Discretization I

S. Eggl[1]

[1]Institute for Astronomy,
University of Vienna,
Vienna, Austria.

Practical in numerical Astronomy
Vienna

March 2010

Outline

Why Numerics? I

What do we want to do?

- describe nature

How do we do it?

- mathematics

Why Numerics? II

Numerics?

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

Why Numerics? III

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?

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

So?

We undo the ingenious step (by Leibnitz):

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

$\rightarrow$

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

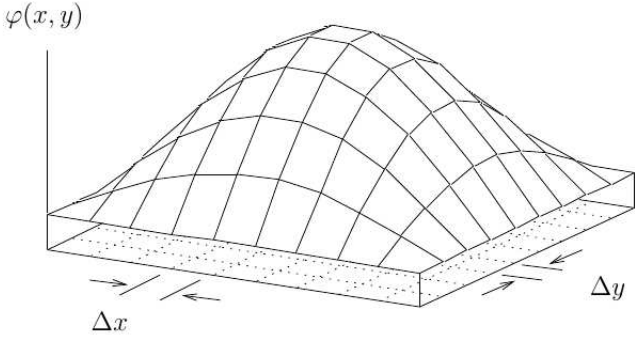
e.g.

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

with:

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

Discretization



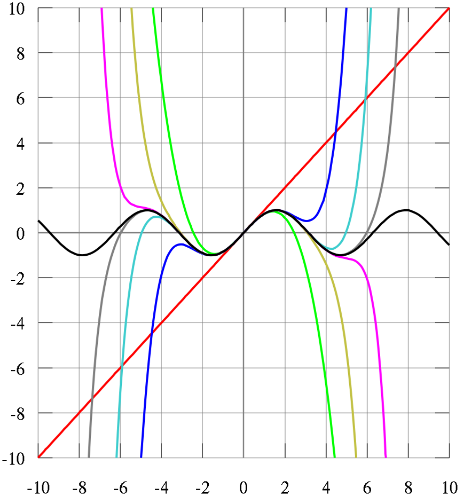
First - once again Taylor...

with:

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

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

Taylor II



Taylor as we will use it...

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

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

differencing and approximations of derivatives

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

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

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

higher derivatives I

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

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

Two "philosophies"

- Taylor-based
- Geometry-based

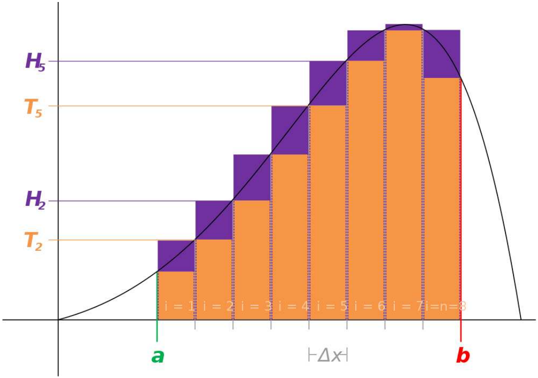
Taylor-based

Euler's method

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

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

Geometry-based



Upper,lower Sum, Trapezoidal Rule, Simpson Rule → Newton-Cotes rules

Thank you for your attention