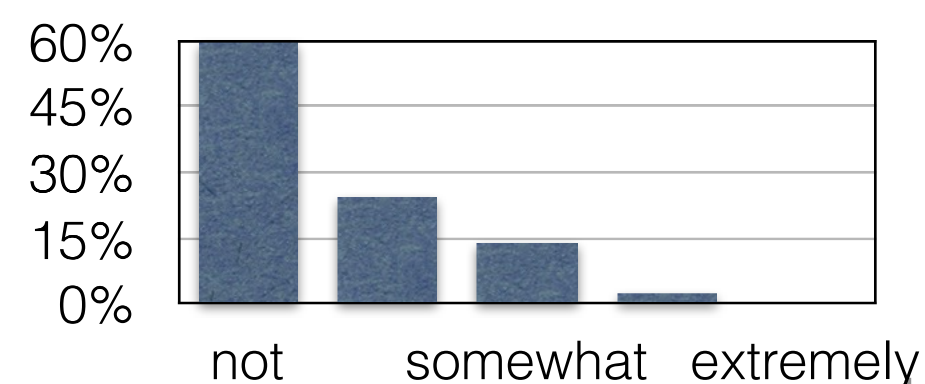
• Muddiest Points from Class 01/18

- *“I wasn't sure where you got the "general form equation" of the Ax"+Bx"+Cx'+...+G, was it just something defined to talk about the B^2-4AC?”*
- *“Slide 19 : 2D model PDE consists of only spacial derivatives. What is the scheme to classify when there are time derivatives as well?”*
- *“When determining the PDE types in the helicopter example, I noticed that here B^2-4*A*C=4*(M^2-1)<0, then M<1 instead of M^2<1. Is that because Mach number should always be a positive number?”*

  - The model equation is simply the combination of all possible second-, first-, and no-derivative terms for a second-order PDE with two independent variables.
  - The independent variables can be anything, space or time, or something else
  - The Mach number, as used in the equation, is always positive.

- *“[…] I noticed that the lectures are uploaded as PDF's but I was wondering if you can do that as PowerPoints files instead so we can write notes on a specific slide. Also PowerPoint lets you export into PDF but there isn't a way to reverse that process while maintaining the formats for the symbols correctly.”*

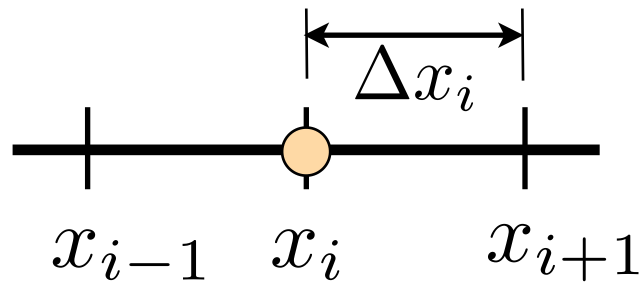
  - I don’t use Powerpoint to generate the notes, so I can’t upload a Powerpoint file. However, there are many PDF annotation tools/apps that let you annotate/write on the PDF slides.



1) Approximate spatial derivates by **finite differences**

- Example #1:

$$\left.\frac{\partial f}{\partial x}\right|_{x_i}$$



$$\Delta x_i = x_{i+1} - x_i$$

- How? **Taylor Series!**

$$f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)\left.\frac{df}{dx}\right|_{x_i} + \frac{1}{2}(x_{i+1} - x_i)^2 \left.\frac{d^2 f}{dx^2}\right|_{x_i} + \ldots$$

or

$$f_{i+1} = f_i + \Delta x_i f_i' + \frac{1}{2}\Delta x_i^2 f_i'' + \ldots$$

let's assume $\Delta x_i = const. = h$

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

solve for f_i':

order

$$f_i' = \frac{f_{i+1} - f_i}{h} - \frac{1}{2} h f_i'' + \ldots \quad \Leftrightarrow \quad \boxed{f_i' = \frac{f_{i+1} - f_i}{h} + O(h)}$$

Forward difference

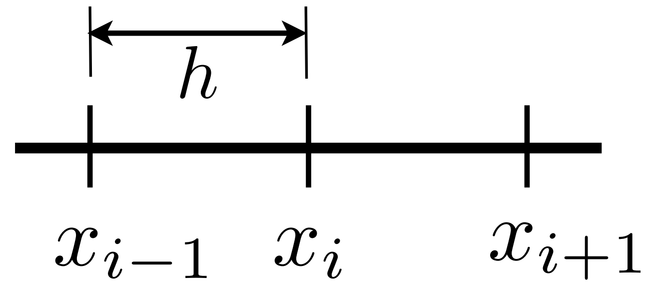
- Forward difference

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

  - exponent of *h* in *O(h)* is the **order of accuracy** of the method
    - here: order = 1
  - the order indicates how fast the error (the *O(h)* term) decreases with a reduction in *h*
    - here: reduce *h* by a factor 2 ⇒ error reduces by a factor $2^1 = 2$
  - Note: only leading order error term is important!
    Higher order error terms decrease faster = are smaller
    (provided h is sufficiently small)

- Example #2:

$$\left.\frac{\partial f}{\partial x}\right|_{x_i}$$ again, but TS for f_{i-1}



$$h = x_i - x_{i-1}$$

$$f(x_{i-1}) = f(x_i) + (x_{i-1} - x_i)\left.\frac{df}{dx}\right|_{x_i} + \frac{1}{2}(x_{i-1} - x_i)^2\left.\frac{d^2 f}{dx^2}\right|_{x_i} + \ldots$$

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

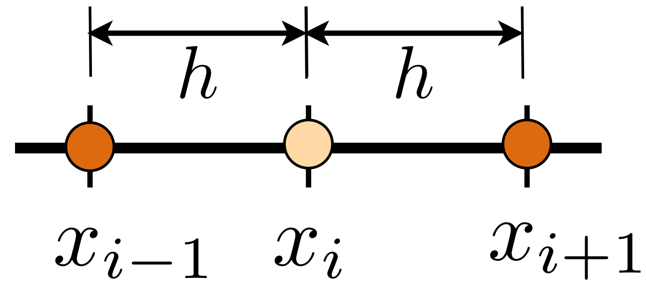
$$\Leftrightarrow \quad f_i' = \frac{f_i - f_{i-1}}{h} + O(h)$$

Backward difference

Question: What's the order? Answer: 1

- Example #3:

$$\left.\frac{\partial f}{\partial x}\right|_{x_i}$$ again, but TS for f_{i+1} & f_{i-1}



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

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

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

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

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

Central difference

Question: What's the order? Answer: 2

$$\text{as } h \to \frac{h}{2} : \text{ error} \to \frac{\text{error}}{4}$$

- General PDE

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

  - 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

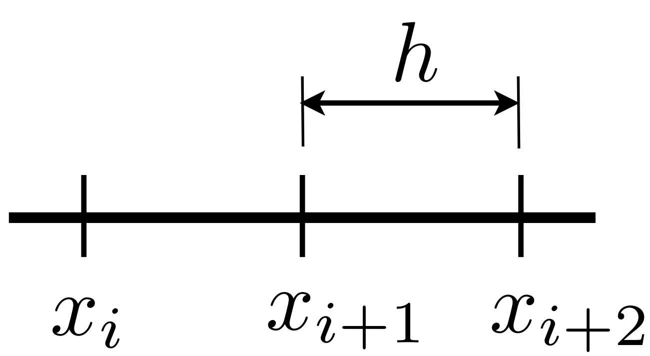
  - However, the derivation of these finite difference formulas was very ad-hoc
  - Need a more general technique

- 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:



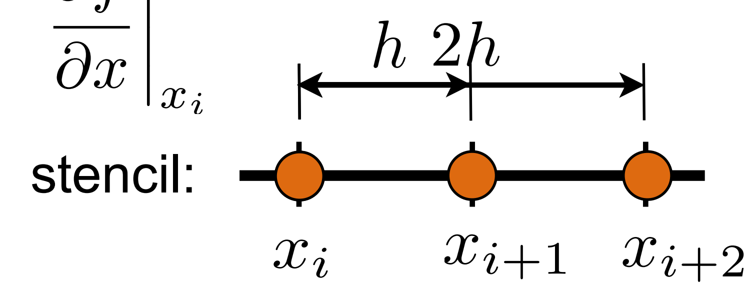
or $f'_i + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = O(?)$

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 $O(h^{n-1})$

$$\left.\frac{\partial f}{\partial x}\right|_{x_i}$$



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

$$f_i = f_i$$

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

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

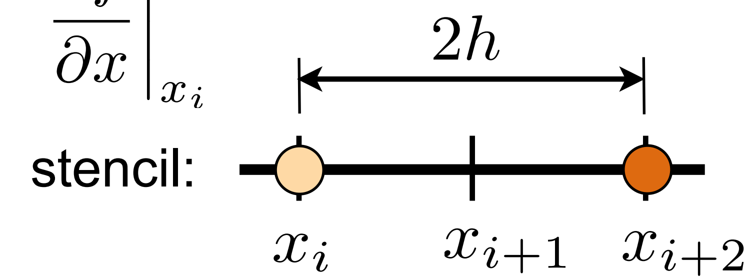
- Step 2: Put into Taylor table (can combine with step 1)

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

$$\left.\frac{\partial f}{\partial x}\right|_{x_i}$$



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

$$f_i = f_i$$

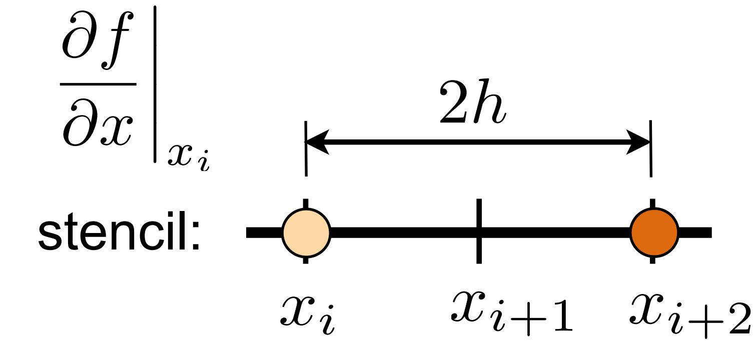
$$f_{i+1} = f_i + hf_i' + \frac{1}{2}h^2 f_i'' + \frac{1}{6}h^3 f_i''' + \ldots$$

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

- 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

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

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

- 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): $a_0 = \dfrac{3}{2h}$ $\quad a_1 = -\dfrac{2}{h}$ $\quad a_2 = \dfrac{1}{2h}$

- Step 4: Substitute solution back in

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = f_i' + \frac{3}{2h} f_i - \frac{2}{h} f_{i+1} + \frac{1}{2h} f_{i+2}$$

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

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

Solve for target derivative f'_i:

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

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

Order? 2nd order!

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

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

- Another example Taylor table: calculate f''' at i using stencil i-2, i-1, i+2, i+3, i+4

Step 0: Write the sum of the target derivative + linear combination of all stencil f values

$$f_i''' + a_0 f_{i-2} + a_1 f_{i-1} + a_2 f_{i+2} + a_3 f_{i+3} + a_4 f_{i+4} = O(?)$$

Step 1: Write Taylor series for f at each stencil point

Step 2: Put into Taylor table

f_i'''	
$a_0 f_{i-2}$	
$a_1 f_{i-1}$	
$a_2 f_{i+2}$	
$a_3 f_{i+3}$	
$a_4 f_{i+4}$	

The header column is simply each term from step 0

- Another example Taylor table: calculate f''' at i using stencil i-2, i-1, i+2, i+3, i+4

Step 0: Write the sum of the target derivative + linear combination of all stencil f values

$$f_i''' + a_0 f_{i-2} + a_1 f_{i-1} + a_2 f_{i+2} + a_3 f_{i+3} + a_4 f_{i+4} = O(?)$$

Step 1: Write Taylor series for f at each stencil point

Step 2: Put into Taylor table

	f_i	f_i'	f_i''	f_i'''	$f_i^{(IV)}$	$f_i^{(V)}$
f_i'''						
$a_0 f_{i-2}$						
$a_1 f_{i-1}$						
$a_2 f_{i+2}$						
$a_3 f_{i+3}$						
$a_4 f_{i+4}$						

The header row simply contains the derivates from the Taylor series from step 1

But how many terms/columns?

At least so many that the final leading order error term is included
(there are really infinitely many terms)

- Another Example Taylor table: calculate f''' at i using stencil i-2, i-1, i+2, i+3, i+4

Step 0: Write the sum of the target derivative + linear combination of all stencil f values

$$f_i''' + a_0 f_{i-2} + a_1 f_{i-1} + a_2 f_{i+2} + a_3 f_{i+3} + a_4 f_{i+4} = O(?)$$

Step 1: Write Taylor series for f at each stencil point

Step 2: Put into Taylor table

	f_i	f_i'	f_i''	f_i'''	$f_i^{(IV)}$	$f_i^{(V)}$
f_i'''	0	0	0	1	0	0
$a_0 f_{i-2}$						
$a_1 f_{i-1}$						
$a_2 f_{i+2}$						
$a_3 f_{i+3}$						
$a_4 f_{i+4}$						

First row: put 0s everywhere and a 1 in the column of the derivative we want to calculate

Other rows: just fill in using the Taylor series from step 1

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

- Solution:
  - define mesh spacing h and calculate f at mesh points used in finite difference formula using the given f(x)
  - calculate derivative using finite difference formula

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

  - What's the error e? error = exact solution - calculated (numerical) solution

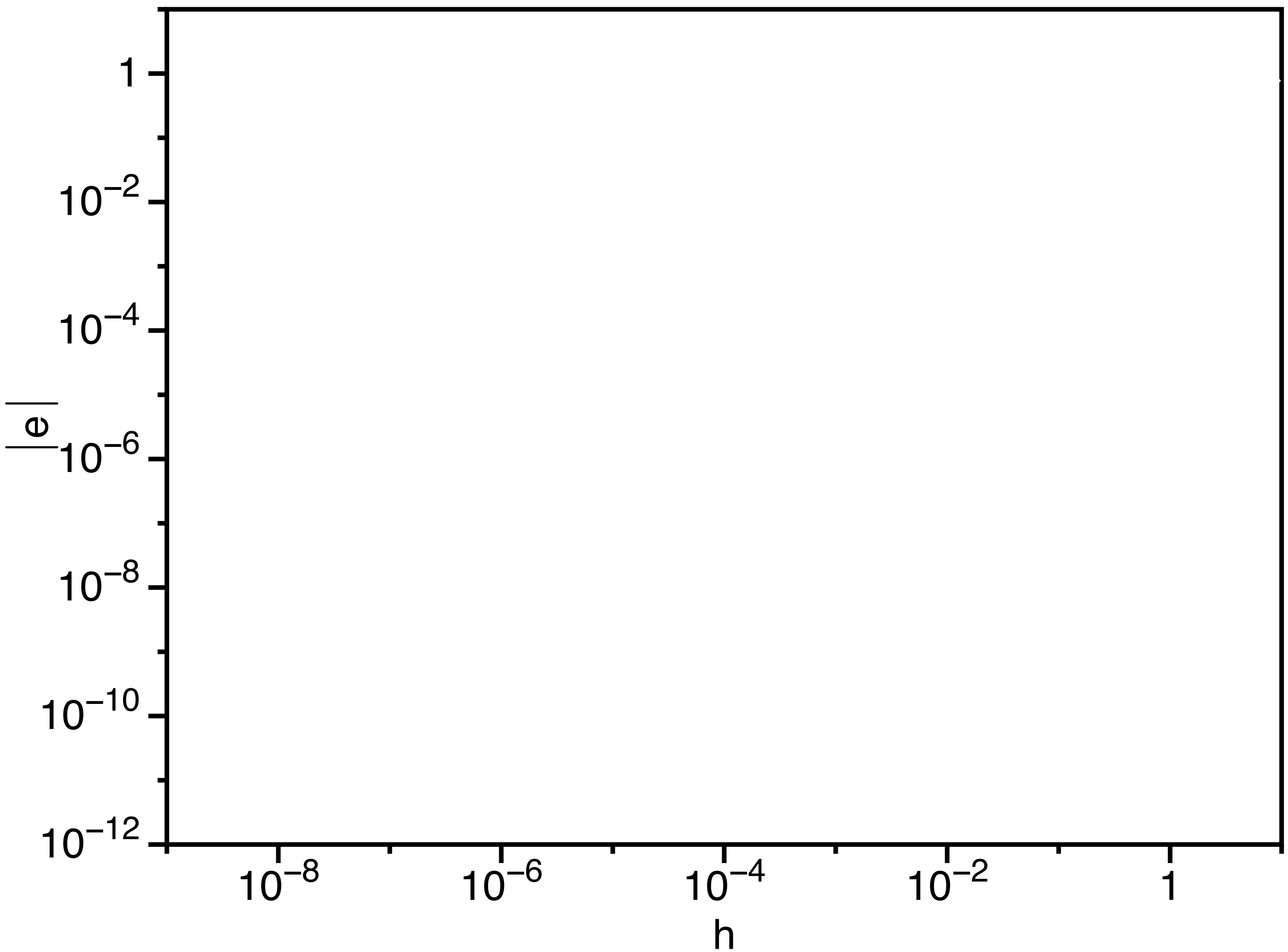
How to calculate the exact solution?
1) determine the analytical derivative of f(x)
2) evaluate the analytical derivative in your code: this is the “exact” solution

But, we can in theory also calculate the exact solution/error using Taylor series

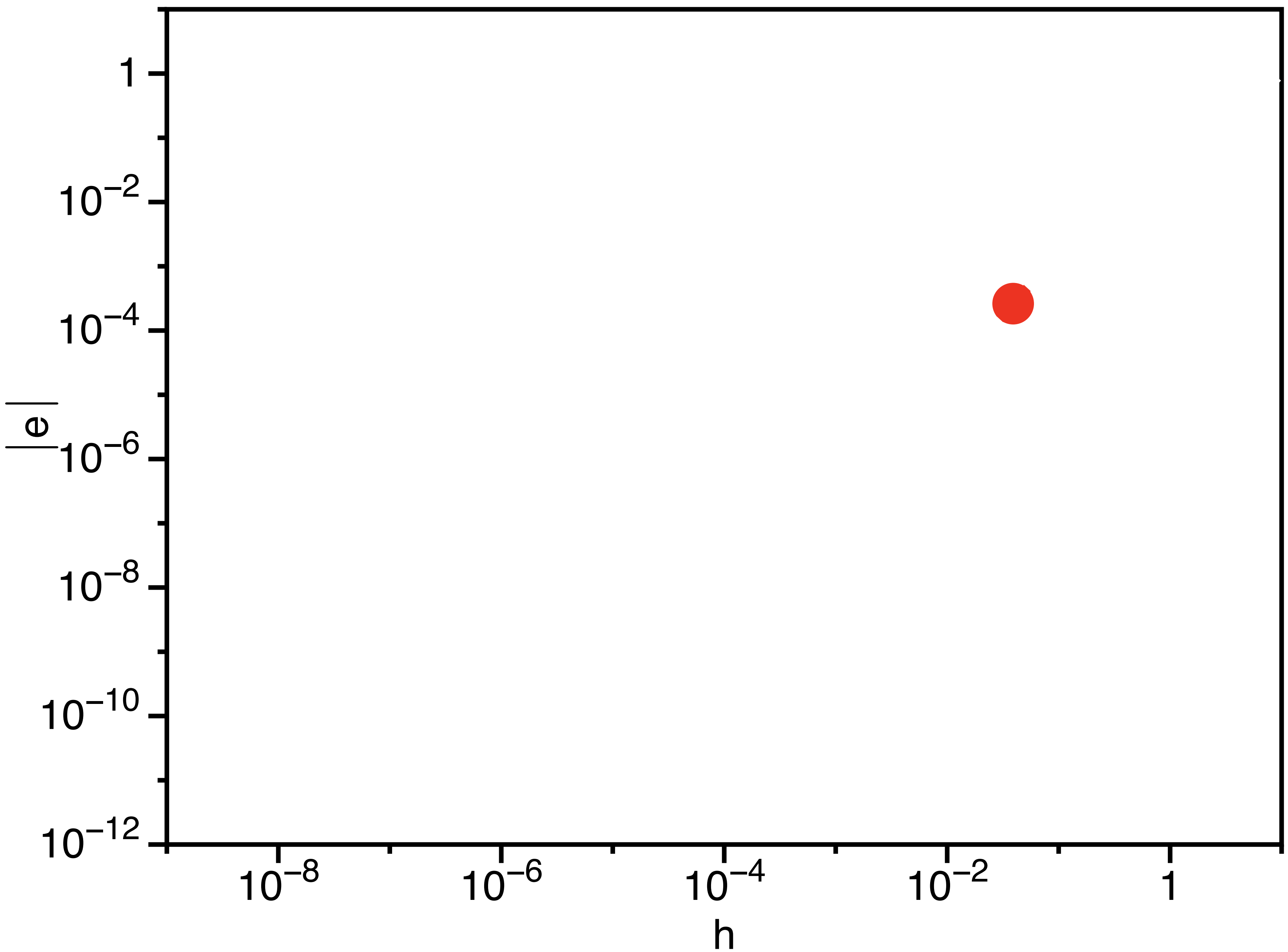
exact f': $$f'(x_i) = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \frac{1}{3}h^2 f_i''' + \frac{1}{4}h^3 f_i^{(IV)} + \frac{7}{60}h^4 f_i^{(V)} + \ldots$$

error: $$e = f'(x_i) - f_i' = \frac{1}{3}h^2 f_i''' + \frac{1}{4}h^3 f_i^{(IV)} + \frac{7}{60}h^4 f_i^{(V)} + \ldots$$

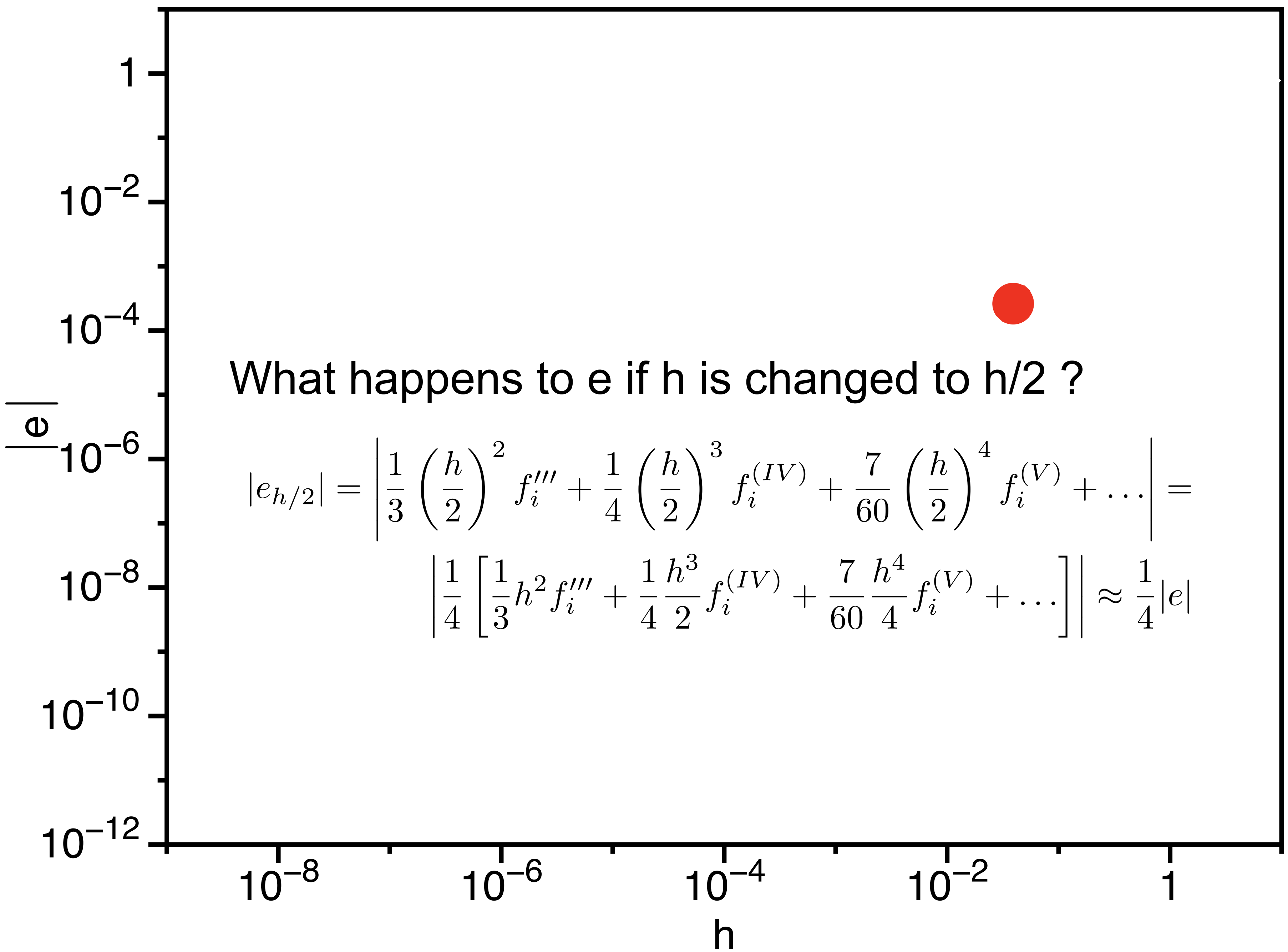
(not useful in practice since it requires infinitely many terms, but instructive for theory)



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



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

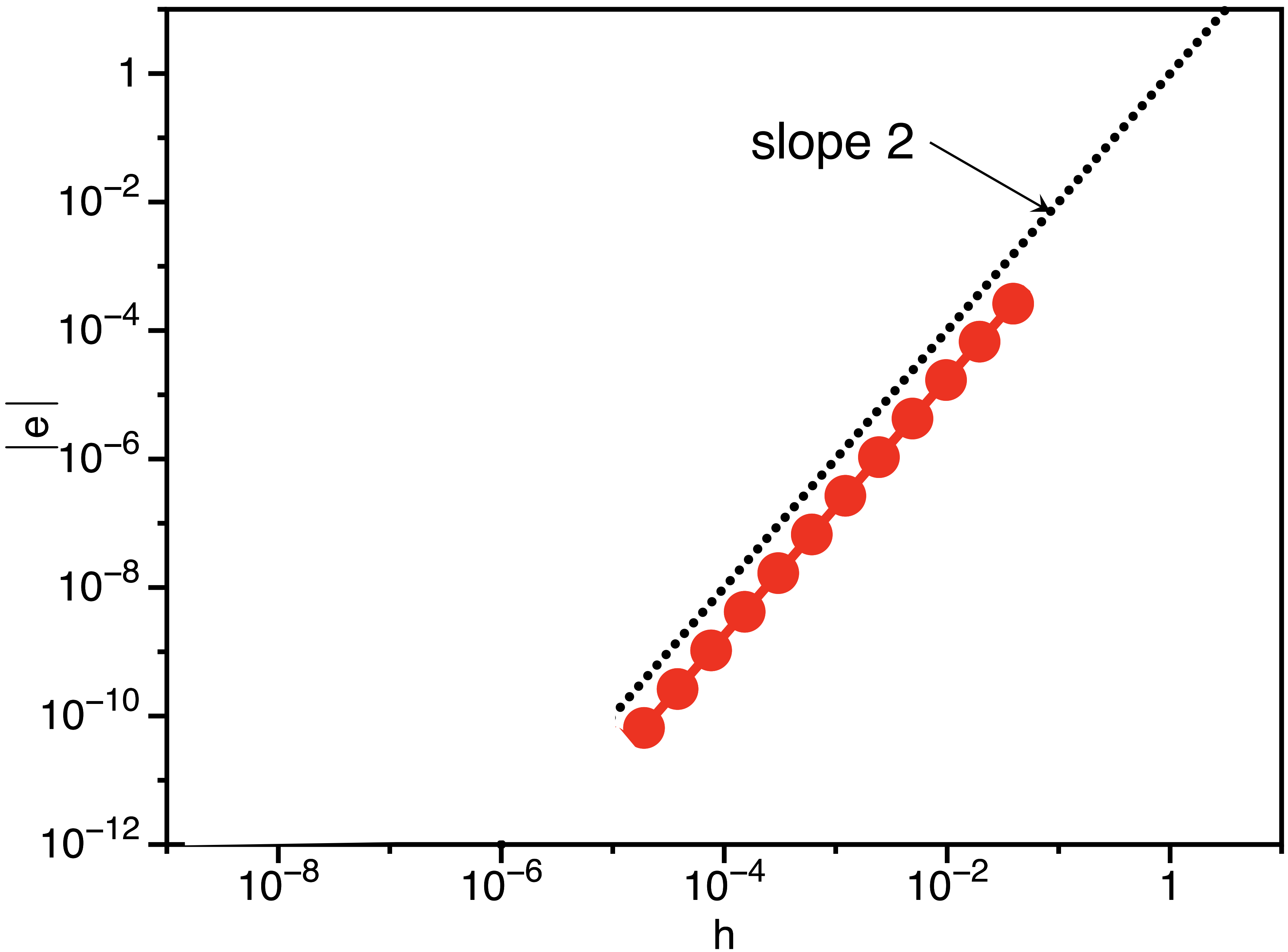


What happens to e if h is changed to h/2 ?

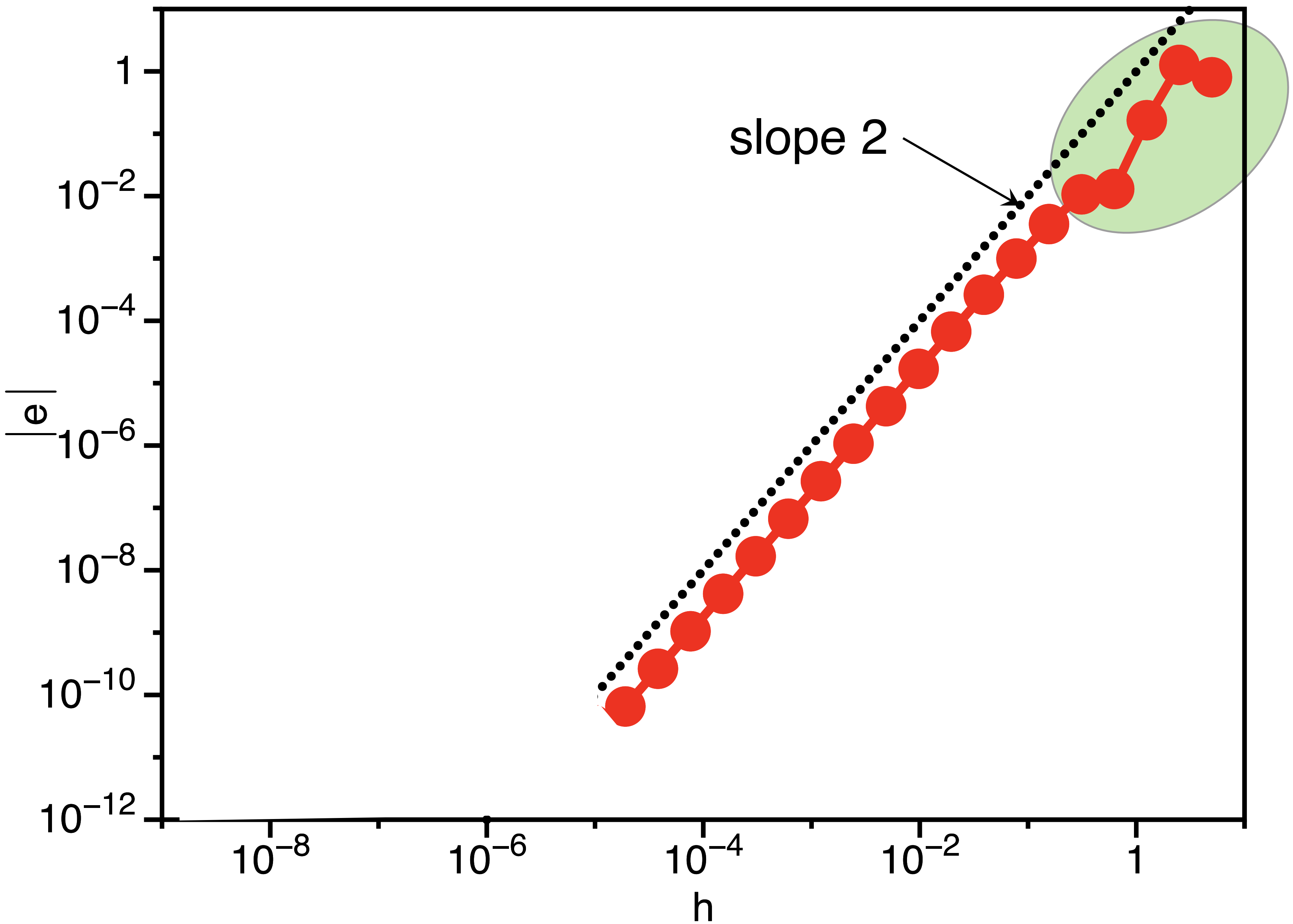
$$|e_{h/2}| = \left| \frac{1}{3}\left(\frac{h}{2}\right)^2 f_i''' + \frac{1}{4}\left(\frac{h}{2}\right)^3 f_i^{(IV)} + \frac{7}{60}\left(\frac{h}{2}\right)^4 f_i^{(V)} + \dots \right| =$$

$$\left| \frac{1}{4}\left[\frac{1}{3}h^2 f_i''' + \frac{1}{4}\frac{h^3}{2} f_i^{(IV)} + \frac{7}{60}\frac{h^4}{4} f_i^{(V)} + \dots\right]\right| \approx \frac{1}{4}|e|$$

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

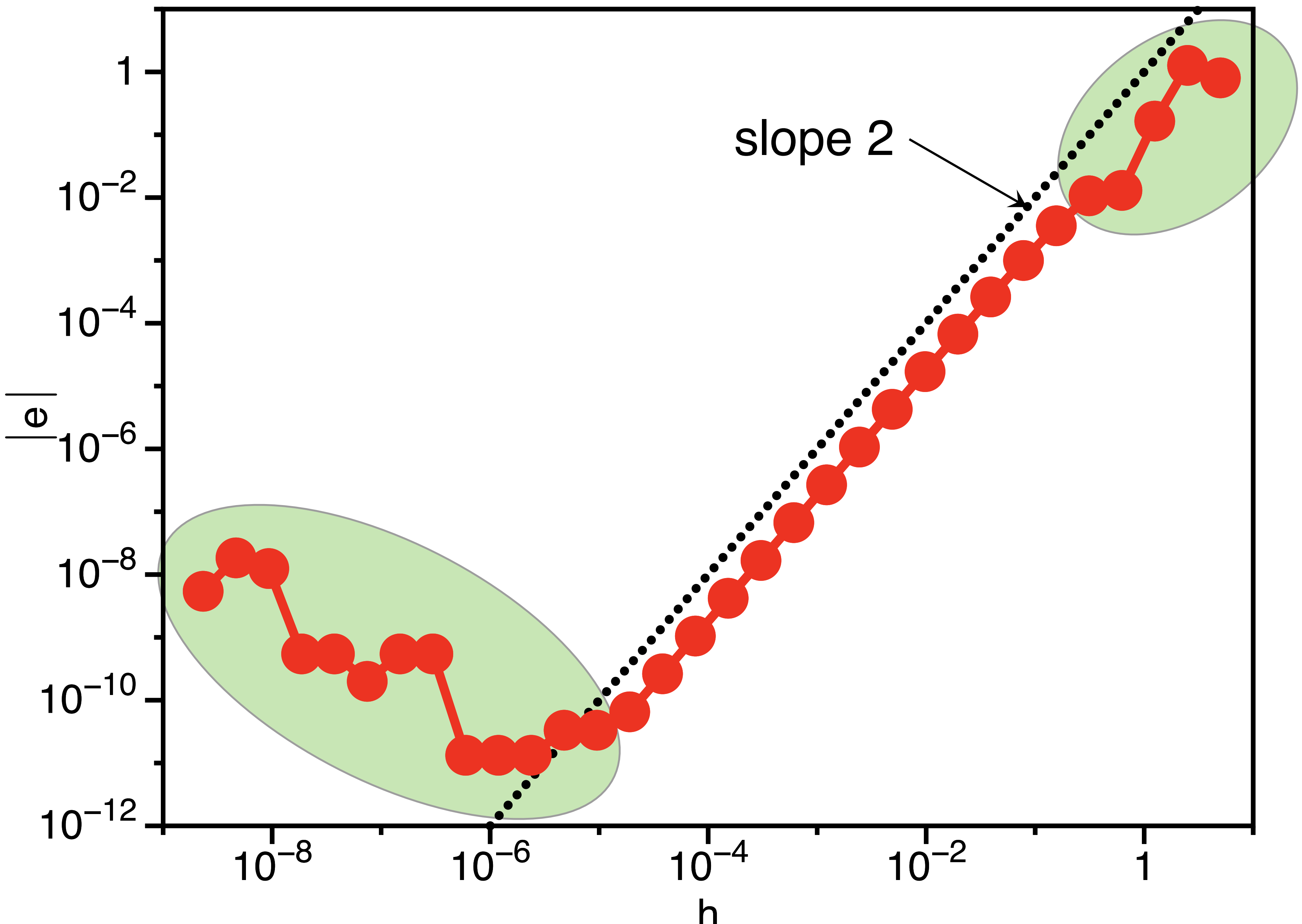


$$|e| = |f'(x_i) - f'_i| = \left| \frac{1}{3} h^2 f'''_i + \frac{1}{4} h^3 f_i^{(IV)} + \frac{7}{60} h^4 f_i^{(V)} + \ldots \right| = O(h^2)$$



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