Notas de aula

Introdução à Física Computacional

Prof. Gerson – UFU – 2019

Atendimento:

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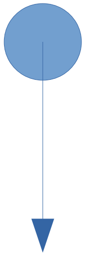
Use: $g = 9$, $\gamma = 0.5$, $v(0) = 0$

Ordinary differential equations

→ initial value problems

Example: free fall and terminal velocity



Forces:

→ gravity
→ drag

$$F = mg - bv^2$$

Applying Newton's 2nd law:

$$\frac{\partial v}{\partial t} = g - \gamma v^2$$

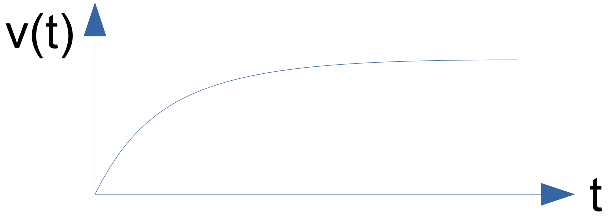
+ initial condition: $v(0) = 0$

Terminal velocity:

$$v = \sqrt{g/\gamma}$$

Full solution:

$$v(t) = \sqrt{\frac{g}{\gamma}} \tanh\left[\sqrt{g\gamma}\, t\right]$$



Ordinary differential equations

→ How to solve it numerically?

1) Euler's method → the "worst"… but very intuitive method

Problem prototype: $$\frac{dy}{dt} = f(t,y)$$ → y = y(t) is the unknown function
→ f(t,y) is a given function that defines the problem

Taylor expansion of y(t + Δt) for Δt → 0

$$y(t+\Delta t) \approx y(t) + \Delta t\, y'(t) + \cancel{\frac{\Delta t^2}{2} y''(t)} + \cdots$$

$$y(t+\Delta t) \approx y(t) + \Delta t\, y'(t) + \mathcal{O}(\Delta t^2)$$

$$\boxed{y'(t) \approx \frac{y(t+\Delta t) - y(t)}{\Delta t} + \mathcal{O}(\Delta t)}$$

Replace the derivative by its forward finite differences stencil

1) The Euler method – how to apply

Given the problem

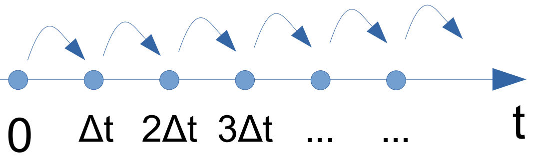
$$\frac{dy}{dt} = f(t, y)$$

… and the initial condition

$$y(0) = y_0$$

Apply Euler's recursion successively

$$y(t + \Delta t) \approx y(t) + \Delta t \; f(t, y(t))$$



initial condition → $y(0) = y_0$

From t=0 to Δt → $y(\Delta t) \approx y(0) + \Delta t \; f(0, y(0))$

From t=Δt to 2Δt → $y(2\Delta t) \approx y(\Delta t) + \Delta t \; f(\Delta t, y(\Delta t))$

From t=2Δt to 3Δt → $y(3\Delta t) \approx y(2\Delta t) + \Delta t \; f(2\Delta t, y(2\Delta t))$

...

Plot the data:

t	y(t)
0	y_0
Δt	y_1
$2\Delta t$	y_2
$3\Delta t$	y_3
...	...

2) The Runge-Kutta methods

[link to Wikipedia]

→ Derivation of the RK2 method on my book
→ Derivation of the **RK4** method on Numerical Calculus books

It's a "simple" variation of Euler's recursion

Problem prototype: $$\frac{dy}{dt} = f(t,y)$$ → y = y(t) is the unknown function
→ f(t,y) is a given function that defines the problem

Jumping from t = n Δt → t = (n+1) Δt

$$\begin{aligned}
\boldsymbol{k}_1 &= \boldsymbol{f}(\boldsymbol{y}_n, t_n), \\
\boldsymbol{k}_2 &= \boldsymbol{f}\left(\boldsymbol{y}_n + \frac{\tau}{2}\boldsymbol{k}_1, t_n + \frac{\tau}{2}\right), \\
\boldsymbol{k}_3 &= \boldsymbol{f}\left(\boldsymbol{y}_n + \frac{\tau}{2}\boldsymbol{k}_2, t_n + \frac{\tau}{2}\right), \\
\boldsymbol{k}_4 &= \boldsymbol{f}\left(\boldsymbol{y}_n + \tau\boldsymbol{k}_3, t_n + \tau\right), \\
\boldsymbol{y}_{n+1} &= \boldsymbol{y}_n + \frac{\tau}{6}\left(\boldsymbol{k}_1 + 2\boldsymbol{k}_2 + 2\boldsymbol{k}_3 + \boldsymbol{k}_4\right).
\end{aligned}$$

Higher precision:

→ while Euler's is a 2nd order method

→ RK4 is a 4th order method

Consequently, the time step

Δt on RK4 can be larger than in Euler

Pendulum: reduction of order

The 2nd order oscillator equation → can be solved using Verlet's method,
but let's try it with Euler and RK4 first

$$\frac{d^2x}{dt^2} = a(t,x)$$

Pendulum → $a(t,x) = -\omega^2 \sin(x)$

initial conditions:

$x(0) = x_0$ $v(0) = v_0$

Reduction of order

$$\vec{y}(t) = \begin{pmatrix} x(t) \\ v(t) \end{pmatrix} \longrightarrow \boxed{\frac{d\vec{y}}{dt} = \vec{f}(t,\vec{y})}$$

Now it has the form of our prototype
… but now with vectors

with $v(t) = \dfrac{dx}{dt}$

$$\vec{f}(t,\vec{y}) = \begin{pmatrix} v \\ a(t,x) \end{pmatrix} = \begin{pmatrix} y_1 \\ a(t,y_0) \end{pmatrix}$$

and $\vec{y}(0) = \begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$

Written in terms of the components of y

Your code is good… but better use scipy!!!

→ the python way… always use a library!

SciPy has methods that implement the adaptive RK4.5

→ solves using RK4

→ uses RK5 to check the error and define the optimal time step

→ scipy.integrate.solve_ivp [link]

Read the docs… check the examples… try to implement the pendulum
… and plot the results.

Tip: consider large initial angles → $x_0 = 0.98\pi$, and $v_0 = 0$

Later, change the acceleration to consider damping:

$$a(t, x, v) = -\omega^2 \sin(x) - \gamma v$$