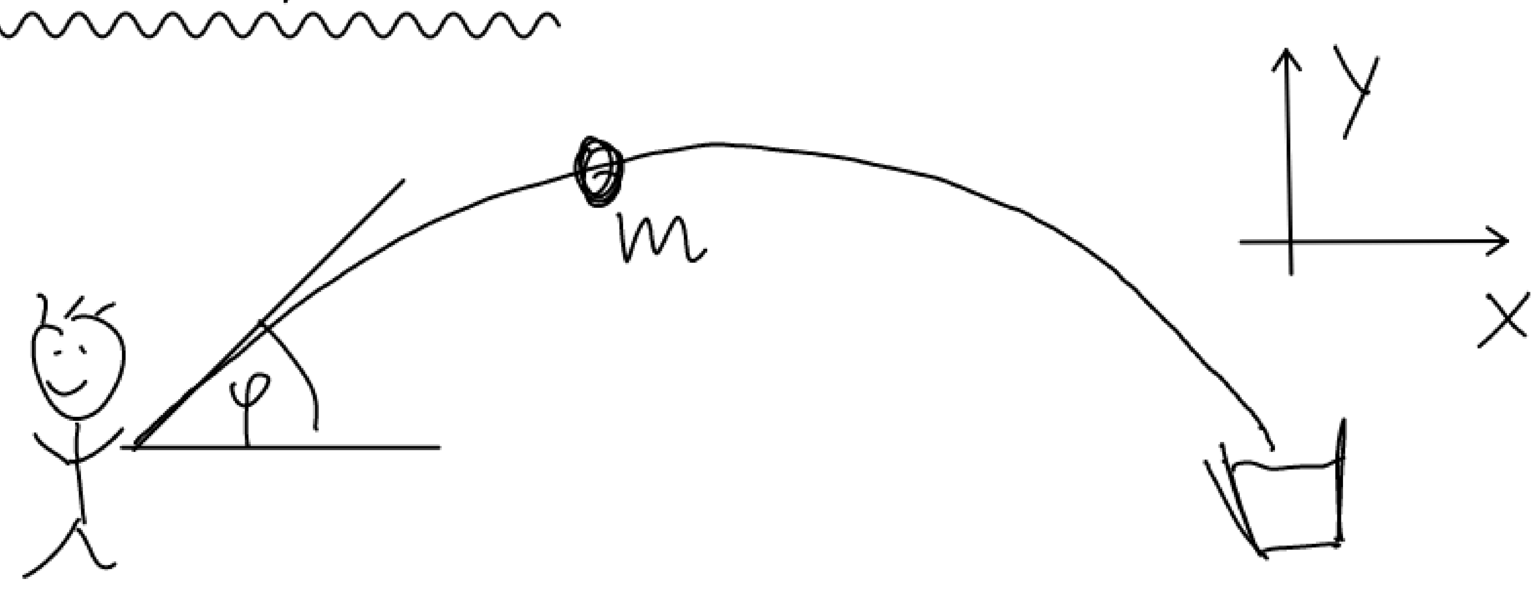
4. Solving Ordinary Differential Equations (ODEs)

Example: throw a ball



$$\vec{a} = \frac{d\vec{v}}{dt} \qquad \vec{v} = \frac{d\vec{x}}{dt}$$

$$\vec{v} = \begin{pmatrix} v_x \\ v_y \end{pmatrix} \qquad \vec{x} = \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\vec{a} = \begin{pmatrix} 0 \\ -g \end{pmatrix} = \begin{pmatrix} \dot{v}_x \\ \dot{v}_y \end{pmatrix} = \begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix}$$

we look at this one first

$$\frac{dv_y}{dt} = -g \quad \rightsquigarrow \quad \underbrace{\Delta v_y}_{\text{change of } v_y \text{ during } -\text{"}-} = -g \underbrace{\Delta t}_{\text{small time step}}$$

$$v_y(t_0 + i\Delta t) = v_i$$

$$\boxed{\begin{aligned} v_{i+1} &= v_i - g \cdot \Delta t \\ y_{i+1} &= y_i + v_i \cdot \Delta t \end{aligned}}$$

the same for y

of course we also have $\quad x_{i+1} = x_i + v_x \cdot \Delta t$

4.1. Euler's method

we have (re)discovered Euler's method

$\longrightarrow$ compare with analytic result

$$v_y(t) = v_y(0) - \int_0^t dt' \, g = v_y(0) - g \cdot t = v_0 - g \cdot t$$

$$y(t) = \int_0^t dt' \, v_y(t) = v_0 \cdot t - \frac{1}{2} g \cdot t^2$$

$$x(t) = \int_0^t dt' \, v_x = v_x \cdot t \qquad \text{because } \dot{v}_x = 0$$

$$\rightsquigarrow \quad t = \frac{x}{v_x} \quad \text{and} \quad y(x) = v_0 \cdot \left(\frac{x}{v_x}\right) - \frac{1}{2} g \cdot \left(\frac{x}{v_x}\right)^2$$

For small larger Δt significant error. Why?

Taylor expansion: $x(t+\Delta t) = x(t) + \dot{x}\,\Delta t + \ddot{x}\frac{\Delta t^2}{2} + \dots$

taken into account

error

error occures in every of $N = \frac{T}{\Delta t}$ steps

$\leadsto$ final error is of order Δt

Question: What happens for higher order ODEs?

like damped harmonic oscillator

$$\ddot{x} = -\omega^2 x - \beta \dot{x} \quad \hat{=} \quad 2 \text{ (coupled) first-order ODEs}$$

$$\left.\begin{aligned} \dot{x} &= v \quad \text{and} \\ \dot{v} &= -\omega^2 x - \beta v \end{aligned}\right\} \text{ we already did this for } \ddot{y} = -g$$

$\longrightarrow$ order n ODE $\hat{=}$ system of n first-order ODEs

$\longrightarrow$ standard form $\boxed{\dot{\vec{x}} = \vec{f}(\vec{x})}$ defines the physical system

for the damped HO $\vec{x} = \begin{pmatrix} x \\ v \end{pmatrix}$ $\quad \vec{f} = \begin{pmatrix} v \\ -\omega^2 x - \beta v \end{pmatrix}$

again analytic solution, assume $\dot{x}(t=0) = v_0$

$x(t=0) = x_0$

$$x(t) = e^{\lambda t}, \quad \dot{x}(t) = \lambda e^{\lambda t}, \quad \ddot{x}(t) = \lambda^2 e^{\lambda t}$$

$$\lambda^2 = -\omega^2 - \beta\lambda \quad \text{or} \quad \lambda^2 + \beta\lambda + \omega^2 = 0$$

$$\lambda_{1/2} = -\frac{\beta}{2} \pm i\sqrt{\omega^2 - \beta^2/4} = -\frac{\beta}{2} \pm i\omega'$$

$$x(t) = c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t} \qquad \begin{aligned} c_1 + c_2 &= x_0 \\ \lambda_1 c_1 + \lambda_2 c_2 &= v_0 \end{aligned}$$

$$\rightsquigarrow \; C_1 = \frac{V_0 - X_0 \lambda_2}{\lambda_1 - \lambda_2}, \quad C_2 = \frac{-V_0 + X_0 \lambda_1}{\lambda_1 - \lambda_2} \quad \text{and therefore}$$

$$X(t) = e^{-t\beta/2}\left[X_0 \cdot \cos(t \cdot \omega') + \frac{V_0 + 2X_0\beta}{\omega'} \sin(t\omega')\right]$$

with $\omega' = \sqrt{\omega^2 - \beta^2/4}$

↯ error grows exponentally $\rightsquigarrow$ $\boxed{\text{Euler method is not stable}}$

4.2. Runge-Kutta method

$x(t)$ = solution of ODE

$f(x,t)$ = derivative of x at time t

$$\ddot{x} = \frac{d}{dt}\dot{x} = \frac{d}{dt} f(x,t) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt}$$

$$= f_t + f_x f$$

deviation from exact result and at next order

$$\dddot{x} = f_{tt} + 2 f f_{tx} + f^2 f_{xx} + f f_x^2 + f_t f_x$$

Now look at the Taylor expansion:

$$(1): \; x(t+\Delta t) = x(t) + f \cdot \Delta t + \frac{\Delta t^2}{2!}(f_t + f_x f) + \frac{\Delta t^3}{3!}(\ldots) + \mathcal{O}(\Delta t^4)$$

which can be written as

$$x(t+\Delta t) = x(t) + \alpha_1 K_1 + \alpha_2 K_2 + \ldots + \alpha_n K_n$$

for some constants $\alpha_1, \ldots, \alpha_n$ and the functions

$$K_1 = f(x,t)\,\Delta t$$

$$K_2 = f(x + \nu_{21} K_1,\; t + \nu_{21}\Delta t)\,\Delta t$$

$\vdots$

$$K_n = f\left(X + \sum_{\ell=1}^{n-1} \nu_{n\ell} k_\ell \, , \, t + \Delta t \sum_{\ell=1}^{n-1} \nu_{n\ell}\right) \Delta t$$

Question: How to fix α_n and $\nu_{n\ell}$?

$\longrightarrow$ Taylor expand $f(x + \ldots, t + \ldots)$

(2): $X(t+\Delta t) = X + \alpha_1 K_1 + \alpha_2 K_2 + \ldots$

$$= X + \alpha_1 f \Delta t + \alpha_2 \big(f \Delta t + \underbrace{[f f_x + f_t]} \nu_{21} \Delta t^2 \big) + \mathcal{O}(t^3)$$

we know this guy and now understand the particular choice of parameterization

Comparing (1) and (2) gives rise to

$$\left.\begin{aligned} \alpha_1 + \alpha_2 &= 1 \\ \alpha_2 \nu_{21} &= \tfrac{1}{2} \end{aligned}\right\}$$ underdetermined but for $\nu_{21} = 1 \longrightarrow \alpha_1 = \alpha_2 = 1/2$

Eventually we obtain:

$$\boxed{\begin{aligned} & X(t+\Delta t) = X + \tfrac{1}{2} K_1 + \tfrac{1}{2} K_2 + \mathcal{O}(\Delta t^3) \\ & \text{with} \quad K_1 = f(x,t)\, \Delta t \\ & \qquad\quad\ \ K_2 = f(X + K_1, t + \Delta t)\, \Delta t \end{aligned}}$$

2^{nd}-order Runge-Kutta method

Numerical error: $\mathcal{O}(\Delta t^3)$ in every step

$\mathcal{O}(\Delta t^2)$ after $N = \frac{\tau}{\Delta t}$ steps

We could also choose $\alpha_1 = 0$, $\alpha_2 = 1$ and $\nu_{21} = \frac{1}{2}$ with

$$X(t+\Delta t) = X(t) + \Delta t \, f\left(X + \tfrac{1}{2} K_1, t + \tfrac{1}{2}\Delta t\right).$$

As you can guess, we can continue the expansions above to generate higher-order versions. 4^{th}-order usually offers a good compromise between speed and stability/precision

There are also more sophisticated algorithms with dynamic step size. From now on, we will use

scipy.integrate.odeint