

Lecture 03 - B

§4.3 Extrapolation

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Goals

We will answer these questions:

- What exactly is truncation error?
- What is Richardson extrapolation?
- What are the two sources of error when implementing a finite difference scheme on the computer?
- How do you approximate the 2nd derivative $f''(x)$?



Understanding Truncation Error



Truncation Error

- If we wrote the full Taylor series with no approximation

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

- Then rearranged to get forward difference

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

- The error is |true—approx|

Truncation Error

The truncation error is an *infinite* series

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



Leading Order Term

Large n

- Recall that the worst-case cost of bubble sort is

$$f(n) = \frac{n^2}{2} - \frac{n}{2}$$

but we express this in Big-O notation as $\mathcal{O}(n^2)$ as $n \rightarrow \infty$

- When $n \gg 0$, the $n^2/2$ term dominates the $n/2$ term



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- When $n \gg 0$, the $n^2/2$ term dominates the $n/2$ term

Small h

- In the forward difference error

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

the term $h^2/2f''(x)$ dominates as $h \rightarrow 0$

Leading Order Term

- If h is small, then

$$E = \underbrace{\frac{h}{2}f''(x)}_{\text{small}} + \underbrace{\frac{h^2}{6}f'''(x)}_{\text{tiny}} + \underbrace{\frac{h^3}{24}f^{(4)}(x)}_{\text{very tiny}} \dots$$

- In the limit $h \rightarrow 0$ the term that dominates is

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

- For **truncation error** we only care about the *smallest* power of h which in this case is

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



Asymptotics

- Consider the function $f(x) = x + x^2 + x^3$

- In the limit as $x \rightarrow \infty$,

$$f(x) = \mathcal{O}(x^3)$$

- In the limit as $x \rightarrow 0$,

$$f(x) = \mathcal{O}(x)$$

Key Idea

When considering truncation error (small h) the term that vanishes the slowest is the leading order term.



Main Idea

- We use Taylor expansions to derive equations such as

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



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- Identify the true value, the approximation, and the error

$$\underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{approx}} = \underbrace{f'(x)}_{\text{true}} + \underbrace{\frac{h}{2}f''(x) + \frac{h^2}{6}f'''(x) + \frac{h^3}{24}f^{(4)}(x) \cdots}_{\text{error}}$$



Main Idea

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$$\underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{approx}} = \underbrace{f'(x)}_{\text{true}} + \underbrace{\frac{h}{2}f''(x) + \frac{h^2}{6}f'''(x) + \frac{h^3}{24}f^{(4)}(x) \dots}_{\text{error}}$$

- In the limit as $h \rightarrow 0$, the lowest power of h dominates

$$E = \underbrace{\frac{h}{2}f''(x)}_{\text{dominant}} + \underbrace{\frac{h^2}{6}f'''(x) + \frac{h^3}{24}f^{(4)}(x) \dots}_{\text{asymptotically insignificant}} = \mathcal{O}(h)$$



Extrapolation



Improving the Method

- Suppose you want to approximate $f'(x)$
- Suppose you already have one scheme $\phi(h) \approx f'(x)$
- For example $\phi(h) = \frac{f(x+h)-f(x)}{h}$

Question

Can you develop an improvement $\psi(x)$ over the original ϕ using a linear combination, e.g.

$$\psi(h) = w_1\phi(c_1h) + w_2\phi(c_2h)$$



Even Smarter?

- Let's try to improve centered difference

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



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

- We know that truncation error has *even powers* of h

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x-h)}{2h} + c_2h^2 + c_4h^4 + c_6h^6 + \dots \\ &= \phi(h) + c_2h^2 + c_4h^4 + c_6h^6 + \dots \\ \phi(h) &= f'(x) - c_2h^2 - c_4h^4 - c_6h^6 - \dots \end{aligned}$$



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- We expect the error to be reduced by 1/4 when h is cut in half.



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- We know that truncation error has *even powers* of h

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + c_2h^2 + c_4h^4 + c_6h^6 + \dots$$

$$= \phi(h) + c_2h^2 + c_4h^4 + c_6h^6 + \dots$$

$$\phi(h) = f'(x) - c_2h^2 - c_4h^4 - c_6h^6 - \dots$$

- We expect the error to be reduced by 1/4 when h is cut in half.
- Utilize this!

$$\phi(h) = f'(x) - c_2h^2 - c_4h^4 - c_6h^6 - \dots$$

$$\phi(h/2) = f'(x) - c_2(h/2)^2 - c_4(h/2)^4 - c_6(h/2)^6 - \dots$$



Richardson Extrapolation

- Utilize this!

$$\phi(h) = f'(x) - c_2h^2 - c_4h^4 - c_6h^6 - \dots$$

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$$\phi(h/2) = f'(x) - c_2(h/2)^2 - c_4(h/2)^4 - c_6(h/2)^6 - \dots$$

- Combine these to eliminate the “ c_2 ” term:

$$\phi(h) - 4\phi(h/2) = -3f'(x) - (3/4)c_4h^4 - (15/16)c_6h^6 - \dots$$



Richardson Extrapolation

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- Dividing by -3 , and regrouping terms,

$$\phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) = f'(x) + (1/4)c_4h^4 + (5/16)c_6h^6 - \dots$$



Richardson Extrapolation

- Utilize this!

$$\begin{aligned}\phi(h) &= f'(x) - c_2 h^2 - c_4 h^4 - c_6 h^6 - \dots \\ \phi(h/2) &= f'(x) - c_2 (h/2)^2 - c_4 (h/2)^4 - c_6 (h/2)^6 - \dots\end{aligned}$$

- Combine these to eliminate the “ c_2 ” term:

$$\phi(h) - 4\phi(h/2) = -3f'(x) - (3/4)c_4 h^4 - (15/16)c_6 h^6 - \dots$$

- Dividing by -3 , and regrouping terms,

$$\phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) = f'(x) + (1/4)c_4 h^4 + (5/16)c_6 h^6 - \dots$$

- Result:

$$\underbrace{\phi(h/2) + (1/3)(\phi(h/2) - \phi(h))}_{\text{scheme}} = \underbrace{f'(x)}_{\text{true}} + \underbrace{(1/4)c_4 h^4 + (5/16)c_6 h^6 - \dots}_{\text{error}}$$



Improvement in Accuracy

Original Scheme

We started with $\phi(h)$ 2nd order accurate

$$\begin{aligned}f'(x) &= \frac{f(x+h) - f(x-h)}{2h} + c_2h^2 + c_4h^4 + c_6h^6 + \dots \\&= \phi(h) + \mathcal{O}(h^2)\end{aligned}$$

Fourth Order Richardson Extrapolation

We obtained $\psi(x)$ 4th order accurate

$$\begin{aligned}f'(x) &= \phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) + (1/4)c_4h^4 + (5/16)c_6h^6 - \dots \\&= \psi(x) + \mathcal{O}(h^4)\end{aligned}$$

Key Idea

We eliminated the leading order error c_2h^2 to increase the accuracy.

And better?

Question

What's stopping us from doing Richardson extrapolation again?



And better?

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What's stopping us from doing Richardson extrapolation again?

- We can extend the Richardson extrapolation idea to any order.
- Idea: use $\psi(h) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h))$ to annihilate the fourth order error term:



And better?

Question

What's stopping us from doing Richardson extrapolation again?

- We can extend the Richardson extrapolation idea to any order.
- Idea: use $\psi(h) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h))$ to annihilate the fourth order error term:
- Giving us

Sixth Order Richardson Extrapolation

$$f'(x) = \psi(h/2) + (1/15)(\psi(h/2) - \psi(h)) + \mathcal{O}(h^6)$$

where $\psi(h)$ is the fourth order Richardson extrapolation.



Richardson Extrapolation

Fourth Order Richardson Extrapolation

$$f'(x) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) + \mathcal{O}(h^4)$$

where $\phi(h)$ is the central difference approximation.

Sixth Order Richardson Extrapolation

$$f'(x) = \psi(h/2) + (1/15)(\psi(h/2) - \psi(h)) + \mathcal{O}(h^6)$$

where $\psi(h)$ is the fourth order Richardson extrapolation.

Method: Richardson Extrapolation

- **Given:** Derivative approximation $\phi(h) \approx f'(x)$
- **Output:** Improved approximation $\psi(h)$
- **Idea:** General technique to improve upon existing scheme.

Example

Suppose you use the 4th order Richardson to approximate $f'(x)$ with a small h and you obtain the error E . How much smaller will the error be if h is reduced by half?

- We begin by finding a formula for E

$$E = \mathcal{O}(h^4) \approx Ch^4$$

- If we halve h then

$$E_{1/2} = \mathcal{O}((h/2)^4) \approx C \frac{h^4}{2^4} = C \frac{h^4}{16}$$

- Since $E = Ch^4$ we have

$$E_{1/2} = \frac{Ch^4}{16} = \frac{E}{16}$$

so $E_{1/2}$ is *sixteen* times smaller than E



Rounding vs. Truncation Error



- Consider

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

- Run code to approximate $f'(x) = \pi \cos(\pi x)$ using

$$f'(x) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) + \mathcal{O}(h^4)$$

with

$$h = 0.01$$



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- We see that $p \approx 3.9999$, so its $\mathcal{O}(h^4)$ accurate!



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- Next lower stepsize to $h = 0.001$



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with

$$h = 0.01$$

- We see that $p \approx 3.9999$, so its $\mathcal{O}(h^4)$ accurate!
- Next lower stepsize to $h = 0.001$

!!!

Decreasing h to 0.001 made the error worse instead of improving it!

Truncation Error

Truncation Error

- **Definition:** The error that arises when an infinite series is approximated by a finite sum.
- **Example:** Using the forward difference formula:

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

The term $-\frac{h}{2}f''(\xi)$ represents truncation error.

- **How to Reduce:** Use higher-order methods such as the central difference or Richardson extrapolation.

Truncation error is a mathematical error introduced in the development of the scheme.



Rounding Error

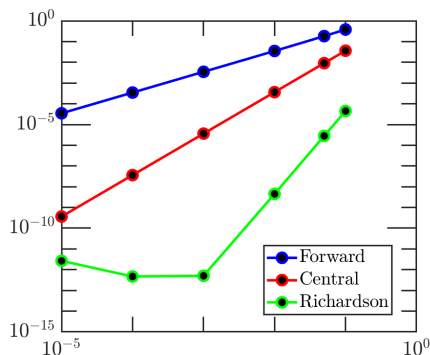
Rounding Error

- **Definition:** The error due to finite precision arithmetic in computers, which leads to small inaccuracies in calculations.
- **Example:** If h is too small, subtracting nearly equal numbers (e.g., $f(x+h) - f(x)$) can lead to significant loss of precision due to floating-point rounding errors.
- **How to Reduce:** Choose an optimal step size h —not too large (to minimize truncation error) and not too small (to minimize rounding error).

Rounding error is a numerical error introduced in the implementation of the scheme.



Caution About Tuning h



- Richardson error converges to zero the most rapidly
- Richardson error starts to rise after going lower than critical value of h
- The error computed in Matlab contains a mix of truncation error AND rounding error



- **Truncation Error** is theoretical

$$E_{\text{trunc}} = \left| f'(x) - \frac{f(x+h) - f(x)}{h} \right|$$

- **Round-off Error** happens when you use floating-point numbers

$$E_{\text{round}} = \left| \frac{f(x+h) - f(x)}{h} - \text{fl} \left(\frac{f(x+h) - f(x)}{h} \right) \right|$$

- The total error is the sum of both errors

$$E_{\text{total}} = E_{\text{trunc}} + E_{\text{round}}$$



Total Error

Total Error

Approximating $f'(a)$ on the computer will contain a mixture of truncation error *and* rounding error.

Key Idea

The truncation error decreases as we make the parameter h smaller. However, when h is too small rounding error will take over and cause the error to rise.



Total Error

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Approximating $f'(a)$ on the computer will contain a mixture of truncation error *and* rounding error.

Key Idea

The truncation error decreases as we make the parameter h smaller. However, when h is too small rounding error will take over and cause the error to rise.

How do you know how small to make h ?



Total Error

Total Error

Approximating $f'(a)$ on the computer will contain a mixture of truncation error *and* rounding error.

Key Idea

The truncation error decreases as we make the parameter h smaller. However, when h is too small rounding error will take over and cause the error to rise.

How do you know how small to make h ? **Homework!**



Second Order Derivative



Derivative Approximations

Forward Difference

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

Backward Difference

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

Central Difference

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

Question

How do we approximate $f''(x)$?

Derivation

- Look at the Forward AND Backward Taylor series together

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

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



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

- Add them:

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



Derivation

- Look at the Forward AND Backward Taylor series together

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

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

- Add them:

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

- Subtract

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



Derivation

- Look at the Forward AND Backward Taylor series together

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

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

- Add them:

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

- Subtract

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

- Divide

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



2nd Order Central Difference

Scheme

$$f''(x) = \underbrace{\frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}_{\text{scheme}} + \underbrace{\frac{h^2}{12}f''''(\xi)}_{\text{error}}$$

Method: 2nd Order Central Difference

- **Given:** function $f(x)$, step parameter h
- **Output:** approximation to $f''(x)$
- **Idea:** This scheme approximates $f''(x)$ knowing nothing about $f'(x)$

Note: Since the error term contains $f''''(\xi)$ this formula has *zero error* if $f(x)$ is a 3rd order polynomial.



Hand Calculations



Forward Difference

Example

Approximate $f'(1)$ for $f(x) = x^3$ using the forward difference with $h = \frac{1}{2}$.

- True derivative:

$$f'(x) = 3x^2 \Rightarrow f'(1) = 3$$

- Forward difference:

$$f'(1) \approx \frac{f(1+h) - f(1)}{h}$$

- Compute:

$$\frac{(3/2)^3 - 1^3}{1/2} = \frac{\frac{27}{8} - 1}{1/2} = \frac{\frac{19}{8}}{1/2} = \frac{19}{4} = 4.75$$

- Error:

$$|4.75 - 3| = 1.75$$

Key Idea

Forward difference can be very inaccurate for moderate h .

1st Order Central Difference

Example

Approximate $f'(1)$ for $f(x) = x^3$ using the central difference with $h = \frac{1}{2}$.

- Central difference:

$$f'(1) \approx \frac{f(1+h) - f(1-h)}{2h}$$

- Compute:

$$\frac{(3/2)^3 - (1/2)^3}{1} = \frac{\frac{27}{8} - \frac{1}{8}}{1} = \frac{26}{8} = \frac{13}{4} = 3.25$$

- Error:

$$|3.25 - 3| = 0.25$$



Comparison

Problem

Approximate $f'(1)$ for $f(x)$ using $h = 1/2$.

Method	Approximation	Error
Forward Difference	$\frac{19}{4}$	1.75
Central Difference	$\frac{13}{4}$	0.25

Key Idea

Central difference is much more accurate at the same h .



2nd Order Central Difference

Example

Approximate $f''(1)$ for $f(x) = x^3$ using the second-order central difference with $h = \frac{1}{2}$.

- True second derivative:

$$f''(x) = 6x \quad \Rightarrow \quad f''(1) = 6$$

- Approximation:

$$f''(1) \approx \frac{f(1+h) - 2f(1) + f(1-h)}{h^2}$$

- Compute:

$$\frac{\frac{27}{8} - 2(1) + \frac{1}{8}}{(1/2)^2} = \frac{\frac{28}{8} - 2}{1/4} = \frac{3.5 - 2}{1/4} = \frac{1.5}{1/4} = 6$$



2nd Order Central Difference

Example

Approximate $f''(1)$ for $f(x) = x^3$ using the second-order central difference with $h = \frac{1}{2}$.

- True second derivative:

$$f''(x) = 6x \quad \Rightarrow \quad f''(1) = 6$$

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- Compute:

$$\frac{\frac{27}{8} - 2(1) + \frac{1}{8}}{(1/2)^2} = \frac{\frac{28}{8} - 2}{1/4} = \frac{3.5 - 2}{1/4} = \frac{1.5}{1/4} = 6$$

There is NO error for approximating the derivative!



Why is there no error?

Scheme

$$f''(x) = \underbrace{\frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}_{\text{scheme}} + \underbrace{\frac{h^2}{12}f''''(\xi)}_{\text{error}}$$

- The leading order term contains $f''''(\xi)$
- The function we approximated was $f(x) = x^3$
- The derivatives are:

$$f'(x) = 3x^2$$

$$f''(x) = 6x$$

$$f'''(x) = 6$$

$$f''''(x) = 0$$



Why is there no error?

Scheme

$$f''(x) = \underbrace{\frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}_{\text{scheme}} + \underbrace{\frac{h^2}{12}f''''(\xi)}_{\text{error}}$$

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$$f''(x) = 6x$$

$$f'''(x) = 6$$

$$f''''(x) = 0$$

Key Idea

The central difference will never have any truncation error if the function is a polynomial of degree 3 or less.