

# Numerical Analysis

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# Course Overview, Numerical Differentiation

- ▶ Course Overview
- ▶ Finite differences and truncation error
- ▶ Finite differences and rounding errors
- ▶ Richardson's extrapolation
- ▶ Method of undetermined coefficients
- ▶ Stencil, nonuniform mesh, curvilinear mesh
- ▶ Compact finite differences
- ▶ Estimating expressions with finite differences
- ▶ Finite differences in multidimension
- ▶ Differentiation matrix, convolution, mask, mollifier, smoothing kernel
- ▶ Application to edge detection
- ▶ Q & A

# Numerical Analysis, Course Overview 1

- ▶ Course format: 2L + 2TTF

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- [illegible]



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- ▶ Learning outcomes: **apply knowledge and skills**
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  - ▶ select suitable method of solution, analyze and prove their properties
  - ▶ **apply numerical methods to selected practical problems**

## QUESTIONS ?

- ▶ which slide? please give slide number
- ▶ which theorem?
- ▶ which example?
- ▶ which ...?



# Examples of Functions 1

- ▶ Polynomial  $P_n(x) = \sum_{i=0}^n a_i x^i$ ,  $x, a_i \in \mathbb{R}, i = 0, 1, \dots, n$
- ▶ Trigonometric  
 $T(x) = \sum_{i=0}^n (a_i \sin(x) + b_i \cos(x))$ ,  $x, a_i \in \mathbb{R}, i = 0, 1, \dots, n$
- ▶ Rational  $R_{n,m}(x) = \frac{\sum_{i=0}^n a_i x^i}{\sum_{i=0}^m b_i x^i}$ , etc.

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- ▶ Average temperature in the classroom is a function of time  
(Temperature - dependent, time independent variable)

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- ▶ Water channel on campus: cross section's average flow velocity is a function of time and distance from its origin

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- ▶ Lake on campus: depth is a function of Cartesian coordinates with origin e.g. ...

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- ▶ Digital image: piece-wise constant function of Cartesian coordinates, origin - left lower corner

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- ▶ Thomas algorithm for tridiagonal matrices - almost perfect why?

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  - ▶ accurate enough
  - ▶ fast enough
  - ▶ low cost, acceptable cost

## QUESTIONS ?

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- ▶ which theorem?
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# Computing function derivatives

## Example 1.2

►  $f(x)$  is continuously differentiable function (CALCULUS)

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$$f'(x) = \lim_{h \rightarrow 0+} \frac{f(x+h) - f(x)}{h}$$

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  - ▶ Are these formulas good for any parameter  $h$ ?
  - ▶ Can I apriori estimate accuracy with respect to  $h$ ?



# Computing function derivatives: exact vs approximate

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Source: J.V. Lambers, A.C. Summer, Explorations in Numerical Analysis, p.226


$$f(x) = \frac{\sin^2\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right)}{\sin\left(\frac{\sqrt{x-1}}{\sqrt{x^2+1}}\right)}$$

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$$f'(x) = \frac{2 \sin\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right) \cos\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right) \left[ \frac{2x+1}{2\sqrt{x^2+1}(\cos x - x)} + \frac{\sqrt{x^2+1}(\sin x + 1)}{(\cos x - x)^2} \right]}{\sin\left(\frac{\sqrt{x-1}}{\sqrt{x^2+1}}\right)} - \frac{\sin\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right) \cos\left(\frac{\sqrt{x-1}}{\sqrt{x^2+1}}\right) \left[ \frac{1}{2\sqrt{x}\sqrt{x^2+1}} - \frac{x(\sqrt{x-1})}{(x^2+1)^{3/2}} \right]}{\sin^2\left(\frac{\sqrt{x-1}}{\sqrt{x^2+1}}\right)}$$

$$\blacktriangleright f'(0.25) = -9.066698770$$

# Computing function derivatives: exact vs approximate

## Example 1.3

Source: J.V. Lambers, A.C. Summer, Explorations in Numerical Analysis, p.226

$$f(x) = \frac{\sin^2\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right)}{\sin\left(\frac{\sqrt{x-1}}{\sqrt{x^2+1}}\right)}$$

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►  $f'(0.25) = -9.066698770$

►  $f'(x) \approx f'_{\text{centralFD}}(x) = \frac{f(x+h) - f(x-h)}{2h}$

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- ▶  $h = 0.005, f'_{\text{centralFD}}(0.25) = -9.067464295$

# Computing function derivatives: exact vs approximate

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- ▶  $|f'_{\text{centralFD}}(0.25) - f'(0.25)| \approx 7.7 \cdot 10^{-4}$

# Computing function derivatives: exact vs approximate

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- ▶ **Conclusions:**

# Computing function derivatives: exact vs approximate

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- ▶  $|f'_{\text{centralFD}}(0.25) - f'(0.25)| \approx 7.7 \cdot 10^{-4}$
- ▶ **Conclusions:** fast? accurate enough? low cost?



# Estimating accuracy of finite differences

## Definition 1.4

Taylor's formula

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

# Estimating accuracy of finite differences

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## Example 1.5



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

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## Example 1.5



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



$$\left| f'(x_0) - \frac{f(x_0 + h) - f(x_0)}{h} \right| \approx O(h)$$

► **Conclusions:**

# Estimating accuracy of finite differences

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

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Conclusions:

▶ Formula is first order accurate wrt  $h$

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### Conclusions:

- ▶ Formula is first order accurate wrt  $h$
- ▶ For estimating first order derivative  $f$  should be twice continuously differentiable

# Estimating accuracy of finite differences

## Definition 1.4

Taylor's formula

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

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### ▶ Conclusions:

- ▶ Formula is first order accurate wrt  $h$
- ▶ For estimating first order derivative  $f$  should be twice continuously differentiable

### ▶ Question: what if $f$ is continuously differentiable only?

# Finite differences for second order derivatives

## Definition 1.6

Taylor's formula

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(x_0) + \dots \\ + \frac{h^n}{n!}f^{(n)}(x_0) + O(h^{n+1})$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(x_0) + \dots \\ + \frac{(-h)^n}{n!}f^{(n)}(x_0) + O(h^{n+1})$$

# Finite differences for second order derivatives

## Definition 1.6

Taylor's formula

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(x_0) + \dots \\ + \frac{h^n}{n!}f^{(n)}(x_0) + O(h^{n+1})$$

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## Example 1.7



$$\frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} = f''(x_0) + \frac{2h^2}{4!}f^{(4)}(x_0) + O(h^4)$$



# Finite differences for second order derivatives

## Definition 1.6

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## Example 1.7



$$\frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} = f''(x_0) + \frac{2h^2}{4!}f^{(4)}(x_0) + O(h^4)$$

► Question: what is accuracy of  $\frac{f(x_0) - 2f(x_0+h) + f(x_0+2h)}{h^2}$  at  $x_0$ ?

## QUESTIONS ?

- ▶ which slide? please give slide number
- ▶ which theorem?
- ▶ which example?
- ▶ which ...?

# Richardson's extrapolation 1

## Definition 1.8

Taylor's formula

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x) + \dots + \frac{h^n}{n!}f^{(n)}(x_0) + O(h^{n+1})$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(x) - \frac{h^5}{5!}f^{(5)}(x) + \dots + \frac{(-h)^n}{n!}f^{(n)}(x_0) + O(h^{n+1})$$


# Richardson's extrapolation 1

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$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!}f^{(3)}(x) - \frac{h^4}{5!}f^{(5)}(x) + O(h^6)$$

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►  $f'(x) = f'_{\text{centralFD}}(x, h) + b_2h^2 + b_4h^4 + O(h^6)$

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- ▶  $b_2, b_4$  does not depend on  $h$

## Richardson's extrapolation 2



$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!}f^{(3)}(x) - \frac{h^4}{5!}f^{(5)}(x) + O(h^6)$$

- ▶  $f'(x) = f'_{centralFD}(x, h) + b_2h^2 + b_4h^4 + O(h^6)$
- ▶  $Error(h) = E(h) = b_2h^2 + b_4h^4 + O(h^6)$
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## Richardson's extrapolation 2



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## Richardson's extrapolation 2



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- ▶  $\text{Error}(2h) = E(2h) = b_24h^2 + b_416h^4 + O(h^6)$
- ▶  $4f'(x) = 4f'_{\text{centralFD}}(x, h) + b_24h^2 + b_44h^4 + O(h^6)$

## Richardson's extrapolation 2



$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!}f^{(3)}(x) - \frac{h^4}{5!}f^{(5)}(x) + O(h^6)$$

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## Richardson's extrapolation 2



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- ▶  $\text{Error}(2h) = E(2h) = b_24h^2 + b_416h^4 + O(h^6)$
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- ▶  $3f'(x) = 4f'_{\text{centralFD}}(x, h) - f'_{\text{centralFD}}(x, 2h) - b_412h^4 + O(h^6)$

## Richardson's extrapolation 2



$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!}f^{(3)}(x) - \frac{h^4}{5!}f^{(5)}(x) + O(h^6)$$

- ▶  $f'(x) = f'_{\text{centralFD}}(x, h) + b_2h^2 + b_4h^4 + O(h^6)$
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## Richardson's extrapolation 3

$$\blacktriangleright f'(x) = \frac{4f'_{\text{centralFD}}(x,h) - f'_{\text{centralFD}}(x,2h)}{3} + O(h^4)$$

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## ▶ Conclusions

- ▶ Richardson's extrapolation achieves high order accuracy by means of combining lower order formulas

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- ▶ Formal high order accuracy requires high order derivatives from the function under consideration

## ▶ Questions

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- ▶ Using Richardson's extrapolation can you obtain FD formula having accuracy  $O(h^{2k})$ ,  $k > 2$

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## ▶ Conclusions

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## ▶ Questions

- ▶ Using Richardson's extrapolation can you obtain FD formula having accuracy  $O(h^{2k})$ ,  $k > 2$
- ▶ Is Richardson's extrapolation valid for computing second order derivatives?

## QUESTIONS ?

- ▶ which slide? please give slide number
- ▶ which theorem?
- ▶ which example?
- ▶ which ...?

# Finding undetermined coefficients 1

Considered approaches can be generalized in the following algorithm

## Algorithm 1.9

Finding undetermined coefficients

1. Consider formula

$$f'(x) \approx \frac{1}{h} \sum_{i=1}^m c_i f(x + p_i h) \quad (1)$$

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$$f'(x) - \frac{1}{h} \sum_{i=1}^m c_i f(x + p_i h) = O(h^k) \quad (2)$$

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# Undetermined coefficients related

## QUESTIONS ?

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Q & A