Discretization |

Introduction Numerics vs Analytics

Discretizatio

Numerical Derivatives

Numerical Integration

#### Discretization I

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#### Outline

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Numerical Derivative

- 1 Introduction
  Numerics vs Analytics
- 2 Discretization
- 3 Numerical Derivatives
- 4 Numerical Integration

# Why Numerics? I

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Numerical Integration What do we want to do?

describe nature

How do we do it?

mathematics

# Why Numerics? II

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#### Numerics?

- is a branch of mathematics
- deals with numbers (of finite precision)
- may be synonymous for "the art of approximation"

# Why Numerics? III

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#### Approximations?

- $+, -, \cdot, /$  work very well on defined fields (discrete operations)
- representation of functions at discrete points tricky
- operations that require continuity of operands, e.g.  $\int dx, \, \frac{d}{dx}$  may be more difficult

# Are we lazy or stupid?

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Numerical Integratio Instead of finding analytical solutions to be valid:

- for all times
- for all initial conditions

we aim for:

- calculation of results just for some points (discreteness)
- approximate evolution of a system (e.g. a single set of initial conditions in phase space (single trajectory))

#### We are finite creatures

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#### So?

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Numerical Integration We undo the ingenious step (by Leibnitz):

$$\lim_{h\to 0}\frac{f(x+h)-f(x)}{h}=\dot{f}(x)$$

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$$\frac{f(x+h) - f(x)}{h} \simeq \dot{f}(x)$$

e.g.

$$\frac{d\vec{r}}{dt} \to \frac{\Delta \vec{r}}{\Delta t} = \vec{v}$$

with:

$$\frac{\Delta \vec{r}}{\Delta t} = \frac{\vec{r}(t_1) - \vec{r}(t_0)}{\Delta t} = \vec{v}$$

#### Discretization

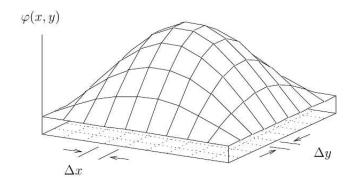
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#### Discretization

Numerical Derivative



# First - once again Taylor...

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Numerical Integration with:

$$f(x) = f(a) + f'(a)(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \dots + \frac{f^{(n)}(a)}{n!}(x - a)^n + R_n(x)$$

$$|R_n(x)| \le M_n \frac{r^{n+1}}{(n+1)!}$$

# Taylor II

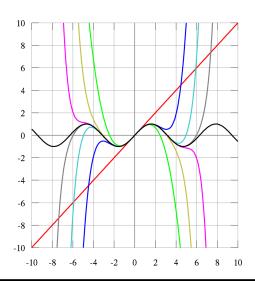
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#### Taylor as we will use it...

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$$f(x+h) \approx f(x) + f'(x)(h) + \frac{f''(x)}{2!}(h)^2 + \dots + \frac{f^{(n)}(x)}{n!}(h)^n + O(h^{n+1})$$

$$f(x-h) \approx f(x) - f'(x)(h) + \frac{f''(x)}{2!}(h)^2 - \dots + \frac{f^{(n)}(x)}{n!}(h)^n + O(h^{n+1})$$

# differencing and approximations of derivatives

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Numerical Integration forward differencing

$$\frac{f(x+h) - f(x)}{h} = f'(x) + O(h^?)$$

backward differencing

$$\frac{f(x) - f(x - h)}{h} = f'(x) + O(h^?)$$

centered differencing I

$$\frac{f(x+h) - f(x-h)}{h} = f'(x) + O(h^?)$$

# differencing and approximations of derivatives II

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forward differencing

$$\Delta_h[f](x) = f(x+h) - f(x)$$

backward differencing

$$\nabla_h[f](x) = f(x) - f(x - h))$$

centered differencing II

$$\delta_h[f](x) = f(x + \frac{1}{2}h) - f(x - \frac{1}{2}h)$$

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# higher derivatives I

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Numerical Integration forward differencing

$$\Delta_h^n[f](x) = \sum_{i=0}^n (-1)^i \binom{n}{i} f(x + (n-i)h),$$

backward differencing

$$\nabla_h^n[f](x) = \sum_{i=0}^n (-1)^i \binom{n}{i} f(x-ih)$$

centered differencing II

$$\delta_h^n[f](x) = \sum_{i=0}^n (-1)^i \binom{n}{i} f\left(x + \left(\frac{n}{2} - i\right)h\right)$$

# higher derivatives II

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Numerical Integration second derivatives using central differencing II

$$f''(x) \approx \frac{\delta_h^2[f](x)}{h^2} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

higher derivatives

$$\frac{d^n f}{dx^n}(x) = \frac{\Delta_h^n[f](x)}{h^n} + O(h) = \frac{\nabla_h^n[f](x)}{h^n} + O(h) = \frac{\delta_h^n[f](x)}{h^n} + O(h^2).$$

#### Numerical Integration

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Numerical Integration Two "philosophies"

- Taylor-based
- Geometry-based

#### Taylor-based

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Numerical Integration Euler's method

$$f(x+h) \simeq f(x) + h \cdot \dot{f}(x)$$

Predictor-Corrector, Runge Kutta, Lie-Series,...

# Geometry-based

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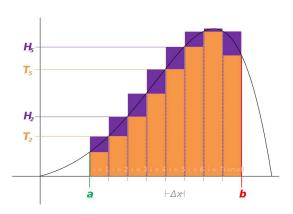
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Upper,lower Sum, Trapezoidal Rule, Simpson Rule  $\rightarrow$  Newton-Cotes rules

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Numerical Integration Thank you for your attention

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