VL 18.4.2023

Runge-Kutta Methods

General from RK2 (2nd order) $\mathcal{O}(\Delta t^3)$

$$\dot{x} = f(x_1, t_1)$$

- $K_1 = \Delta t\, f(t_n, x_n)$
- $K_2 = \Delta t\, f(t_n + \alpha \Delta t_1, x_n + \beta K_1)$

$$x_{n+1} = x_n + a K_1 + b K_2$$

$a, b, \alpha, \beta = ?$ → Constants subject to constraints.

Taylor series in Δt

$$x_{n+1} = x(t_n + \Delta t) = x_n(t_n) + \Delta t\, \dot{x}(t_n) + \frac{(\Delta t)^2}{2} \ddot{x}(t_n) + \dots$$

① $$x_{n+1} = x_n + \Delta t f(t_n, x_n) + \frac{(\Delta t)^2}{2}\left[f_t(t_n, x_n) + f(t_n, x_n) f_x(t_n, x_n)\right]$$

f_t: time; f_x: space derivatives

Compare eq. 1 with 2:

$$\left.\begin{array}{l} a+b=1 \\ \alpha b = 1/2 \\ a\beta = 1/2 \end{array}\right\} \text{constraints}$$

Examples: Modified Euler's Method

① $a = b = 1/2$, $\alpha = \beta = 1$

$K_1 = \Delta t\, f(t_n, x_n)$, $K_2 = \Delta t\, f(t_n + \Delta t_1, x_n + K_1)$

$x_{n+1} = x_n + \frac{1}{2}(K_1 + K_2)$

② Mid point: $\alpha = \beta = 1/2$ $b = 1$, $a = 0$

$K_1 = \Delta t\, f(t_n, x_n)$, $K_2 = \Delta t\, f(t_n + \frac{1}{2}\Delta t, x_n + \frac{1}{2}K_1)$

$x_{n+1} = x_n + K_2$

Higher Order RKs:

RK3:

$$\dot{x} = f(x, t)$$

3 stages
$$\left[\begin{array}{l} K_1 = \Delta t\, f(t_n, x_n) \\ K_2 = \Delta t\, f(t_n + \alpha \Delta t_1, x_1 + \beta K_1) \\ K_3 = \Delta t\, f(t_n + \gamma \Delta t_1, x_n + \theta K_1 + \epsilon K_2) \end{array}\right.$$

$$x_{n+1} = x_n + aK_1 + bK_2 + cK_3$$

Order:	2	3	4	5	6	7	8
Stages:	2	3	4	6	7	9	11

Central question: How to find a proper value for Δt?

Dormand-Prince Method: (Matlab)

5th order RK / 4th order RK

$O(\Delta t^6)$ / $O(\Delta t^5)$ → Calculate $x_n \to x_{n+1}$ / $\hat{x}_{n+1}$

ϵ → tolerance = desired error

$e_n = |x_n - \hat{x}_{n+1}| \sim \mathcal{O}(\Delta t^5)$

$$\frac{e_n}{e} = \frac{(\Delta t)^5}{(\Delta \tau)^5} = \Delta\tau = s \cdot \Delta t \left(\frac{\epsilon}{e_n}\right)^{1/5}$$

Δt → Δt I used

$\Delta\tau$ → Time step I should have used.

s → safety factor $s \approx 0.9$

→ two scenarios:
① $e_n > t$ → reject
② $e_{n+1} < t$ → accept & rescale

Stiff differential equation

$$y'(x) = \frac{y(x) - y(x-h)}{h}, \quad y(x) = y(x-h) + h f(x, y), \quad y(x+h) = y(x) + \underbrace{h f(x+h, y+h)}_{\text{root solving problem}}$$ → Implicit method

Implicit methods are unconditionally stable.
↪ h independent

Examples:

$y' = -50(y - \cos x)$ (slow, fast)

Adams-Moulton

$y_{n+1} = y_n + \frac{1}{2}$

Newtons equation of motion (Hamiltonian dynamics)

$\dot{\vec{r}} = \vec{v}$, $\dot{\vec{v}} = \frac{1}{m}\vec{F}(\vec{r}, t) = \vec{a}(\vec{r}, t)$

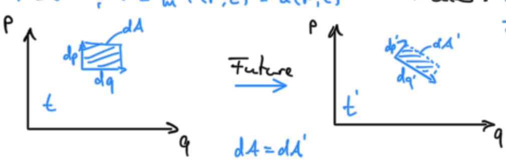
Euler:
$$\left.\begin{array}{l} \vec{r}_{n+1} = \vec{r}_n + \vec{v}_n h + \mathcal{O}(h^2) \\ \vec{v}_{n+1} = \vec{v}_n + \vec{a}_n h + \mathcal{O}(h^2) \end{array}\right\}$$

↪ $\vec{a}_{n+1}$ Euler-Cromer (1st order)

→ Problem: Space and momentum defined at the same time
→ inherently unstable

QM: $[q, p] = i\hbar$ → Classical: $\{q, p\} = 1$

→ RK, RK4 are not time reversible → not symplectic



$dA = dA'$

Position Verlet $\ddot{r} = \frac{F}{m}$, $\ddot{r}_n = \frac{r_{n+1} - 2r_n + r_{n-1}}{h^2}$, $r_{n+1} = 2r_n - r_{n-1} + a_n h^2 + \mathcal{O}(h^4)$

$v_n = \frac{1}{2h}(r_{n+1} - r_{n-1})$ →