the truncation error. The truncation error tells use the order of accuracy.

Backward Difference



Backward Difference

- Let's derive another differentiation scheme with the backward Taylor expansion

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



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

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



Backward Difference

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

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



Backward Difference

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$$\frac{f(x) - f(x-h)}{h} = f'(x) - \frac{h}{2}f''(\xi)$$



Backward Difference

- Let's derive another differentiation scheme with the backward Taylor expansion

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

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

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

$$\frac{f(x) - f(x-h)}{h} = f'(x) - \frac{h}{2}f''(\xi)$$

- We have a new scheme

$$\underbrace{\frac{f(x) - f(x-h)}{h}}_{\text{approx}} = \underbrace{f'(x)}_{\text{true}} - \underbrace{\frac{h}{2}f''(\xi)}_{\text{ignore}}$$



Backward Difference

- This approximation is called the **backward difference scheme**

$$f'(x) \approx \frac{f(x) - f(x - h)}{h}$$

- Error is also first-order accurate

$$\text{error} = \frac{h}{2}f''(\xi) = \mathcal{O}(h)$$

Method: Backward Difference

- **Given:** function $f(x)$, step parameter h
- **Output:** approximation to $f'(x)$
- **Idea:** Similar to forward difference but it looks at a prior point



Central Difference



Can we do better?

- Look at the Forward AND Backward Taylor series together

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

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



Can we do better?

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- Subtract them:

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \mathcal{O}(h^4)$$



Can we do better?

- Look at the Forward AND Backward Taylor series together

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

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- Subtract them:

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \mathcal{O}(h^4)$$

- Thus

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



Truncation Error

- Subtracting $f(x+h)$ and $f(x-h)$ cancels out even powers and odd powers

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

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

- The truncation error (true - approx) has the form

$$\begin{aligned} f'(x) - \frac{f(x+h) - f(x-h)}{2h} &= -\frac{h^2}{3!}f'''(x) - \frac{h^4}{5!}f^{(5)}(x) - \frac{h^6}{7!}f^{(7)}(x) - \dots \\ &= c_2h^2 + c_4h^4 + \dots \end{aligned}$$



Central Difference - The Method

Approximation

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

with truncation error of

$$\text{error} = -\frac{h^2}{6}f'''(\xi) = \mathcal{O}(h^2)$$

Method: Central Difference

- **Given:** function $f(x)$, step parameter h
- **Output:** approximation to $f'(x)$
- **Idea:** improvement over the forward and backward difference methods



What's with the Names?

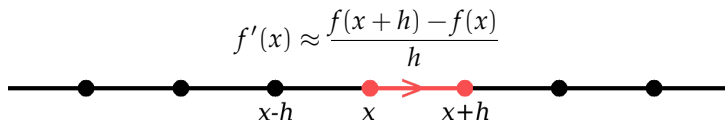
- Forward difference looks forward

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

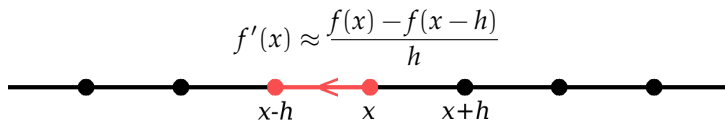



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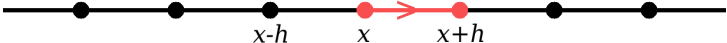


- Backward difference looks backward

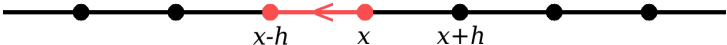


What's with the Names?

- Forward difference looks forward

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


- Backward difference looks backward

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$


- Central difference centers the subtraction around x

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




Performance?

- In theory, the error for forward difference is

$$E_{fwd} = \frac{h}{2}|f''(\xi)|$$

- Error for central difference is

$$E_{cen} = \frac{h^2}{6}|f'''(\xi)|$$

Question

- What does this mean about the two algorithms?
- Which one is better?



Same test as before

- Consider

$$f(x) = \sin(\pi x) \text{ on } [-1, 1]$$

- Use centered difference

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

- Calculate

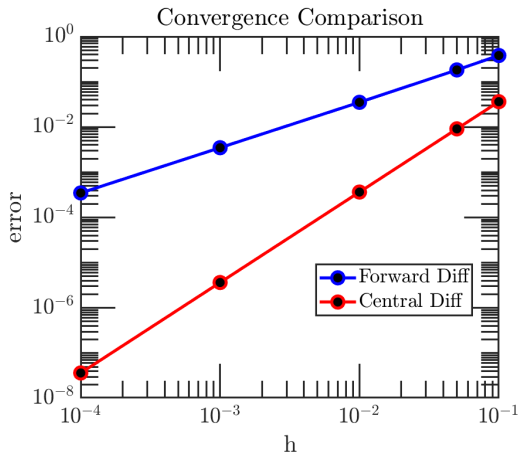
$$p = \frac{\log(\text{err}_k / \text{err}_j)}{\log(h_k / h_j)}$$

- We are expecting $p \approx 2$

See diff_central.m



Comparison in Convergence



Key Idea

Since central difference is 2nd-order accurate, its error plummets to much faster as $h \rightarrow 0^+$.

Moving Forward

- Are there schemes that go beyond $\mathcal{O}(h^2)$?
- Can we approximate higher order derivatives $f''(x)$?
- How should the parameter h be chosen in practice?

