- Recap from last class:

$$\frac{\partial}{\partial t}(\ldots) + \text{spatial derivatives} = 0$$

  - approximate spatial derivatives

$$f_i' = \frac{f_{i+1} - f_i}{h} + O(h)$$ Forward difference: 1st order

$$f_i' = \frac{f_i - f_{i-1}}{h} + O(h)$$ Backward difference: 1st order

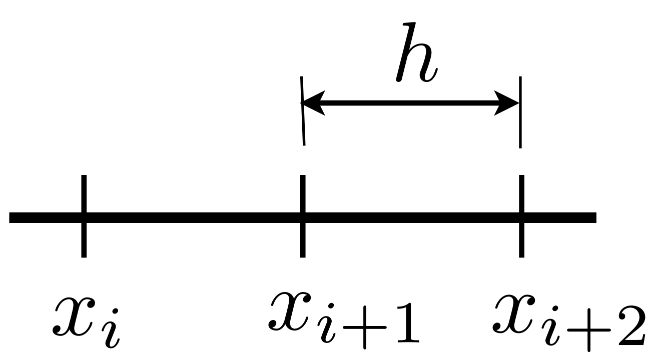
$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$$ Central difference: 2nd order

  - However, the derivation of these finite difference formulas was very ad-hoc
  - Need a more general technique

- General technique
  - Goal: derive most accurate formula for f'_i using a given set of grid points
  - given set of grid points = **stencil**
  - assume constant grid point spacing h
  - Example 4:

find $\left.\dfrac{\partial f}{\partial x}\right|_{x_i}$ using only grid points $x_i,\ x_{i+1},\ x_{i+2}$

stencil:

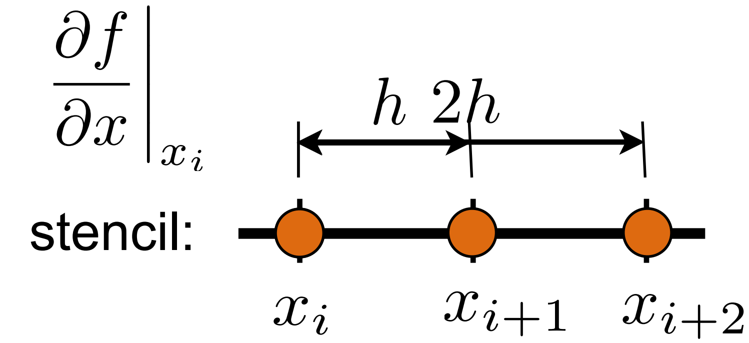


or $f'_i + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = O(?)$

Task: find a_0, a_1, a_2 for maximum order

- Step 1: Write Taylor series for each stencil point around point where derivative is requested
- Step 2: Put into Taylor table (can combine with step 1)
- Step 3: Set as many of the lower order terms on the right hand side to zero as possible
- Step 4: Substitute solution back in

- **This works for higher derivatives as well!**
- However: for a stencil of n points, the approximation f'_i is at most $O(h^{n-1})$



- Step 1: Write Taylor series for each stencil point around point where derivative is requested

$$f_i = f_i$$

$$f_{i+1} = f_i + hf_i' + \frac{1}{2}h^2 f_i'' + \frac{1}{6}h^3 f_i''' + \ldots$$

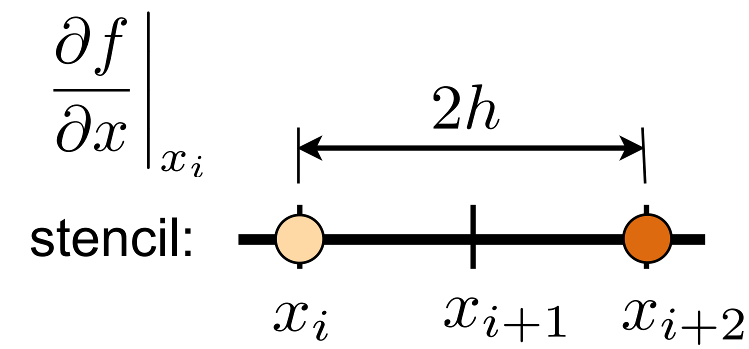
$$f_{i+2} = f_i + 2hf_i' + \frac{1}{2}(2h)^2 f_i'' + \frac{1}{6}(2h)^3 f_i''' + \ldots$$

- Step 2: Put into Taylor table (can combine with step 1)

	f_i	f_i'	f_i''	f_i'''
f_i'				
$a_0 f_i$				
$a_1 f_{i+1}$				
$a_2 f_{i+2}$				

derivates in Taylor series expansion

terms from target formula $f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2}$



- Step 1: Write Taylor series for each stencil point around point where derivative is requested

$$f_i = f_i$$

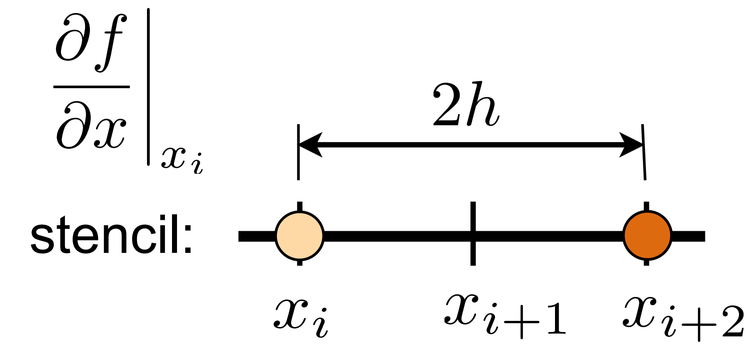
$$f_{i+1} = f_i + hf_i' + \frac{1}{2}h^2 f_i'' + \frac{1}{6}h^3 f_i''' + \ldots$$

$$f_{i+2} = f_i + 2hf_i' + \frac{1}{2}(2h)^2 f_i'' + \frac{1}{6}(2h)^3 f_i''' + \ldots$$

- Step 2: Put into Taylor table (can combine with step 1)

	f_i	f_i'	f_i''	f_i'''
f_i'				
$a_0 f_i$				
$a_1 f_{i+1}$				
$a_2 f_{i+2}$				

fill table with linear combination coefficients,
such that
header column = linear combination of header row



- Step 1: Write Taylor series for each stencil point around point where derivative is requested

$$f_i = f_i$$

$$f_{i+1} = f_i + h f_i' + \frac{1}{2} h^2 f_i'' + \frac{1}{6} h^3 f_i''' + \dots$$

$$f_{i+2} = f_i + 2h f_i' + \frac{1}{2} (2h)^2 f_i'' + \frac{1}{6} (2h)^3 f_i''' + \dots$$

- Step 2: Put into Taylor table (can combine with step 1)

	f_i	f_i'	f_i''	f_i'''	
f_i'	0	1	0	0	$f_i' = f_i'$ derivative we want
$a_0 f_i$	a_0	0	0	0	use 1st TS
$a_1 f_{i+1}$	a_1	$a_1 h$	$\frac{1}{2} a_1 h^2$	$\frac{1}{6} a_1 h^3$	use 2nd TS
$a_2 f_{i+2}$	a_2	$a_2 2h$	$a_2 2h^2$	$\frac{4}{3} a_2 h^3$	use 3rd TS

	f_i	f'_i	f''_i	f'''_i
f'_i	0	1	0	0
$a_0 f_i$	a_0	0	0	0
$a_1 f_{i+1}$	a_1	$a_1 h$	$\frac{1}{2} a_1 h^2$	$\frac{1}{6} a_1 h^3$
$a_2 f_{i+2}$	a_2	$a_2 2h$	$a_2 2h^2$	$\frac{4}{3} a_2 h^3$

write: sum of header column = sum of each table column * header row entry

$$f'_i + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = (a_0 + a_1 + a_2) f_i + (1 + a_1 h + 2a_2 h) f'_i + \left(\frac{1}{2} a_1 h^2 + 2a_2 h^2\right) f''_i + \left(\frac{1}{6} a_1 h^3 + \frac{4}{3} a_2 h^3\right) f'''_i + \dots$$

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = \cancel{(a_0 + a_1 + a_2) f_i} + \cancel{(1 + a_1 h + 2a_2 h) f_i'} +$$
$$\cancel{\left(\frac{1}{2}a_1 h^2 + 2a_2 h^2\right)} f_i'' + \left(\frac{1}{6}a_1 h^3 + \frac{4}{3}a_2 h^3\right) f_i''' + \ldots$$

- Step 3: Set as many of the lower order terms on the right hand side to zero as possible

$$a_0 + a_1 + a_2 = 0$$

$$1 + a_1 h + 2a_2 h = 0$$

3 equations for 3 unknowns ($a_0,\ a_1,\ a_2$)

$$\frac{1}{2}a_1 h^2 + 2a_2 h^2 = 0$$

Solve! (Linear Algebra): $a_0 = \frac{3}{2h}$ $a_1 = -\frac{2}{h}$ $a_2 = \frac{1}{2h}$

- Step 4: Substitute solution back in

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = f_i' + \frac{3}{2h} f_i - \frac{2}{h} f_{i+1} + \frac{1}{2h} f_{i+2}$$
$$= \left(-\frac{1}{6}\frac{2}{h}h^3 + \frac{4}{3}\frac{1}{2h}h^3\right) f_i''' + \ldots = \frac{1}{3}h^2 f_i''' + \ldots$$

$$f_i' + \frac{3}{2h} f_i - \frac{2}{h} f_{i+1} + \frac{1}{2h} f_{i+2} \quad = \frac{1}{3} h^2 f_i''' + \ldots$$

Solve for target derivative f'_i:

$$f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \frac{1}{3} h^2 f_i''' + \ldots$$

$$\boxed{f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + O(h^2)}$$

Order? 2nd order!

But compared to central differences, error is a factor 2 larger:

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{1}{6} h^2 f_i''' + \ldots$$

- Example: calculate the first derivative of f(x) = sin(x) at x=1 using the finite difference formula just derived

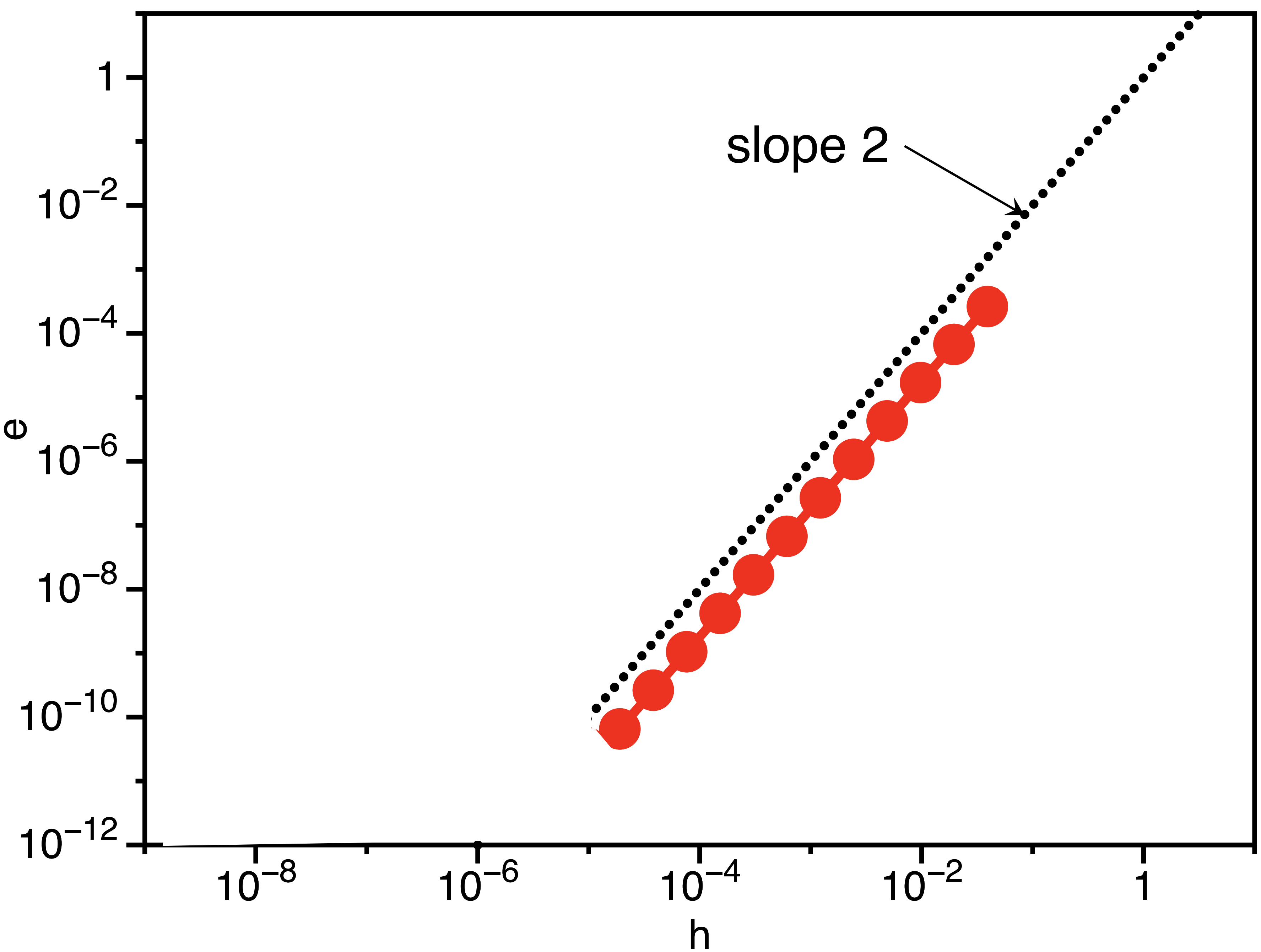
- Solution:
  - define mesh spacing h and calculate f at mesh points used in finite difference formula
  - calculate derivative using finite difference formula

$$f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h}$$

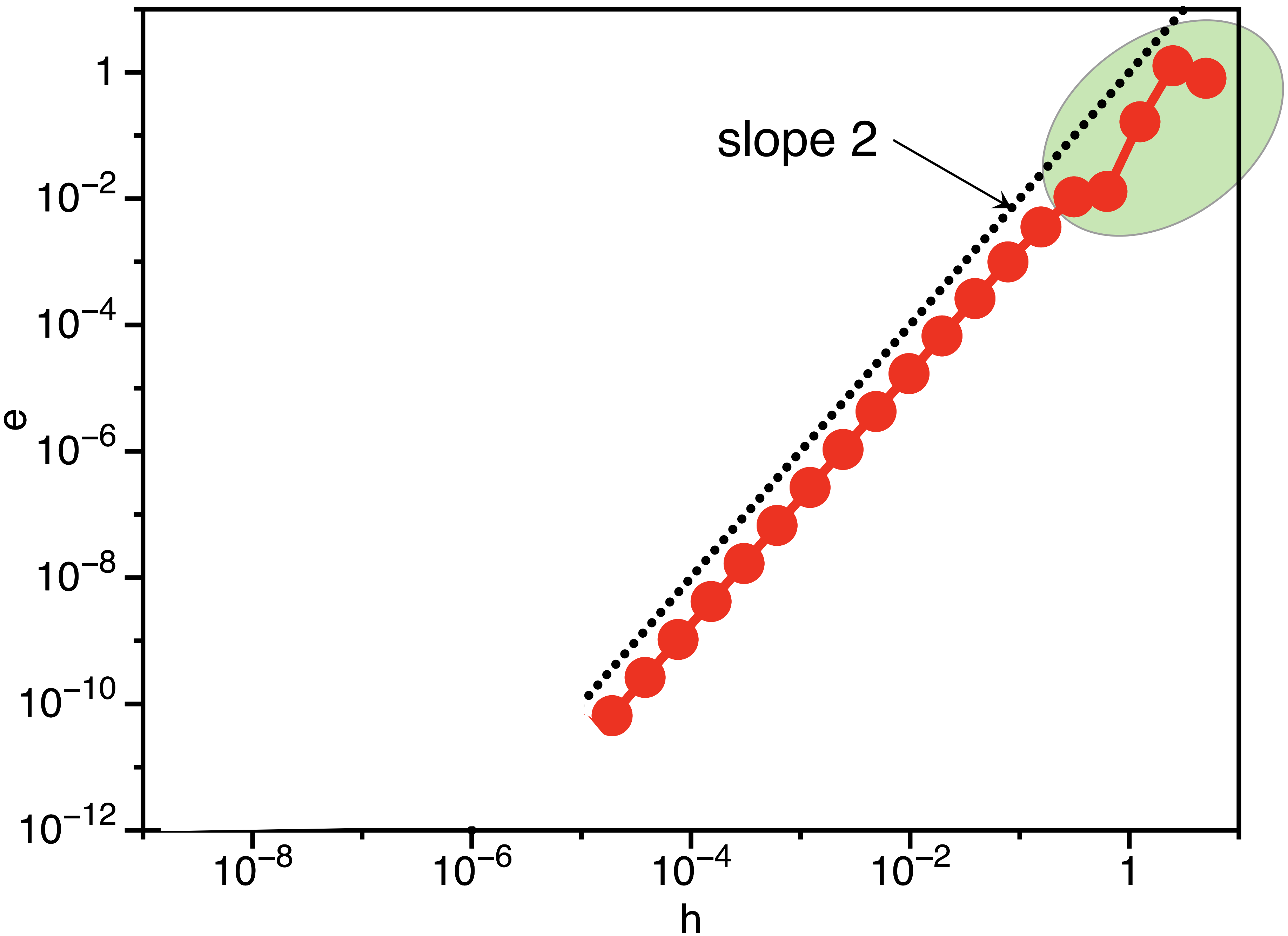
  - What's the error e?

exact f': $$f'(x_i) = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \frac{1}{3}h^2 f_i''' + \frac{1}{4}h^3 f_i^{(IV)} + \frac{7}{60}h^4 f_i^{(V)} + \dots$$

$$e = |f'(x_i) - f_i'| = \left| \frac{1}{3}h^2 f_i''' + \frac{1}{4}h^3 f_i^{(IV)} + \frac{7}{60}h^4 f_i^{(V)} + \dots \right|$$

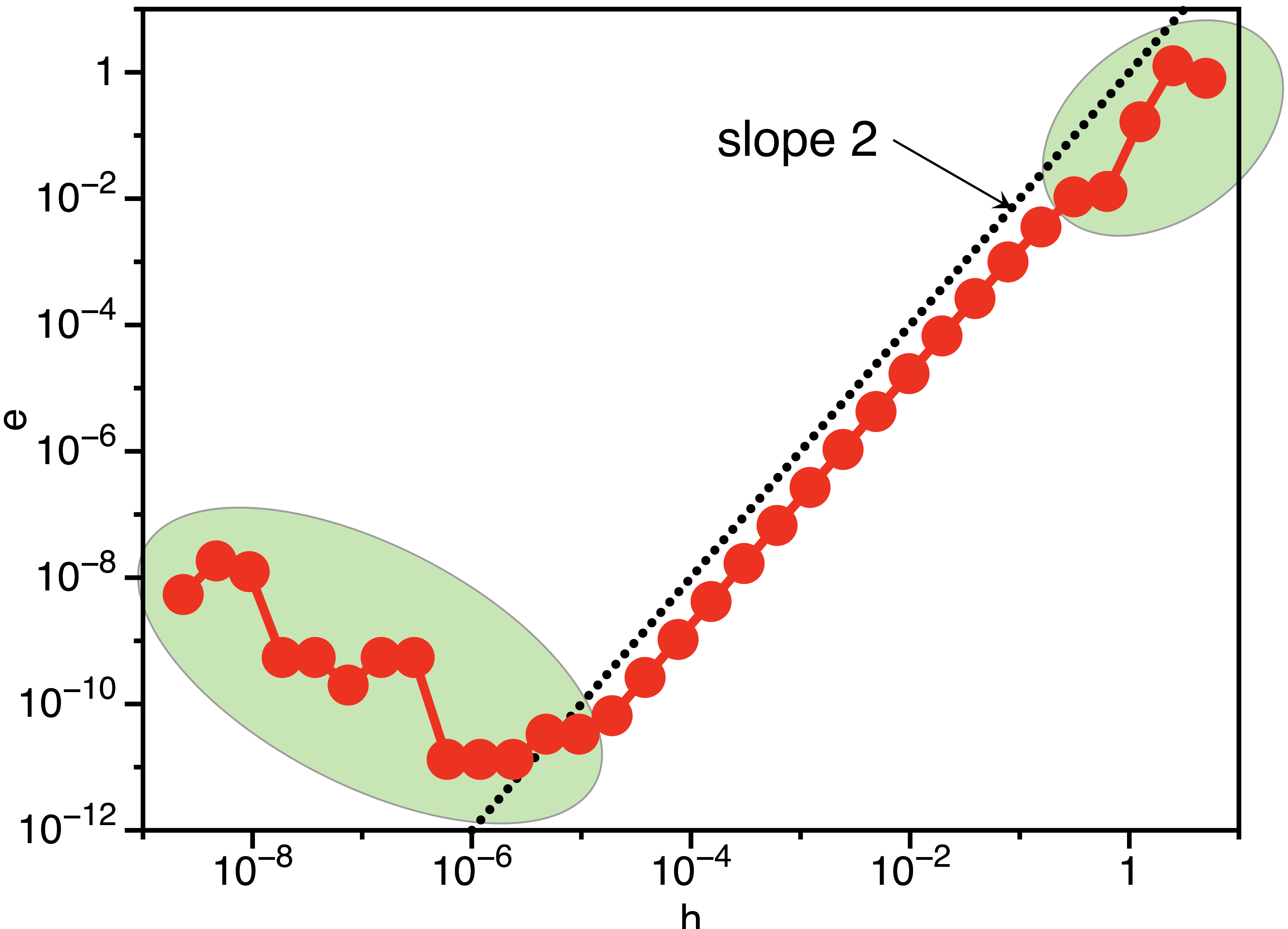


$$e = |f'(x_i) - f'_i| = \left| \frac{1}{3} h^2 f'''_i + \frac{1}{4} h^3 f_i^{(IV)} + \frac{7}{60} h^4 f_i^{(V)} + \ldots \right| = O(h^2)$$



h must be sufficiently small

$$e = |f'(x_i) - f'_i| = \left| \frac{1}{3} h^2 f'''_i + \frac{1}{4} h^3 f_i^{(IV)} + \frac{7}{60} h^4 f_i^{(V)} + \ldots \right| = O(h^2)$$



h must be sufficiently small

$$f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + O(h^2)$$

➡ differences of O(1) numbers

➡ accurate only up to about 1e-16 for double precision (64bit)

➡ still gets divided by ever smaller h ⇒ error increases

- Can we improve on the general technique somehow?
  - Idea: use not only *f* @ stencil points, but also *f'* (PADE)

  - Example 5:

    find $\left.\dfrac{\partial f}{\partial x}\right|_{x_i}$ using only grid points $x_{i-1},\, x_i,\, x_{i+1}$

    or $f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i-1} \boxed{+ a_3 f_{i+1}' + a_4 f_{i-1}'} = O(?)$

- Step 1: Write Taylor series for each stencil point around point where derivative is requested
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- Step 1: Write Taylor series for each stencil point around point where derivative is requested
- Step 2: Put into Taylor table (can combine with step 1)

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i-1} + a_3 f_{i+1}' + a_4 f_{i-1}' = O(?)$$

	f_i	f_i'	f_i''	f_i'''	$f_i^{(IV)}$	$f_i^{(V)}$
f_i'	0	1	0	0	0	0
$a_0 f_i$	a_0	0	0	0	0	0
$a_1 f_{i+1}$	a_1	$a_1 h$	$\frac{1}{2} a_1 h^2$	$\frac{1}{6} a_1 h^3$	$\frac{1}{24} a_1 h^4$	$\frac{1}{120} a_1 h^5$
$a_2 f_{i-1}$	a_2	$-a_2 h$	$\frac{1}{2} a_2 h^2$	$-\frac{1}{6} a_2 h^3$	$\frac{1}{24} a_2 h^4$	$-\frac{1}{120} a_2 h^5$
$a_3 f_{i+1}'$	0	a_3	$a_3 h$	$\frac{1}{2} a_3 h^2$	$\frac{1}{6} a_3 h^3$	$\frac{1}{24} a_3 h^4$
$a_4 f_{i-1}'$						

use TS for f': $f_{i+1}' = f_i' + h f_i'' + \frac{1}{2} h^2 f_i''' + \frac{1}{6} h^3 f_i^{(IV)} + \frac{1}{24} h^4 f_i^{(V)} + \dots$

- Step 1: Write Taylor series for each stencil point around point where derivative is requested
- Step 2: Put into Taylor table (can combine with step 1)

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i-1} + a_3 f_{i+1}' + a_4 f_{i-1}' = O(?)$$

	f_i	f_i'	f_i''	f_i'''	$f_i^{(IV)}$	$f_i^{(V)}$
f_i'	0	1	0	0	0	0
$a_0 f_i$	a_0	0	0	0	0	0
$a_1 f_{i+1}$	a_1	$a_1 h$	$\frac{1}{2} a_1 h^2$	$\frac{1}{6} a_1 h^3$	$\frac{1}{24} a_1 h^4$	$\frac{1}{120} a_1 h^5$
$a_2 f_{i-1}$	a_2	$-a_2 h$	$\frac{1}{2} a_2 h^2$	$-\frac{1}{6} a_2 h^3$	$\frac{1}{24} a_2 h^4$	$-\frac{1}{120} a_2 h^5$
$a_3 f_{i+1}'$	0	a_3	$a_3 h$	$\frac{1}{2} a_3 h^2$	$\frac{1}{6} a_3 h^3$	$\frac{1}{24} a_3 h^4$
$a_4 f_{i-1}'$	0	a_4	$-a_4 h$	$\frac{1}{2} a_4 h^2$	$-\frac{1}{6} a_4 h^3$	$\frac{1}{24} a_4 h^4$

	f_i	f_i'	f_i''	f_i'''	$f_i^{(IV)}$	$f_i^{(V)}$
f_i'	0	1	0	0	0	0
$a_0 f_i$	a_0	0	0	0	0	0
$a_1 f_{i+1}$	a_1	$a_1 h$	$\frac{1}{2}a_1 h^2$	$\frac{1}{6}a_1 h^3$	$\frac{1}{24}a_1 h^4$	$\frac{1}{120}a_1 h^5$
$a_2 f_{i-1}$	a_2	$-a_2 h$	$\frac{1}{2}a_2 h^2$	$-\frac{1}{6}a_2 h^3$	$\frac{1}{24}a_2 h^4$	$-\frac{1}{120}a_2 h^5$
$a_3 f_{i+1}'$	0	a_3	$a_3 h$	$\frac{1}{2}a_3 h^2$	$\frac{1}{6}a_3 h^3$	$\frac{1}{24}a_3 h^4$
$a_4 f_{i-1}'$	0	a_4	$-a_4 h$	$\frac{1}{2}a_4 h^2$	$-\frac{1}{6}a_4 h^3$	$\frac{1}{24}a_4 h^4$
	$=0$	$=0$	$=0$	$=0$	$=0$	

- Step 3: Set as many of the lower order terms on the right hand side to zero as possible

$$a_0 + a_1 + a_2 = 0$$

$$1 + a_1 h - a_2 h + a_3 + a_4 = 0$$

$$\frac{1}{2}a_1 h^2 + \frac{1}{2}a_2 h^2 + a_3 h - a_4 h = 0$$

$$\frac{1}{6}a_1 h^3 - \frac{1}{6}a_2 h^3 + \frac{1}{2}a_3 h^2 + \frac{1}{2}a_4 h^2 = 0$$

$$\frac{1}{24}a_1 h^4 + \frac{1}{24}a_2 h^4 + \frac{1}{6}a_3 h^3 - \frac{1}{6}a_4 h^3 = 0$$

$$a_0 + a_1 + a_2 = 0$$

$$1 + a_1 h - a_2 h + a_3 + a_4 = 0$$

$$\frac{1}{2}a_1 h^2 + \frac{1}{2}a_2 h^2 + a_3 h - a_4 h = 0$$

$$\frac{1}{6}a_1 h^3 - \frac{1}{6}a_2 h^3 + \frac{1}{2}a_3 h^2 + \frac{1}{2}a_4 h^2 = 0$$

$$\frac{1}{24}a_1 h^4 + \frac{1}{24}a_2 h^4 + \frac{1}{6}a_3 h^3 - \frac{1}{6}a_4 h^3 = 0$$

Solve this 5x5 system: $a_0 = 0,\ a_1 = -\frac{3}{4h},\ a_2 = \frac{3}{4h},\ a_3 = \frac{1}{4},\ a_4 = \frac{1}{4}$

- Step 4: Substitute solution back in

$$f_i' - \frac{3}{4h}f_{i+1} + \frac{3}{4h}f_{i-1} + \frac{1}{4}f_{i+1}' + \frac{1}{4}f_{i-1}' = \alpha h^4 f^{(IV)} + \dots$$

multiply by 4 and resort:

$$\boxed{f_{i-1}' + 4f_i' + f_{i+1}' = \frac{3}{h}\left(f_{i+1} - f_{i-1}\right) + O(h^4)}$$

Order? 4th order!