CEGM1000
Modelling, Uncertainty and Data for Engineers

Week 1.2
Numerical modelling (Fundamentals)

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Based on a previous version from Jaime Arriaga and the rest of the MUDE team

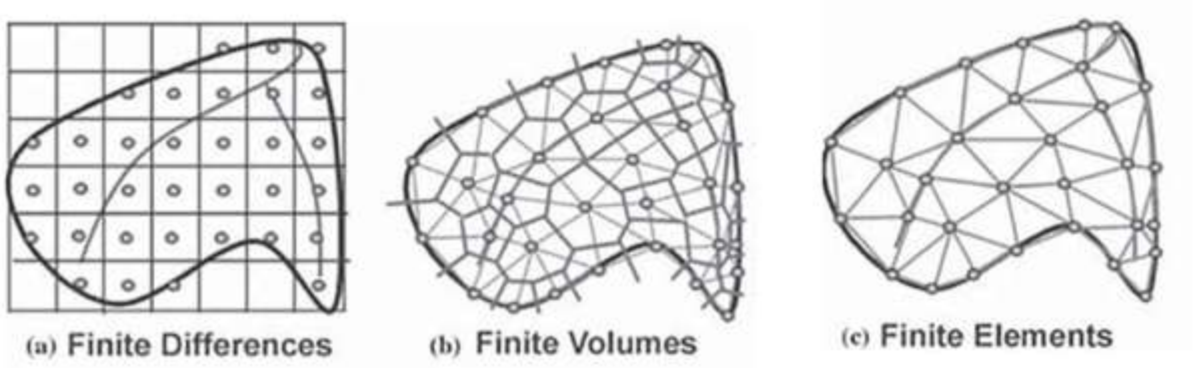
TU Delft

Learning objectives

At the end of this lecture, you should be able to

- Discuss the relevance of numerical modelling keeping in mind its pitfalls
- Use Taylor series to find approximations of derivatives and its accuracy
- Apply numerical integration methods to functions using pen and paper.

Methods



MUDE
Q1

MUDE
Q2

Other methods:

- Based on characteristics
- Boundary elements
- Physics-informed neural networks

Q3, Q4 and beyond (depending on your track)
(e.g. CIEM2110 Numerical Modelling in Geotechnical Engineering)

*What relationship do you **expect** to get with numerical models?*

Developer / creator	0%
User (occasionally)	0%
Super user (daily)	0%
Decision maker	0%

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Showing Results

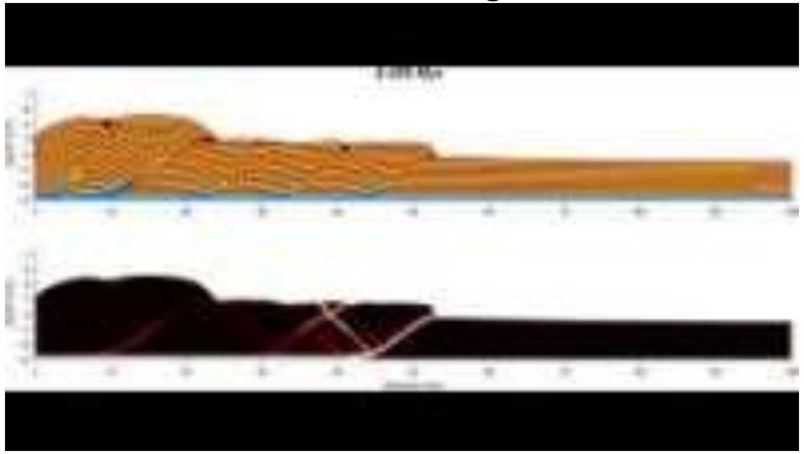
What relationship do you ***expect*** *to get with numerical models?*

Developer / creator	0%
User (occasionally)	0%
Super user (daily)	0%
Decision maker	0%

RESULTS SLIDE

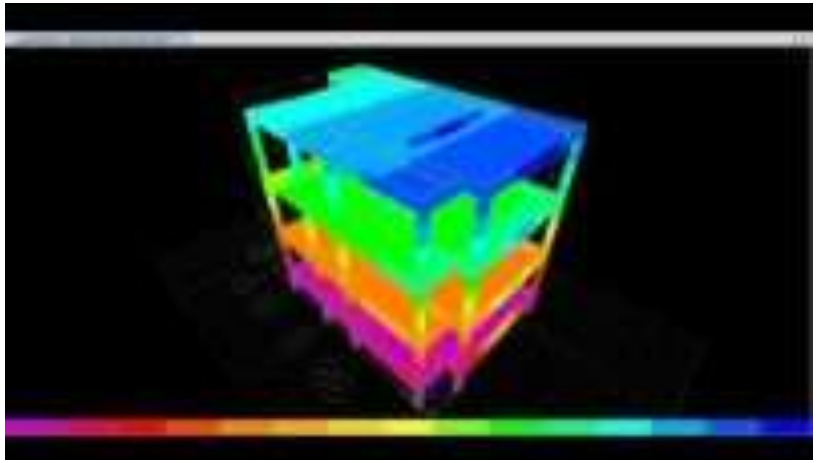
Some applications

Mountain building



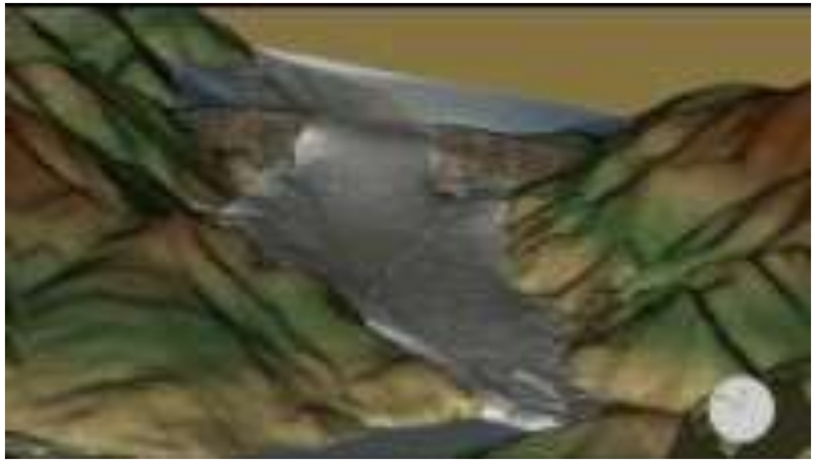
Garrett Apuzen-Ito. (2016, Nov 16). *Numerical model of mountain building* [Video]. Youtube. https://www.youtube.com/watch?v=HUn8lzdDmfk

Building Deformation



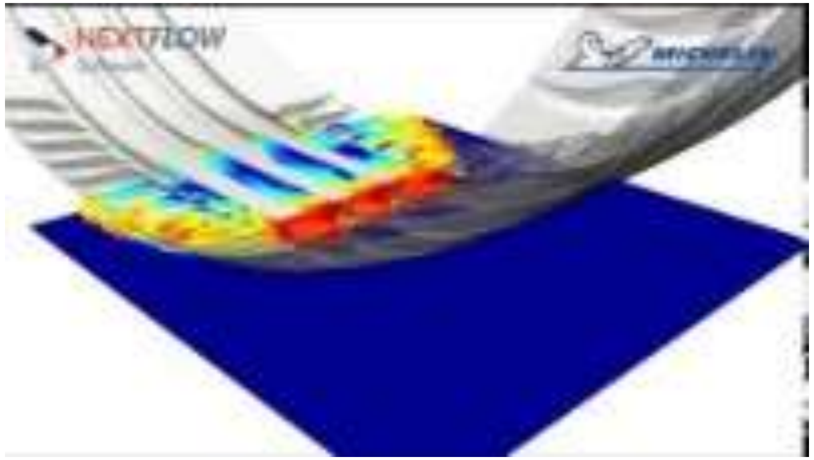
ONKAR CHAUHAN. (2018, Jan 7). *3D Animation of deformation of Building after analysis in ETABS* [Video]. Youtube. https://www.youtube.com/watch?v=RJZRtdINSms

Dam Break Simulation



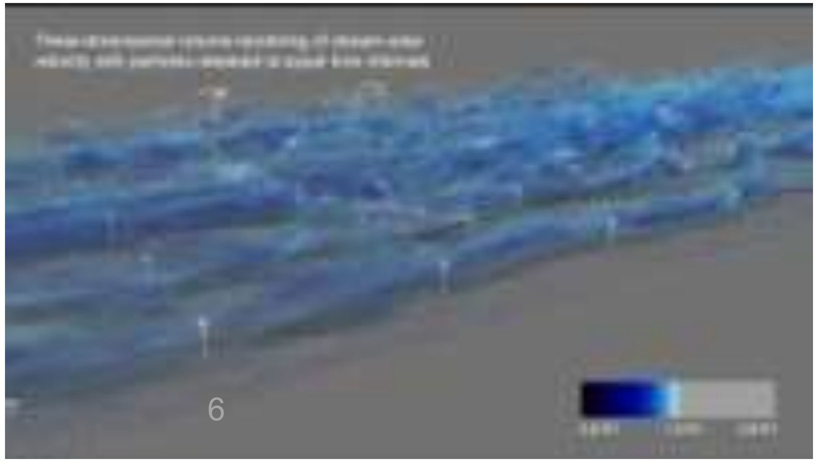
XC ENGINEERING. (2016, Mar 17). *Damn break simulation with FLOW-3D* [Video]. Youtube. https://www.youtube.com/watch?v=3q8EY4zBf3w

Tire - hydroplaning



Nextflow Software. (2019, Mar 14). *Tyre Hydroplanning simulation* [Video]. Youtubehttps://www.youtube.com/watch?v=0sVCOn_hoGU

Large eddy simulation of a Wind Farm



Physics of Fluids Group University of Twente. (2016, October 27). *Large eddy simulation of a Wind Farm- Explanatory clip* [Video]. Youtube. https://www.youtube.com/watch?v=qEtcCjln-0Q

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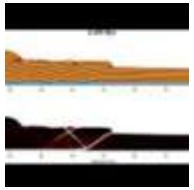
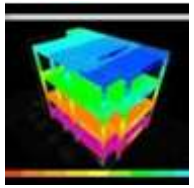
*Which simulation do you **feel** is more reliable?*

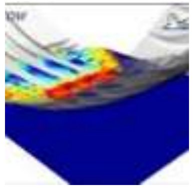


Mountain building — 0%



Structure deformation — 0%

Dam break — 0%



Hydroplaning — 0%

Wind field simulation — 0%

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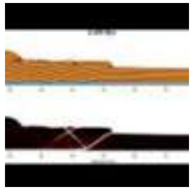
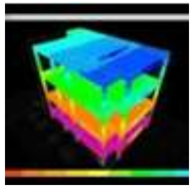
Preparing Results

*Which simulation do you **feel** is more reliable?*



Mountain building

0%

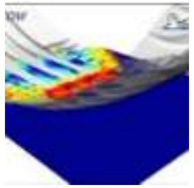


Structure deformation

0%

Dam break

0%



Hydroplaning

0%

Wind field simulation

0%

RESULTS SLIDE

A short discussion about numerical models

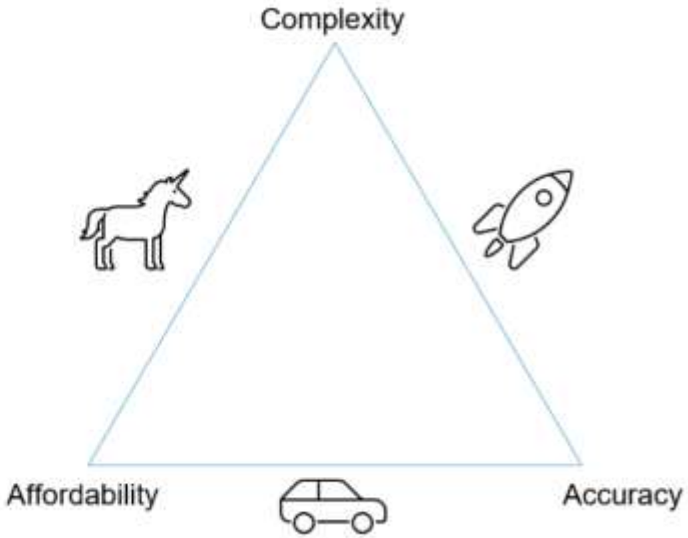
Some Pros

1. Design checks
2. Future scenarios
3. Non-existent situations
4. Some experiments cannot be scaled

Some Cons

1. May give credibility to incorrect results
2. Good modellers are scarce
3. Can take a lot of effort

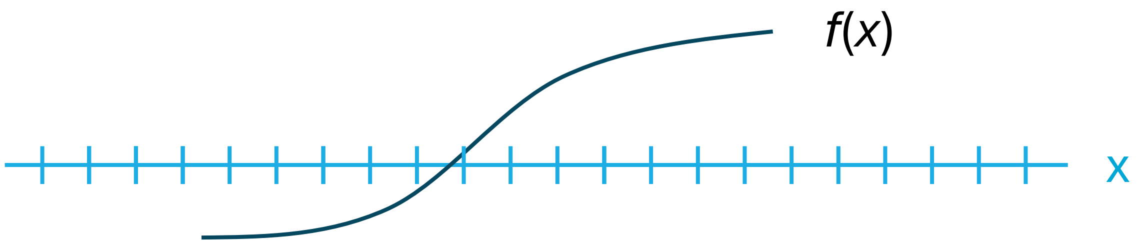
"All models are wrong, but some are useful" (after George Box)



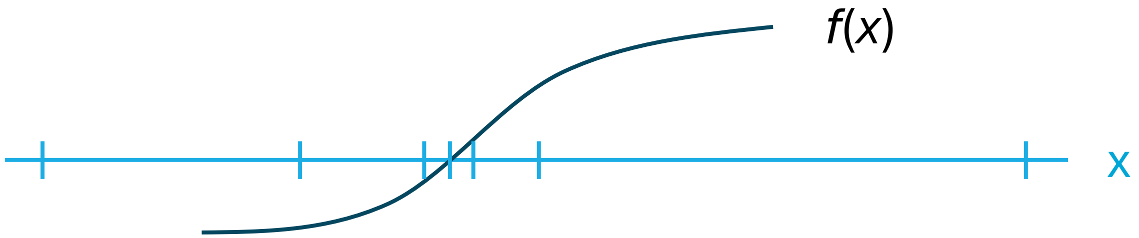
"When all you have is a hammer, everything looks like a nail" (after Abraham Kaplan)

Root finding: Numerical solutions for $f(x) = 0$ (which x?)

1. Stepping method
   (fixed interval)

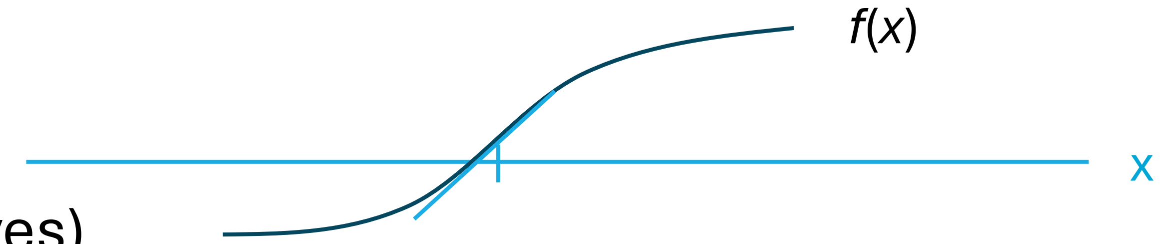


2. Bisection method



3. Newton-Raphson

   (taking advantage of derivatives)



Differential equations – ODEs, PDEs

Ice growth
First order ODE ➔

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water} - T_{air}}{h_{ice}}$$

Beam deformation
Second order ODE ➔

1D consolidation
Second order PDE ➔

Navier Stokes 3D
System on non-linear PDEs ➔

We often ***approximate*** the derivatives ***numerically***!

$$\frac{dh_{ice}}{dt} \approx ?$$

Contents

- Numerical Derivatives
- Taylor Series Expansion
- Numerical Integration

Numerical Derivatives

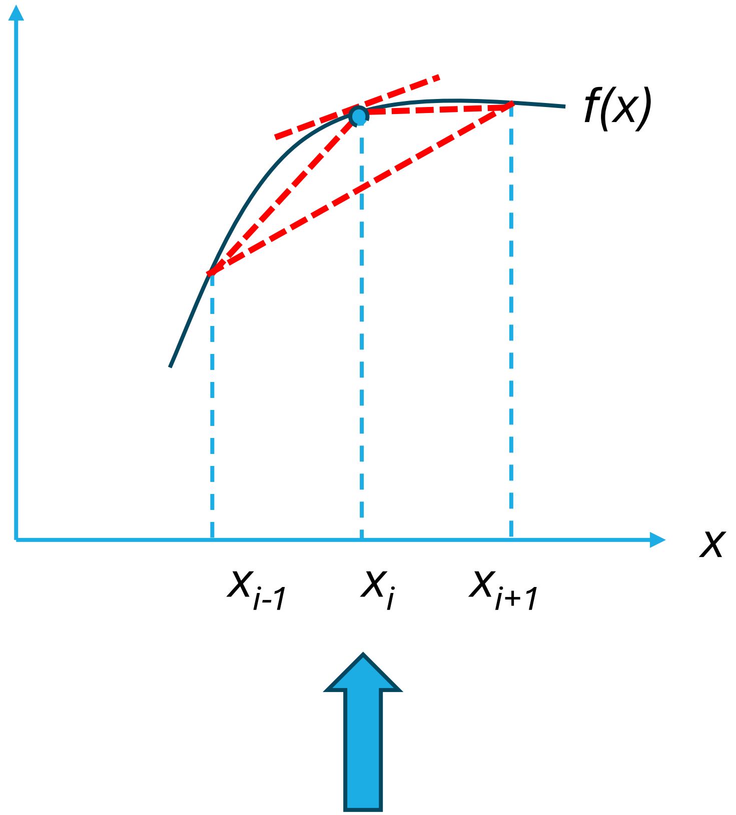
Definition ➔

$$\left.\frac{df}{dx}\right|_{x_0} = f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

Numerically ➔

$$f'(x_0) \approx \frac{f(x) - f(x_0)}{\Delta x}, \text{where } \Delta x = x - x_0$$

More than one way to approximate derivative



$$\text{forward} \quad \left.\frac{df}{dx}\right|_{x_i} \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

$$\text{backward} \quad \left.\frac{df}{dx}\right|_{x_i} \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

$$\text{central} \quad \left.\frac{df}{dx}\right|_{x_i} \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$

Taylor Series Expansions

- The exact value of any function $f(x)$ around $x = x_0$ can be calculated using an infinite number of terms.

$$f(x) = f(x_0) + f'(x_0)\frac{(x - x_0)}{1!} + f''(x_0)\frac{(x - x_0)^2}{2!} + f'''(x_0)\frac{(x - x_0)^3}{3!} + \cdots + f^{(n)}(x_0)\frac{(x - x_0)^n}{n!}$$

The symbol ! means factorial (in Dutch: faculteit): 3! = 1 x 2 x 3 = 6

Taylor Series Expansions

- Compute the Taylor Series Expansion of $f(x) = \sin(x)$ around $x_0 = 0$ with third order accuracy

$$f(x) \approx f(x_0) + f'(x_0)\frac{(x - x_0)}{1!} + f''(x_0)\frac{(x - x_0)^2}{2!} + f'''(x_0)\frac{(x - x_0)^3}{3!}$$

$$\mathrm{f}(0) = \sin(0) \longrightarrow \mathrm{f}(0) = 0$$

$$\mathrm{f}'(0) = \cos(0) \longrightarrow \mathrm{f}'(0) = 1$$

$$\mathrm{f}''(0) = -\sin(0) \longrightarrow \mathrm{f}''(0) = 0$$

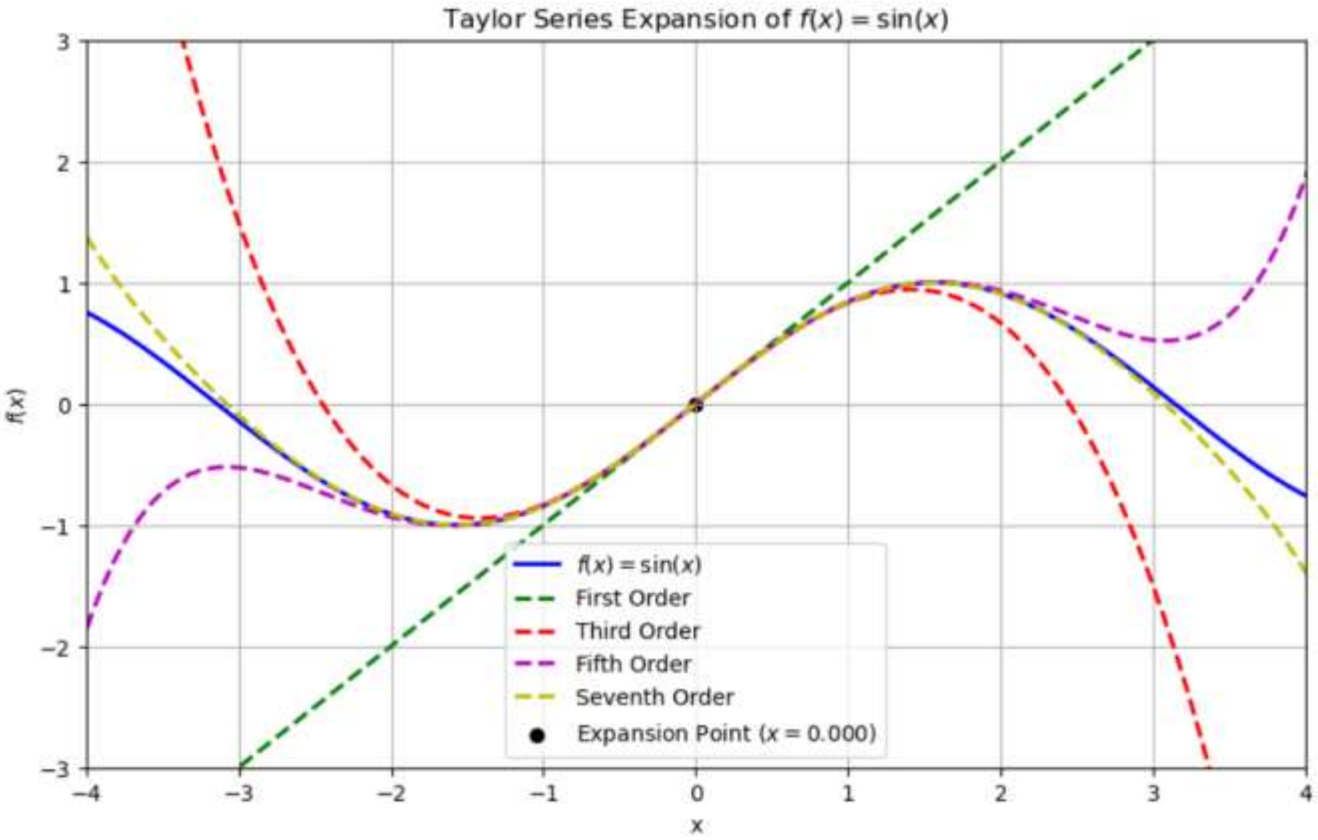
$$\mathrm{f}'''(0) = -\cos(0) \longrightarrow \mathrm{f}'''(0) = -1$$

$$\rightarrow \quad f(x) \approx 0 + (1)\frac{(x - 0)}{1} + 0 + (-1)\frac{(x - 0)^3}{6} = x - \frac{x^3}{6}$$

Taylor Series Expansions

- Compute the Taylor Series Expansion of $f(x) = \sin(x)$ around $x_0 = 0$ with third order accuracy

$$\sin(x) \approx x - \frac{x^3}{6}$$



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Question slide

Which approximation gives the best result at x=10?

1 term

0%

3 terms

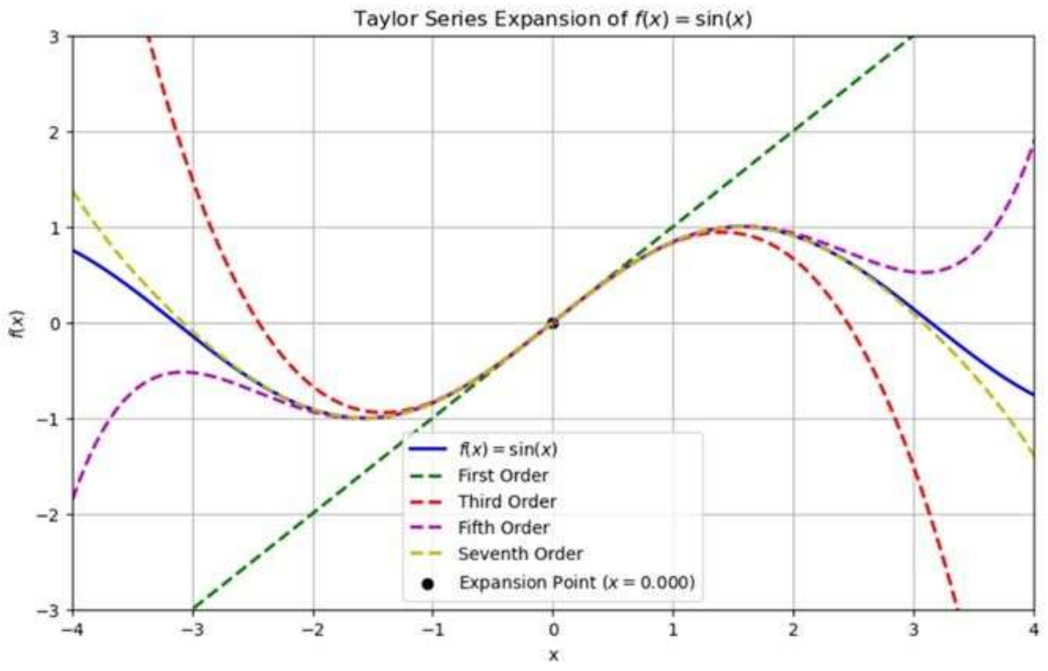
0%

5 terms

0%

7 terms

0%



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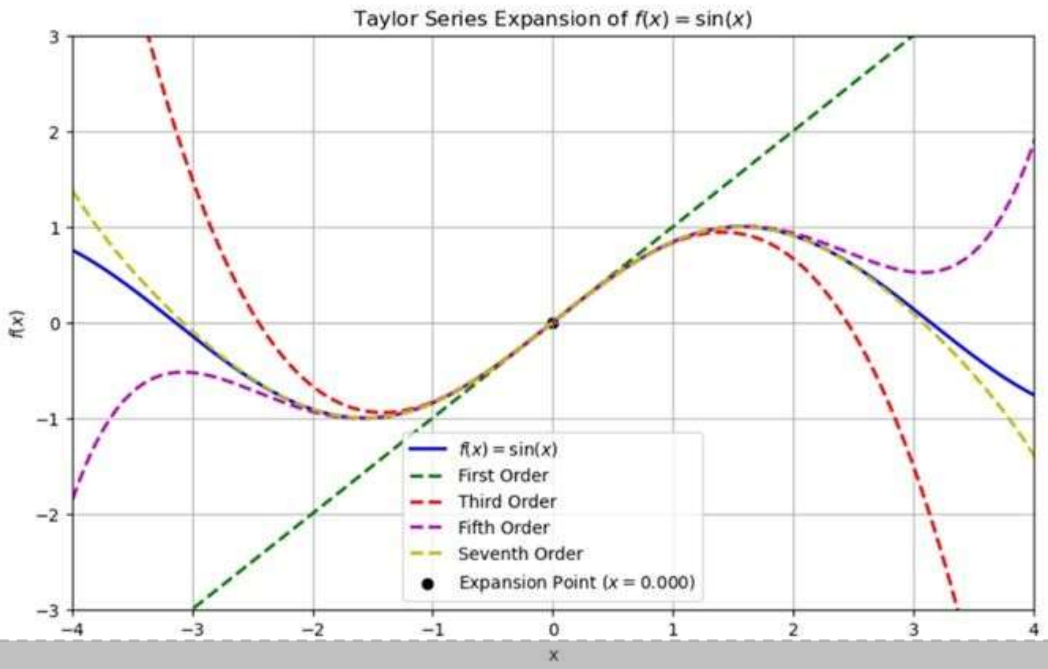
Join at: **vevox.app**

ID: **123-957-664**

Preparing Results

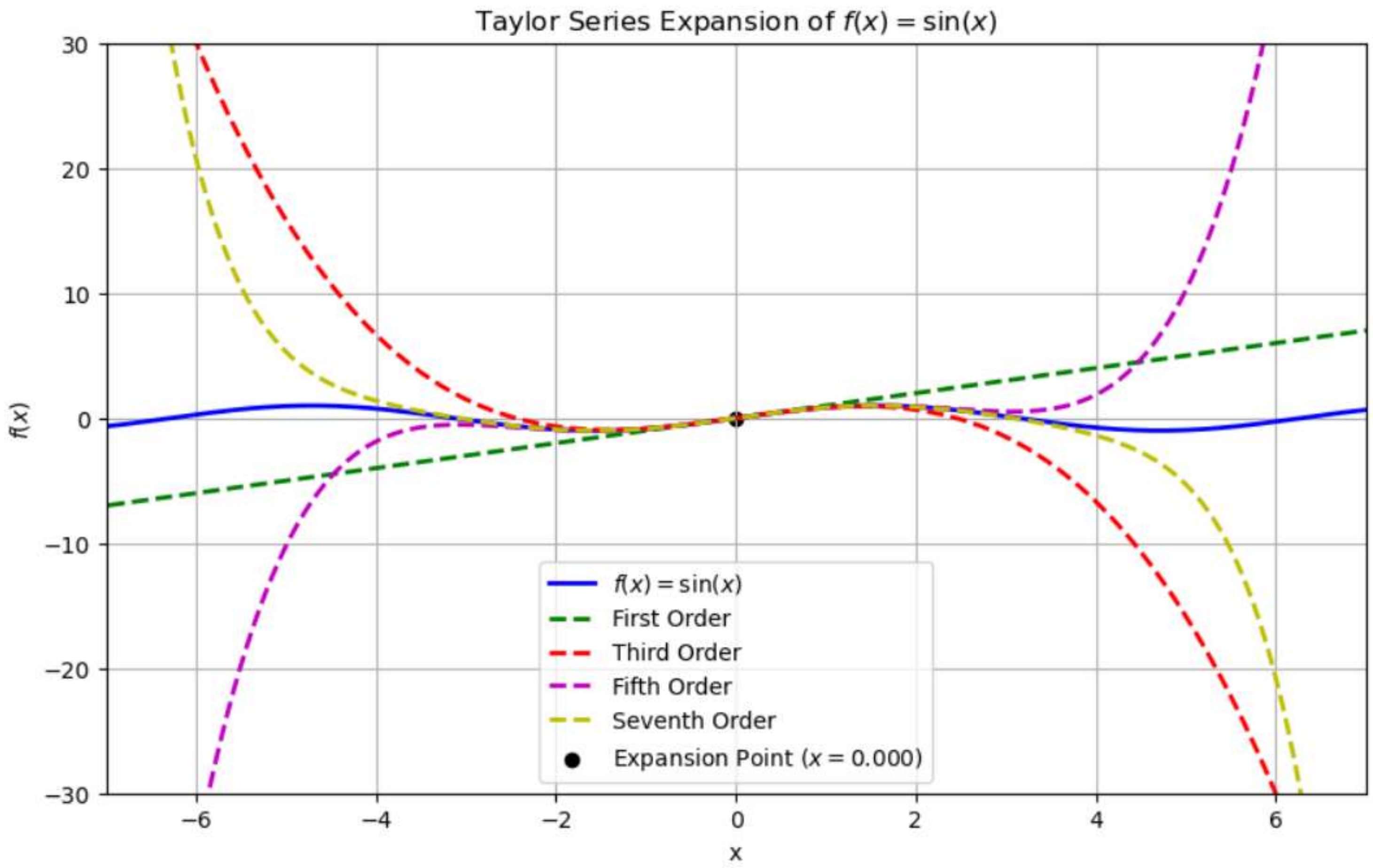
Which approximation gives the best result at x=10?

Option	Result
1 term	0%
3 terms	0%
5 terms	0%
7 terms	0%



RESULTS SLIDE

- The more terms used; the solution will be more accurate near x_0
- The farther from x_0; the error increases



Taylor Series Expansions to get the derivatives

- Basic derivatives
- Higher order Finite Difference
- Second derivative Finite Difference

Taylor expansion – 1 or 2 variables

- Taylor series for a function of one variable *y=f(x)*:

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

- Second degree Taylor Polynomial of a function of two variables, *f(x,y)*

$$f(x,y) \approx f(x_0, y_0) + f'_x(x_0, y_0)(x - x_0) + f'_y(x_0, y_0)(y - y_0) \ +$$

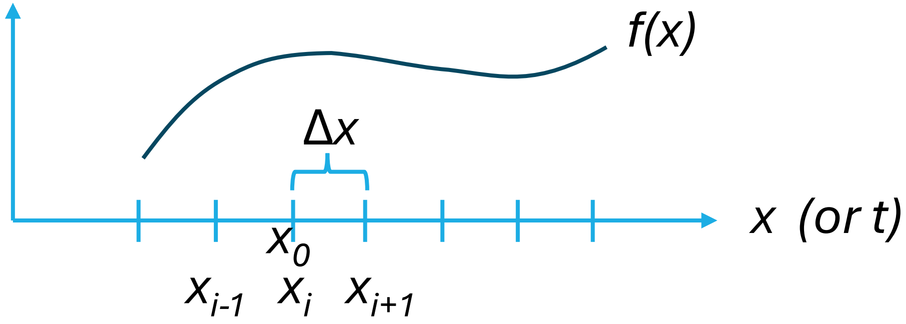
$$\frac{f_x''(x_0, y_0)}{2}(x - x_0)^2 + \frac{f_y''(x_0, y_0)}{2}(y - y_0)^2 + f_{xy}''(x_0, y_0)(x - x_0)(y - y_0)$$

Taylor expansion – Derivation of expression for first derivative

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

Based on TSE, consider a regular interval $(x\text{-}x_0) = \Delta x$ (hence, $x = x_0 + \Delta x$):
Derive an expression for the $O(\Delta x)$-accurate first derivative of function $f(x)$ around x_0

$$f(x_0 + \Delta x) = \ \ldots ?$$



$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x \pm O(\Delta x^2)$$

$$f'(x_0) = \frac{\overset{x_{i+1}}{f(x_0 + \Delta x)} - \overset{x_i}{f(x_0)}}{\Delta x} \pm O(\Delta x)$$

Forward Difference method

$$f'(x_0) = \frac{f(x_0) - \overset{x_{i-1}}{f(x_0 - \Delta x)}}{\Delta x} \pm O(\Delta x)$$

Backward Difference method

Taylor expansion – Derivation of expression for higher-order derivative

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

Derive an expression for the $O(\Delta x^2)$-accurate first derivative of function $f(x)$ around x_0

$$f(x_0 + \Delta x) = \cancel{f(x_0)} + f'(x_0)\Delta x + \cancel{\frac{f''(x_0)}{2}(\Delta x)^2} \pm O(\Delta x^3)$$

$$f(x_0 - \Delta x) = \cancel{f(x_0)} - f'(x_0)\Delta x + \cancel{\frac{f''(x_0)}{2}(\Delta x)^2} \pm O(\Delta x^3)$$

$$f(x_0 + \Delta x) - f(x_0 - \Delta x) = 2 f'(x_0)\Delta x \pm O(\Delta x^3)$$

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

Central Difference method

Taylor expansion – Derivation of

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x -$$

Derive an expression for the second deriv

$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + \frac{f''}{}$$

$$f(x_0) \qquad = f(x_0)$$

$$f(x_0 - \Delta x) = f(x_0) - f'(x_0)\Delta x + \frac{f''}{}$$

$$f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x) =$$

First define a TSE for a point two steps away from x_i:

$$f(x_i + 2\Delta x) = f(x_i) + 2\Delta x f'(x_i) + \frac{(2\Delta x)^2}{2!} f''(x_i) + \mathcal{O}(\Delta x^3).$$

Now multiply the TSE by two for a point one step away from x_i:

$$2f(x_i + \Delta x) = 2f(x_i) + 2\Delta x f'(x_i) + \frac{2\Delta x^2}{2!} f''(x_i) + \mathcal{O}(\Delta x^3).$$

By subtracting the first expression from the second one the first derivative disappears:

$$f(x_i + 2\Delta x) - 2f(x_i + \Delta x) = -f(x_i) + \frac{2\Delta x^2}{2!} f''(x_i) + \mathcal{O}(\Delta x^3).$$

By solving for f'' we obtain the **forward** expression:

$$f''(x_i) = \frac{f(x_i + 2\Delta x) - 2f(x_i + \Delta x) + f(x_i)}{\Delta x^2} + \mathcal{O}(\Delta x).$$

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

Taylor Series Expansions to get the derivatives

- Different numerical **approximations** of the derivative can be found using TSE
- Using TSE, we also find the error order.
  FD/BD are first-order accurate, CD second-order accurate.
- You can find **more accurate approximations** by using more points
- The approximation of the second derivative requires at least one more point of information

Numerical Integration

Numerical Integration

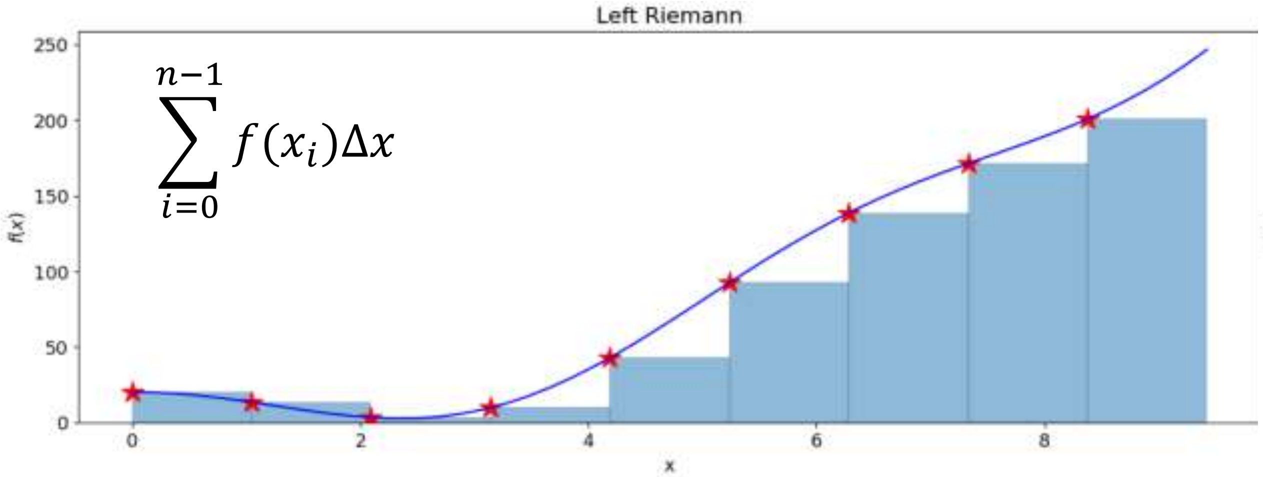
Numerical integration : a technique used to approximate the value of a defined integral, when it is not possible to obtain the exact value.

$$I = \int_a^b f(x)dx$$

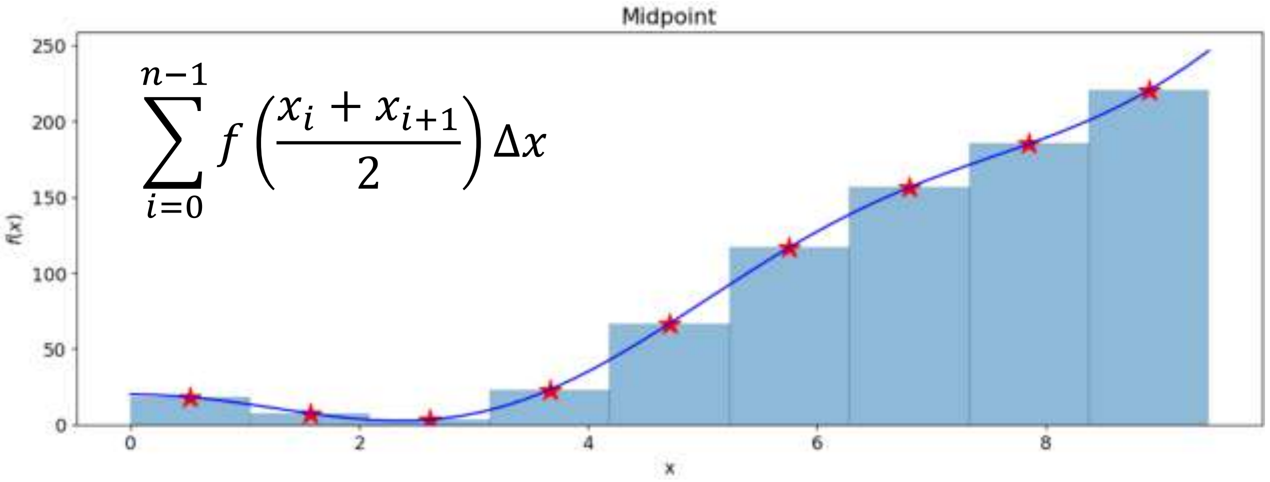
Numerical integration rules :

- Left Riemann
- Right Riemann
- Midpoint rule
- Trapezoidal rule
- …

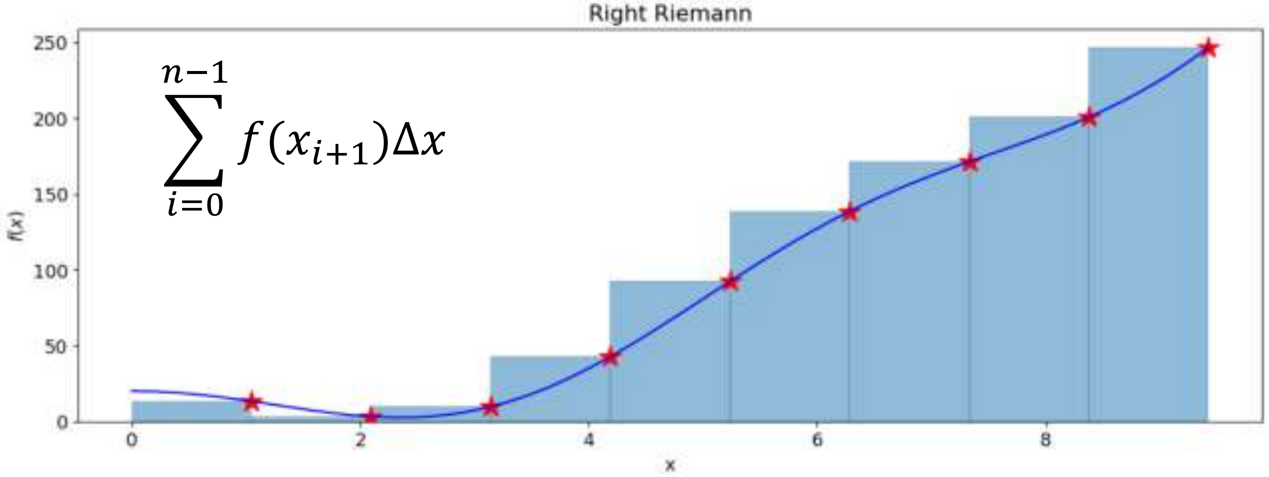
Numerical Integration Methods: $I \approx$



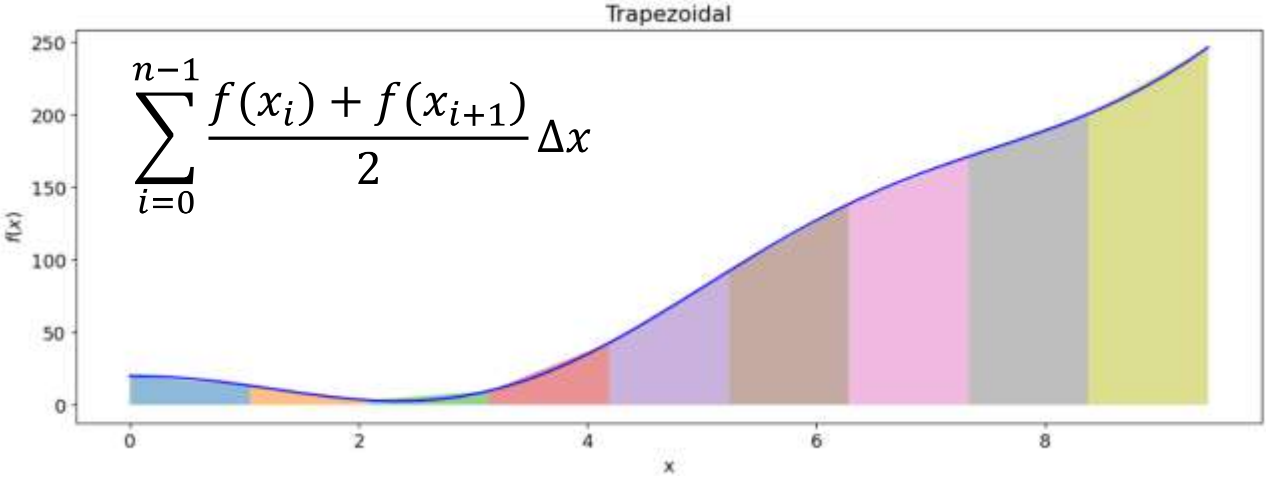
$$\sum_{i=0}^{n-1} f(x_i)\Delta x$$



$$\sum_{i=0}^{n-1} f\left(\frac{x_i + x_{i+1}}{2}\right)\Delta x$$



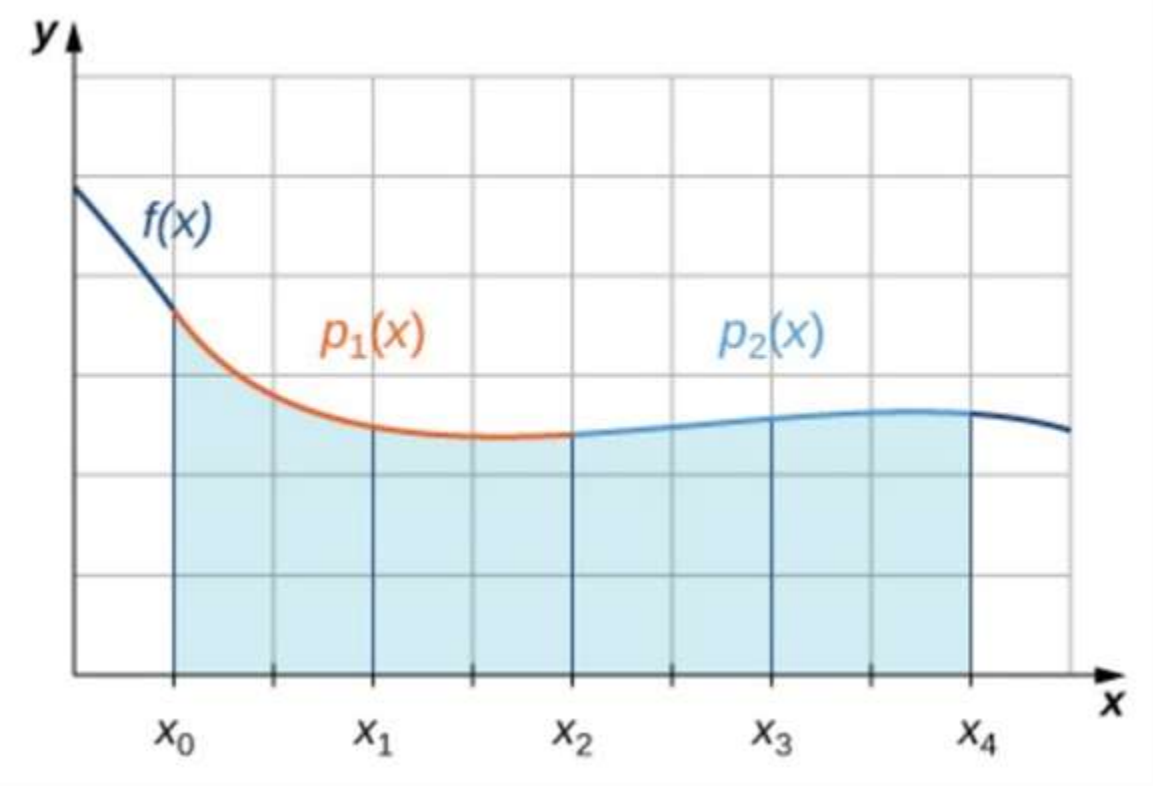
$$\sum_{i=0}^{n-1} f(x_{i+1})\Delta x$$



$$\sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2}\Delta x$$

Numerical Integration Methods: $I \approx$

Simpson's rule:



$$\approx \sum_{i=1}^{n/2} \frac{f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})}{6} 2\Delta x$$

Works only for equally spaced intervals

Numerical Integration Rules

$$\text{Left Riemann Error } = \left| \int_a^b f(x)dx - \sum_{i=0}^{n-1} f(x_i)\Delta x \right|$$

Elaboration using TSE gives:

$$\text{Left Riemann Error } = \left| \bar{f}'(b-a)\Delta x/2 \right| \text{ therefore } \mathcal{O}(\Delta x)$$

$$\text{Right Riemann Error } = \left| \bar{f}'(b-a)\Delta x/2 \right| \text{ therefore } \mathcal{O}(\Delta x)$$

$$\text{Midpoint Error } = \left| \bar{f}''(b-a)\Delta x^2/2 \right| \text{ therefore } \mathcal{O}(\Delta x^2)$$

$$\text{Trapezoidal Error } = \left| \bar{f}''(b-a)\Delta x^2/2 \right| \text{ therefore } \mathcal{O}(\Delta x^2)$$

$$\text{Simpsons Error } = \left| \bar{f}''''(b-a)\Delta x^4/2 \right| \text{ therefore } \mathcal{O}(\Delta x^4)$$

Example: Integration of PDF to obtain CDF

Consider the Standard Gumbel Probability Density Function (PDF) for a stochastic variable: $f(x) = e^{-(x+e^{-x})}$

Calculate the Cumulative Distribution (CDF) for *x* = 0, 2 and 4 by numerical integration

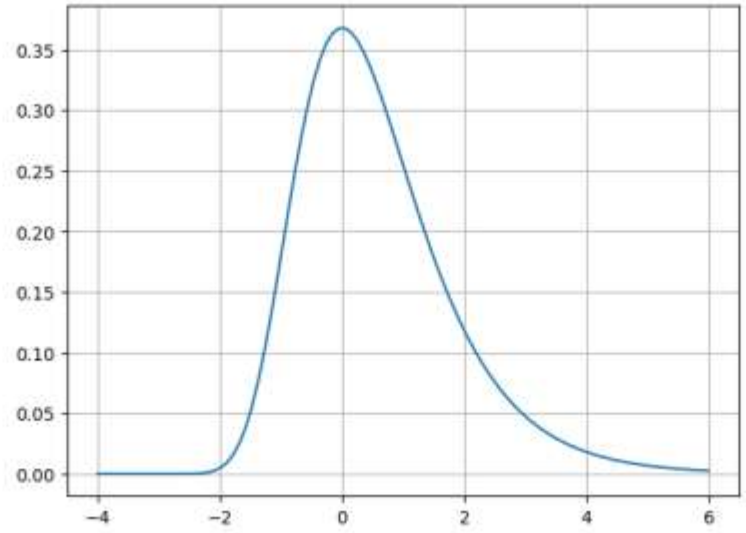
Theoretical solution for CDF:

$$F(x) = \int_{-\infty}^{x} f(x)\,dx = e^{-e^{-x}}$$

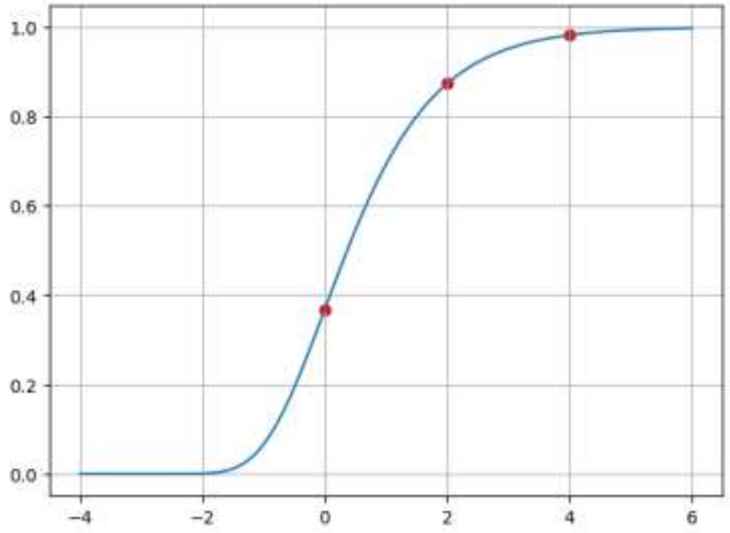
So, for target points:

x = 0: F(0) = 0.36787944
x = 2: F(2) = 0.87342302
x = 4: F(4) = 0.98185107

PDF



CDF



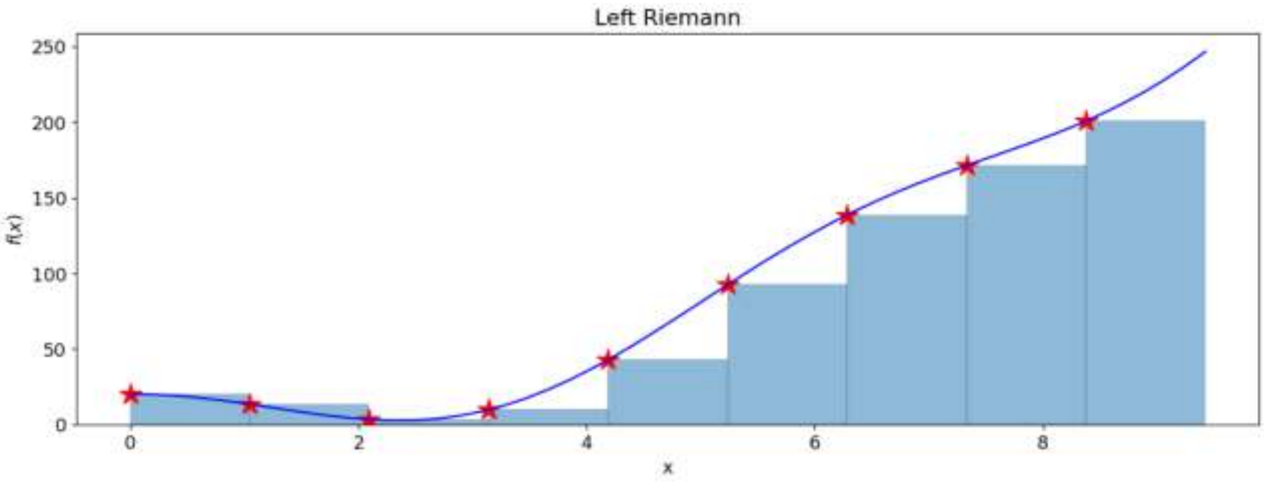
Numerical solutions for Left and Right Riemann, Midpoint and Trapezoidal rule (next slides):

Example: Integration of PDF to obtain CDF

$$F(x) = \int_{-\infty}^{x} f(x)\,dx$$

Left Riemann:

$$\sum_{i=0}^{n-1} f(x_i)\Delta x$$




```
nsteps = 100
Y1 = np.zeros(nsteps+1)

dx = 10. / nsteps
x1 = np.linspace(-4, 6, num=nsteps+1)
for i in range(nsteps):
    Y1[i+1] = Y1[i] + f(x1[i]) * dx
```

Target points (x=0, 2, 4):

```
Left Riemann rule:    [0.34948542 0.8674276  0.9809372 ]
Analytical solution:  [0.36787944 0.11820495 0.01798323]
```

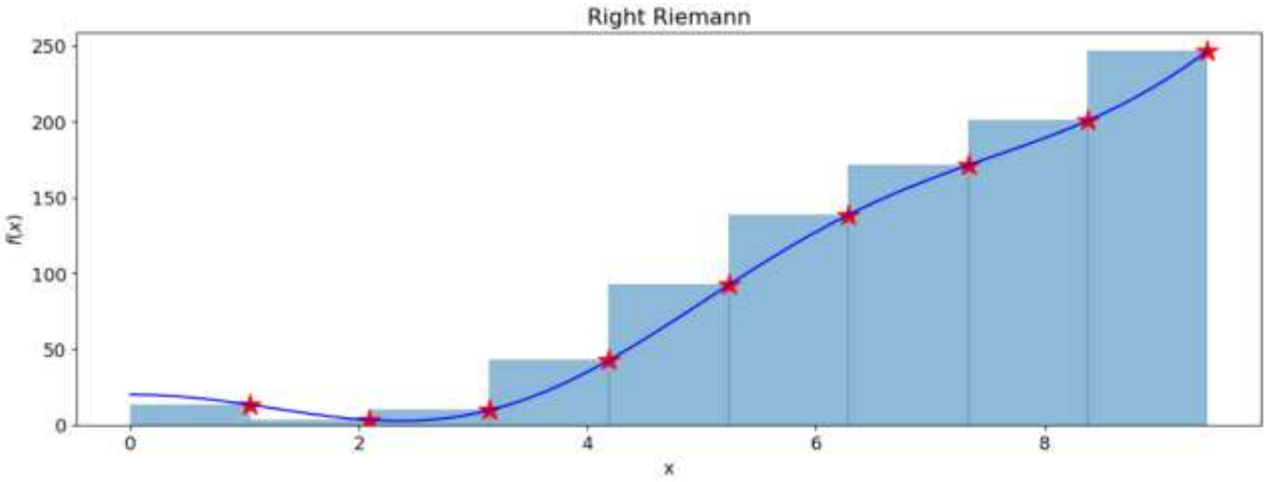
Example: Integration of PDF to obtain CDF

$$F(x) = \int_{-\infty}^{x} f(x)\, dx$$

Right Riemann:

$$\sum_{i=0}^{n-1} f(x_{i+1})\Delta x$$

or $$\sum_{i=1}^{n} f(x_i)\Delta x$$




```
Y1 = np.zeros(nsteps+1)

for i in range(nsteps):
    Y1[i+1] = Y1[i] + f(x1[i+1]) * dx
```

Target points (x=0, 2, 4):

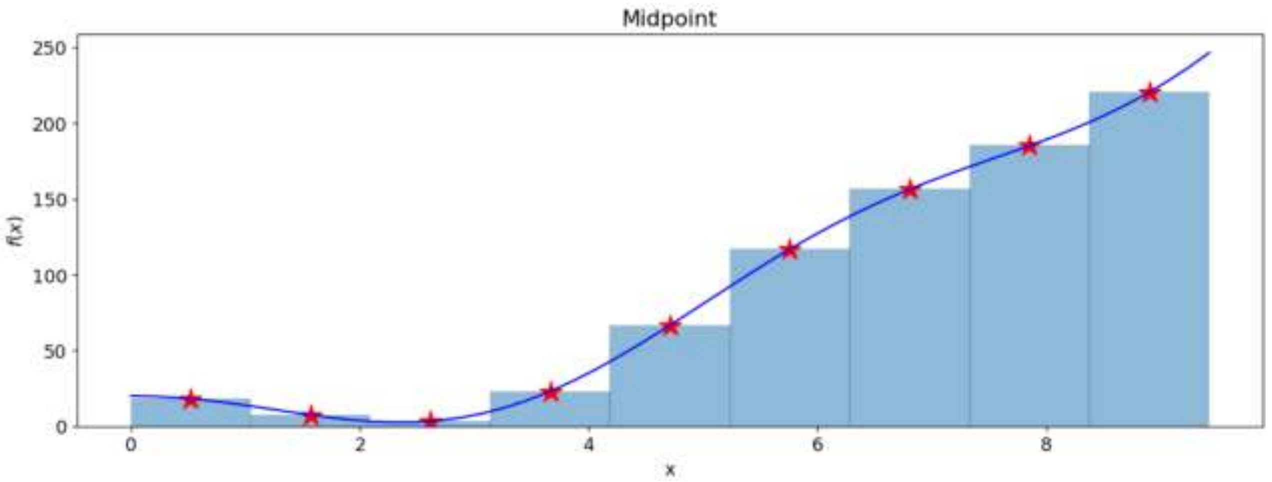
```
Right Riemann rule:    [0.38627336 0.8792481  0.98273553]
Analytical solution:   [0.36787944 0.11820495 0.01798323]
```

Example: Integration of PDF to obtain CDF

$$F(x) = \int_{-\infty}^{x} f(x)\, dx$$

Midpoint rule:

$$\sum_{i=0}^{n-1} f\left(\frac{x_i + x_{i+1}}{2}\right) \Delta x$$




```
Y1 = np.zeros(nsteps+1)

for i in range(nsteps):
    Y1[i+1] = Y1[i] + f((x1[i] + x1[i+1])/2) * dx
```

Target points (x=0, 2, 4):

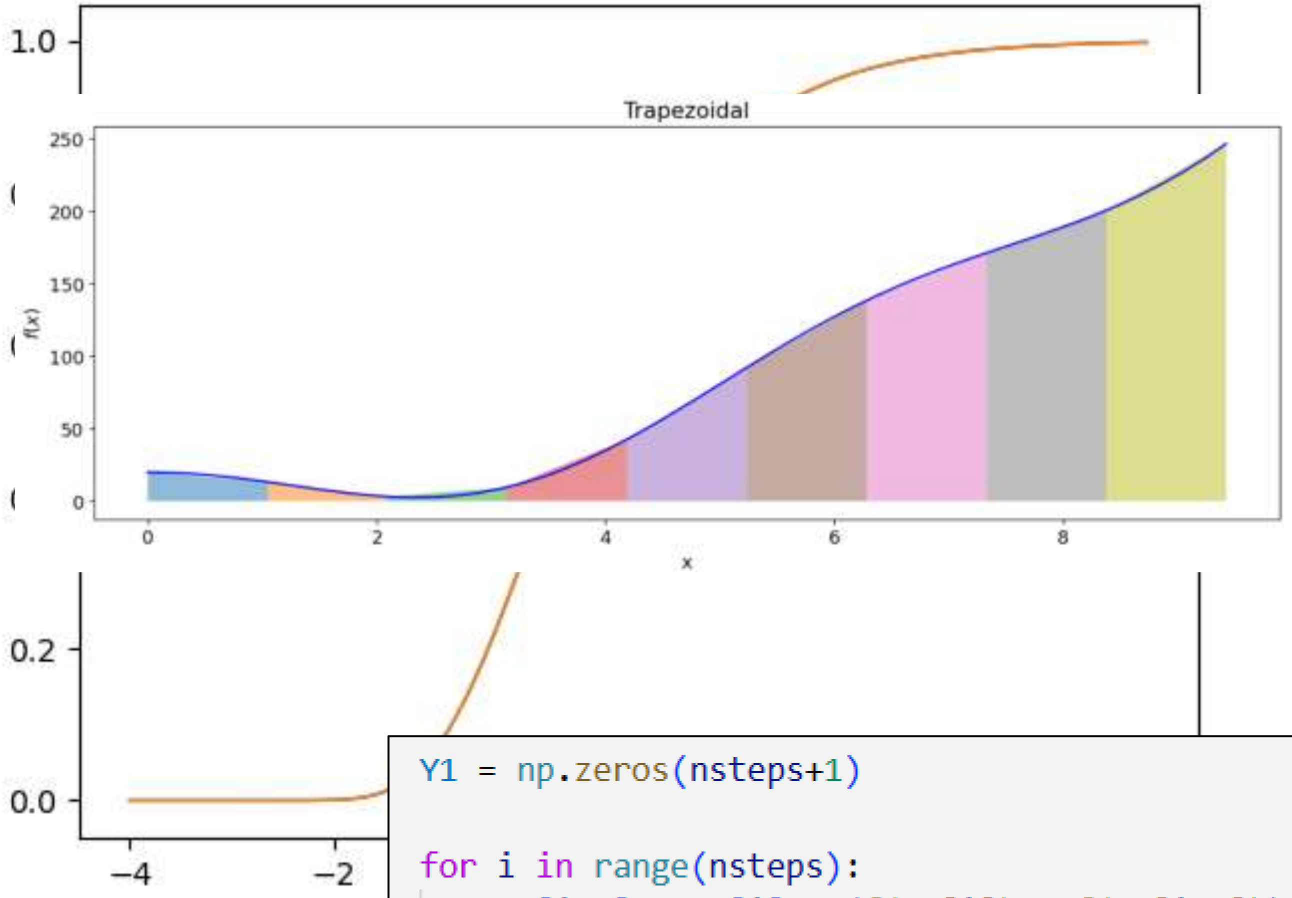
```
Midpoint rule:        [0.36787949 0.8734656  0.98185843]
Analytical solution:  [0.36787944 0.11820495 0.01798323]
```

Example: Integration of PDF to obtain CDF

$$F(x) = \int_{-\infty}^{x} f(x)\, dx$$

Trapezoidal rule:

$$\sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2} \Delta x$$




```python
Y1 = np.zeros(nsteps+1)

for i in range(nsteps):
    Y1[i+1] = Y1[i] + (f(x1[i]) + f(x1[i+1]))/2 * dx
```

In this way, we can integrate up to any intermediate x-value in a range to reproduce the entire CDF by numerical integration

Target points (x=0, 2, 4):

```
Trapezoidal rule:      [0.36787939 0.87333785 0.98183636]
Analytical solution:  [0.36787944 0.11820495 0.01798323]
```

Differential equations – ODEs, PDEs

Ice growth
First order ODE $\rightarrow$

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water} - T_{air}}{h_{ice}}$$

Beam deformation
Second order ODE $\rightarrow$

$$\frac{d^2v}{dz^2} = \frac{-1}{EI}\left(-\frac{qz^2}{2} + qLz - \frac{qL^2}{2}\right)$$

1D consolidation
Second order PDE $\rightarrow$

$$\frac{\partial p}{\partial t} = c_v \frac{\partial^2 p}{\partial z^2}$$

In Q1, we will NOT further consider PDEs !

How many constraints do the following equations need?

1 and 1 — 0%

1 and 2 — 0%

2 and 1 — 0%

1 and 3 — 0%

3 and 1 — 0%

2 and 2 — 0%

2 and 3 — 0%

3 and 2 — 0%

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water} - T_{air}}{h_{ice}}$$

and

$$\frac{d^2v}{dz^2} = \frac{-1}{EI}\left(-\frac{qz^2}{2} + qLz - \frac{qL^2}{2}\right)$$

How many constraints do the following equations need?

1 and 1	0%
1 and 2	0%
2 and 1	0%
1 and 3	0%
3 and 1	0%
2 and 2	0%
2 and 3	0%
3 and 2	0%

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water} - T_{air}}{h_{ice}}$$

and

$$\frac{d^2v}{dz^2} = \frac{-1}{EI}\left(-\frac{qz^2}{2} + qLz - \frac{qL^2}{2}\right)$$

RESULTS SLIDE

Initial Value Problem

$$\frac{dy}{dt} = -y + e^{-t} \quad \rightarrow \quad ?$$

How many solutions do exist for this initial value problem?

How many solutions exist for this initial value problem?

0	0%
1	0%
2	0%
3	0%
5	0%
Infinite	0%

0/1 Join at: **vevox.app** ID: **123-957-664** Preparing Results

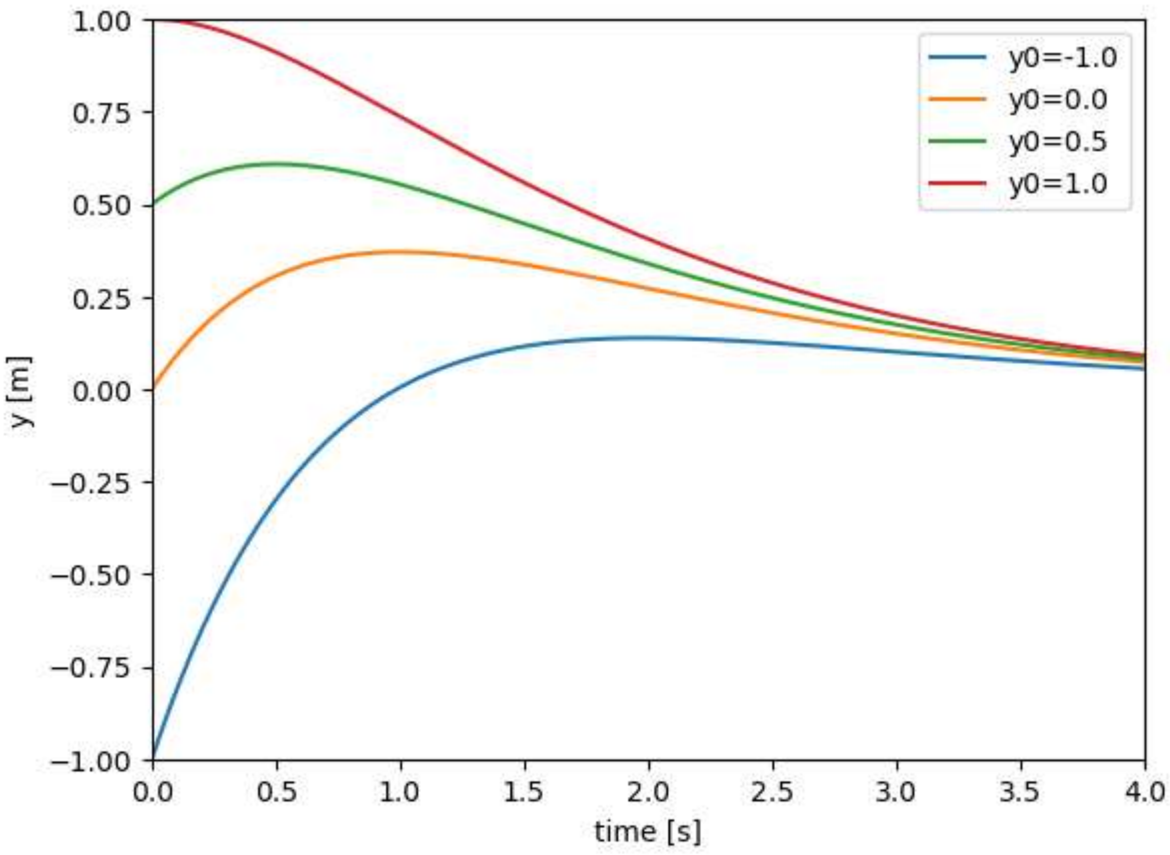
How many solutions exist for this initial value problem?

0	0%
1	0%
2	0%
3	0%
5	0%
Infinite	0%

RESULTS SLIDE

Initial Value Problem

$$\frac{dy}{dt} = -y + e^{-t} \quad \rightarrow$$



Any ODE that has a time dependency, no matter the order, has a solution completely dependent on the initial value!

Summary

- Numerical solutions are used in all kinds of situations
  - Root finding (f(x) = 0)
  - Solving differential equations
  - Numerical integration
- Taylor Series Expansion
  - Derivatives (FD, BD, CD)
  - The relevance of taking higher-order terms into account
  - Accuracy order
- Numerical integration:
  - Left Riemann
  - Right Riemann
  - Midpoint
  - Trapezoidal rule
  - Simpson's rule
- Differential equations (to be continued next week):
  - Initial value problems
  - Boundary value problems

What you can expect further this week…

- Programming Assignment 1.2:
  - Working with GitHub
  - Creating reports with MarkDown
  - Programming: Fundamentals, visualizing a matrix, creating subplots, list comprehension, filling a matrix

- Wednesday 10:45-12:30: Workshop 1.2:
  - Integrating a Probability Density Function (PDF) into a Cumulative Distribution Function (CDF)
  - Integrating and differentiating an earthquake signal

- Friday 9:45-12:30: Group Assignment 1.2:
  - Integrating salt concentration in a river
  - TS approximation of a function
  - TSE approach to function derivatives and accuracy

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