Numerical Integration ODEs I

S. Eggl[1]

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

Practical in numerical Astronomy
Vienna

March 2010

Outline

ODE Definition I

ODEs? Definition?

ODE Definition I

ODEs? Definition?

- relation containing functions

ODE Definition I

ODEs? Definition?

- relation containing functions
- only *one* independent variable

ODE Definition I

ODEs? Definition?

- relation containing functions
- only *one* independent variable
- one or more of their *derivatives* with respect to that variable

Examples

Newton's second law

$$m\frac{d^2x(t)}{dt^2} = F(x(t))$$

Radioactive Decay

$$\frac{du(x)}{dx} = -\frac{1}{\xi}u(x))$$

Anti-Examples

Wave Equation

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \sum_{i=1}^{n}\left(\frac{\partial^2 u}{\partial x_i^2}\right) = 0$$

Poisson's Equation

$$\Delta\phi = f$$

ODE Definition II

$$\Omega \subseteq \mathbb{R} \times (\mathbb{R}^m)^{n+1}, n \in \mathbb{N}$$

$$f : \Omega \longrightarrow \mathbb{R}^m, \text{ f continous}$$

$$f\left(x, y, y', y'', \ldots, y^{(n)}\right) = 0$$

- n-th order
- m-equations

ODE Characterization

explicit

$$y^{(n)} = f\left(x, y, y', y'', \ldots, y^{(n-1)}\right)$$

implicit

$$f\left(x, y, y', y'', \ldots, y^{(n)}\right) = 0$$

ODE Characterization II

initial value problem

$$y(x_0) = y_0,\ y'(x_0) = y_1, \ldots, y^{(n-1)}(x_0) = y_{n-1}$$

boundary value problem

$$y(x_0) = y_0,\ y(x_1) = y_1, \ldots, y(x_n) = y_n$$

ODE Characterization III

autonomous

$$f\left(y, y', y'', \ldots, y^{(n)}\right) = 0$$

inhomogenous (example)

$$f\left(x, y, y', y'', \ldots, y^{(n)}\right) = g(x)$$

ODE Reduction of Order

$$
\begin{aligned}
y_1' &= y_2 \\
y_2' &= y_3 \\
&\vdots \\
y_{n-1}' &= y_n \\
y_n' &= f(x, y_1, y_2, \ldots, y_n)
\end{aligned}
$$

ODE Analytical Solutions

- Ansaetze often very specific
- not much generalization possible
- yet if found they are *exact*

ODE Numerical Solutions

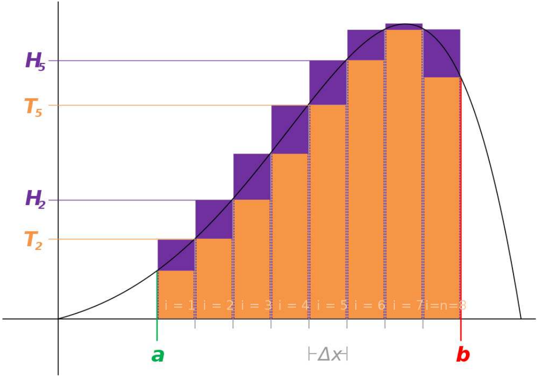
- general Ansaetze available
- not always the best idea to just use them without thinking
- specific *approximations*

Numerical Integration

Two "philosophies"

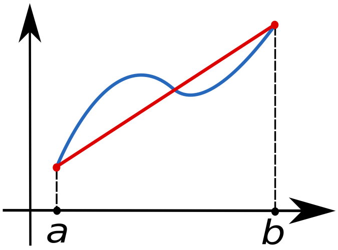
- Geometry-based
- Taylor-based

Geometry-based, Rectangle Rule



$\int_a^b f(x)\,dx \approx f(b)(b-a)$ $\int_a^b f(x)\,dx \approx f(a)(b-a)$

Geometry-based - Trapezoidal Rule



$$\int_a^b f(x)\,dx \approx (b-a)\frac{f(a)+f(b)}{2}$$

Newton - Cotes

$$\int_a^b f(x)\,dx \approx \int_a^b L(x)\,dx =$$

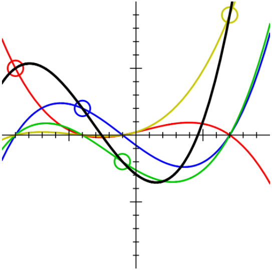
$$\int_a^b \Big(\sum_{i=0}^n f(x_i)\,l_i(x)\Big)\,dx = \sum_{i=0}^n f(x_i) \underbrace{\int_a^b l_i(x)\,dx}_{w_i}$$

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^n w_i\,f(x_i)$$

Lagrange basis polynomials $l_i(x)$

$$L(x) := \sum_{j=0}^{k} y_j \ell_j(x)$$

$$\ell_j(x) := \prod_{f=0,\, f\neq j}^{k} \frac{x-x_f}{x_j-x_f} = \frac{(x-x_0)}{(x_j-x_0)} \cdots \frac{(x-x_{j-1})}{(x_j-x_{j-1})} \frac{(x-x_{j+1})}{(x_j-x_{j+1})} \cdots \frac{(x-x_k)}{(x_j-x_k)}$$



Newton - Cotes II

degree n	name	weights w_i	error
0	Rectangle Rule	0 1	$\frac{h^2}{2} f'(\xi)$
1	Trapezoidal Rule	$\frac{1}{2}$ $\frac{1}{2}$	$\frac{h^3}{12} f''(\xi)$
2	Simpson's Rule	$\frac{1}{6}$ $\frac{4}{6}$ $\frac{1}{6}$	$\frac{(\frac{1}{2}h)^5}{90} f^{(4)}(\xi)$
3	3/8-Rule	$\frac{1}{8}$ $\frac{3}{8}$ $\frac{3}{8}$ $\frac{1}{8}$	$\frac{3(\frac{1}{3}h)^5}{80} f^{(4)}(\xi)$
4	Milne-Rule	$\frac{7}{90}$ $\frac{32}{90}$ $\frac{12}{90}$ $\frac{32}{90}$ $\frac{7}{90}$	$\frac{8(\frac{1}{4}h)^7}{945} f^{(6)}(\xi)$
5	6-Point-Rule	$\frac{19}{288}$ $\frac{75}{288}$ $\frac{50}{288}$ $\frac{50}{288}$ $\frac{75}{288}$ $\frac{19}{288}$	$\frac{275(\frac{1}{5}h)^7}{12096} f^{(6)}(\xi)$

where $t_0 \leq \xi \leq t_0 + h$

Taylor-based

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

Euler's method

$$f(x+h) \simeq f(x) + h \cdot f'(x)$$

Example: Radioactive Decay

$$\frac{du(t)}{dt} = -\frac{1}{\tau}u(t))$$

$$f(u, \dot{u}) = 0$$

explicit Euler's method

$$u^{(n+1)} = u^{(n)} - \frac{h}{\tau}u^{(n)} + O(h^2)$$

Example: Radioactive Decay II

implicit Euler's method

$$u^{(n+1)} = u^{(n)} - \frac{h}{\tau} u^{(n+1)} + O(h^2)$$

$$u^{(n+1)} = \frac{1}{1 + \frac{h}{\tau}} u^{(n)} + O(h^2)$$

Being smart

clever combinations of Taylor Series in different directions

$f(t_0 + h) \simeq f(t_0) + h\dot{f}(t_0)$ and $f(t_0 - h) \simeq f(t_0) - h\dot{f}(t_0)$

Multistep Method

$$f(t_0 + h) = f(t_0 - h) + 2h\dot{f}(t_0)$$

Example: Radioactive Decay III

explicit 2-step method

$$u^{(n+1)} = u^{(n-1)} - 2\frac{h}{\tau}u^{(n)} + O(h^3)$$

Goal

Getting rid of as many Taylor Terms as possible by combining functional values

Runge-Kutta

German mathematicians C.Runge and M.W.Kutta Ansatz:

$$f(t+h) = f(t) + h(a_1 k_1 + a_2 k_2 + a_3 k_3 + a_4 k_4)$$

Runge-Kutta 4th Order

$$f' = g(t, f), \quad f(t_0) = f_0$$

representing an initial value problem, the RK4 algorithm amounts to

$$f_{n+1} = f_n + h\left(\tfrac{1}{6}k_1 + \tfrac{1}{3}k_2 + \tfrac{1}{3}k_3 + \tfrac{1}{6}k_4\right)$$
$$t_{n+1} = t_n + h$$

with the following coefficients.

$$k_1 = g(t_n, f_n)$$
$$k_2 = g(t_n + \tfrac{1}{2}h, f_n + \tfrac{1}{2}hk_1)$$
$$k_3 = g(t_n + \tfrac{1}{2}h, f_n + \tfrac{1}{2}hk_2)$$
$$k_4 = g(t_n + h, f_n + hk_3)$$

Runge-Kutta general

$$\vec{y}_{n+1} = \vec{y}_n + \tau \sum_{l=1}^{s} b_l \vec{k}_l$$

with $\vec{k}_s$, the "intermediate slopes" being defined as:

$$\vec{k}_1 = \tau \vec{f}(t_n, \vec{y}_n)$$

$$\vec{k}_2 = \tau \vec{f}(t_n + c_2\tau, \vec{y}_n + \tau a_{21}\vec{k}_1)$$

$$\vdots$$

$$\vec{k}_s = \tau \vec{f}(t_n + c_s\tau, \vec{y}_n + \tau \sum_{m=1}^{s-1} a_{sm}\vec{k}_m)$$

b_l, c_m and a_{sm} are constants that can be chosen according to the corresponding Butcher tableau.

Butcher Tableau

0	0						
c_2	a_{21}	0					
c_3	a_{31}	a_{32}	0				
c_4	a_{41}	a_{42}	a_{43}	0			
c_5	a_{51}	a_{52}	a_{53}	a_{54}	0		
c_6	a_{61}	a_{62}	a_{63}	a_{64}	a_{65}	0	
0	0						
$\frac{1}{5}$	$\frac{1}{5}$	0					
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$	0				
$\frac{3}{5}$	$\frac{3}{10}$	$-\frac{9}{10}$	$\frac{6}{5}$	0			
1	$-\frac{11}{54}$	$\frac{5}{2}$	$-\frac{70}{27}$	$\frac{35}{27}$	0		
$\frac{7}{8}$	$\frac{1631}{55296}$	$\frac{175}{512}$	$\frac{575}{13824}$	$\frac{44275}{110592}$	$\frac{253}{4096}$	0	
	b_1	b_2	b_3	b_4	b_5	b_6	
	$\frac{37}{378}$	0	$\frac{250}{621}$	$\frac{125}{594}$	0	$\frac{512}{1771}$	order 5
	$\frac{2825}{27648}$	0	$\frac{18575}{48384}$	$\frac{13525}{55296}$	$\frac{277}{14336}$	$\frac{1}{4}$	order 4
	$\frac{19}{54}$	0	$-\frac{10}{27}$	$\frac{55}{54}$	0	0	order 3
	$-\frac{3}{2}$	$\frac{5}{2}$	0	0	0	0	order 2
	1	0	0	0	0	0	order 1

Thank you for your attention