

Numerical solution of ODE & PDE

First order **ordinary differential equation (ODE)**, with initial value

$$\frac{dy}{dx} = f(y(x), x), \quad \text{with initial value } y(x_0) = y_0$$

dy/dx is tangent to solution curve $y = y(x)$ at point x given $x = x_0, y = y_0$.

Possible to convert **second-order ODE** to **two coupled first order ODE**,

$$\frac{d^2x}{dt^2} = -\omega^2 x \Rightarrow v = \frac{dx}{dt} \quad \text{and} \quad \frac{dv}{dt} = -\omega^2 x - \mu v$$

initial conditions being $x(t_0) = x_0$ and $v(t_0) = v_0$.

To solve first order ODEs given an initial condition, the methods we discuss here are

1. **Forward** (explicit) and **Backward** (implicit) **Euler's method**
2. **Predictor-Corrector method**
3. **Runge-Kutta 4th order**

Forward (explicit) Euler

Based on Taylor expansion of $f(x_0 + h)$ about x_0 assuming h is small

$$y(x_0 + h) = y(x_0) + h \left. \frac{dy}{dx} \right|_{x_0} + \frac{h^2}{2!} \left. \frac{d^2y}{dx^2} \right|_{x_0} + \cdots \approx y(x_0) + h f(y(x_0), x_0) + \mathcal{O}(h^2)$$

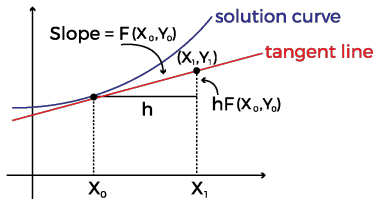
Say $x_1 = x_0 + h$ a small h step away from $x_0 \Rightarrow$ Forward Euler gives

$$y(x_1) = y(x_0) + h f(y(x_0), x_0) + \mathcal{O}(h^2)$$

Continue from x_1 to $x_2 = x_1 + h$, to x_3 etc. After n -th step

$$y(x_n + h) = y(x_n) + h f(y(x_n), x_n) \text{ or, equivalently } y_{n+1} = y_n + \kappa_1$$

where $\kappa_1 = h f(y(x_n), x_n)$ implies slope or tangent at the beginning of the interval boundary $\Rightarrow dy/dx$ calculated at earlier point x_n to obtain solution at the end of interval $x_n + h$.



It is **Forward** because

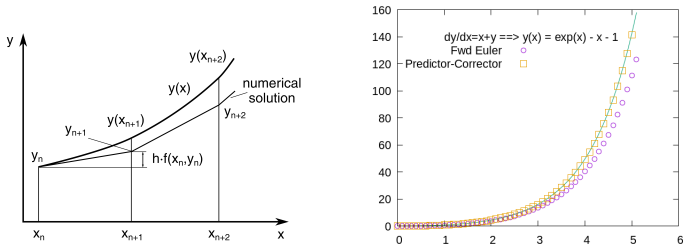
$$\frac{dy}{dx} = \lim_{\Delta x \rightarrow 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \rightarrow 0} \frac{y(x + \Delta x) - y(x)}{\Delta x} = f(y(x), x)$$

\Rightarrow

$$y(x + \Delta x) \approx y(x) + \Delta x f(y(x), x)$$

Forward Euler often returns good approximation to actual solution, but it is extremely slow \rightarrow **h** has to be small to achieve desired accuracy.

Its biggest problem is **stability issue**, can easily veer away from solution.



Left plot \circ is for Forward Euler and \square for Predictor-Corrector.

Stability of Forward Euler is more of a problem than its sluggishness.

Backward (implicit) Euler

Re-define dy/dx in terms of *backward derivative*,

$$\begin{aligned}\frac{\Delta y}{\Delta x} &\approx \frac{y(x) - y(x - \Delta x)}{\Delta x} = f(y(x), x) \Rightarrow y(x) = y(x - \Delta x) + \Delta x f(y(x), x) \\ \Rightarrow &y(x + \Delta x) = y(x) + \Delta x f(y(x + \Delta x), x + \Delta x) \\ \equiv &y(x_n + h) = y(x_n) + h f(y(x_n + h), x_n + h)\end{aligned}$$

$y(x_n + h)$ is determined from the tangent at $x_n + h$, implying strangely that to calculate $y(x_n + h)$ one needs to know $y(x_n + h)$!!

This apparent conflict is resolved by looking it as a **linear equation** and solve it by **Newton-Raphson**,

$$y^{\text{NR}}(x + h) = y(x) + h f(y^{\text{NR}}(x + h), x + h)$$

Hence, solving the differential equation by

$$y(x_n + h) = y(x_n) + h f(y^{\text{NR}}(x_n + h), x_n + h)$$

In spite of having an extra step of **Newton-Raphson**, the **Backward Euler** is advantageous because of better stability.

Predictor-Corrector method

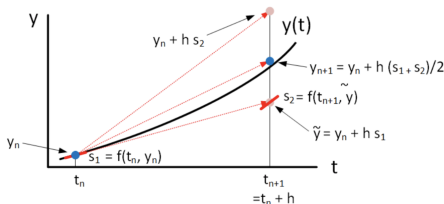
Predicts $y^P(x_n + h)$ using Forward Euler and estimate $f(y^P(x_n + h), x_n + h)$

$$y^P(x_n + h) = y(x_n) + h f(y(x_n), x_n) + \mathcal{O}(h^2)$$

Take the average of the two slopes to obtain correct value $y^C(x_n + h)$,

$$y^C(x_n + h) = y(x_n) + \frac{h}{2} \left[f(y(x_n), x_n) + f(y^P(x_n + h), x_n + h) \right] \equiv y(x_n) + \frac{1}{2} \left[\kappa_1 + \kappa_2 \right]$$

where, $\kappa_1 = h f(y(x_n), x_n)$, $\kappa_2 = h f(y^P(x_n + h), x_n + h)$. The κ_2 denotes predicted slope at the end of interval boundary.



1. Compute slope $\kappa_1 = h f(y(x_n), x_n)$ at x_n .
2. Calculate the predicted $y^P(x_n + h) = y(x_n) + \kappa_1$, hence compute $\kappa_2 = h f(y^P(x_n + h), x_n + h) = h f(y(x_n) + \kappa_1, x_n + h)$.
3. Calculate the corrected solution $y^C(x_n + h) = y(x_n) + (\kappa_1 + \kappa_2)/2$

Runge-Kutta method

Runge-Kutta (RK) methods are based on Taylor expansion and give better algorithms for solutions of ODE for same step size and stability.

$$\begin{aligned}\frac{dy}{dx} &= f(y(x), x) \Rightarrow \int_{y_n}^{y_{n+h}} dy = \int_{x_n}^{x_n+h} f(y(x), x) dx \\ y(x_n + h) &= y(x_n) + \int_{x_n}^{x_n+h} f(y(x), x) dx\end{aligned}$$

Numerical estimate of the integral can come from any of Midpoint, Trapezoidal or Simpson rule. Take Midpoint for instance,

$$\begin{aligned}\bar{x}_n &= [(x_n + h) + x_n]/2 = x_n + h/2 \\ y(x_n + h) &= y(x_n) + h f(y(x_n + h/2), x_n + h/2) + \mathcal{O}(h^3) \\ \text{where, } y(x_n + h/2) &= y(x_n) + \frac{h}{2} f(y(x_n), x_n)\end{aligned}$$

Last step above is Forward Euler, which leads to *second order Runge-Kutta* (RK2)

$$\begin{aligned}\kappa_1 &= h f(y(x_n), x_n) \\ \kappa_2 &= h f(y(x_n) + \kappa_1/2, x_n + h/2) \\ y(x_n + h) &\approx y(x_n) + \kappa_2 + \mathcal{O}(h^3)\end{aligned}$$

Note a couple of points on *RK2* –

1. Difference between previous one-step methods like Euler's and Predictor-Corrector methods is the addition of an intermediate half-step.
2. Order of error follows from the maximum error bound of Midpoint method.
3. Trapezoidal rule reproduces Predictor-Corrector formula with the same error $\mathcal{O}(h^3)$.

Next obvious step is using Simpson rule as integrator to develop famous and by far the most popular method for solving ODE : fourth-order Runge-Kutta (*RK4*).

Unless stated or asked differently, it will always be assumed that *RK4* is used to solve ODE.

Consider the integral equation again, this time using **Simpson** rule,

$$\begin{aligned}y(x_n + h) &= y(x_n) + \int_{x_n}^{x_n+h} f(y(x), x) dx \\&= y(x_n) + \frac{h}{6} \left[f(y(x_n), x_n) + 4f(y(x_n + h/2), x_n + h/2) + f(y(x_n + h), x_n + h) \right] \\&= y(x_n) + \frac{h}{6} \left[f(y(x_n), x_n) + 2f(y(x_n + h/2), x_n + h/2) + \right. \\&\quad \left. 2f(y(x_n + h/2), x_n + h/2) + f(y(x_n + h), x_n + h) \right]\end{aligned}$$

Essentially, expression for slopes are splitted up at interval midpoint $f(y(x_n + h/2), x_n + h/2)$ into two – one **predicts** the tangent at the interval and the later **corrects** it. Define the following,

$$\begin{aligned}\kappa_1 &= h f(y(x_n), x_n) & \kappa_2 &= h f(y(x_n) + \kappa_1/2, x_n + h/2) \\ \kappa_3 &= h f(y(x_n) + \kappa_2/2, x_n + h/2) & \kappa_4 &= h f(y(x_n) + \kappa_3, x_n + h)\end{aligned}$$

Combine these to form the **RK4** solution

$$y(x_n + h) = y(x_n) + \frac{1}{6} (\kappa_1 + 2\kappa_2 + 2\kappa_3 + \kappa_4) + \mathcal{O}(h^5)$$

The error $\mathcal{O}(h^5)$ follows from maximum error bound of Simpson and allow us to use relative coarser interval to arrive at very precise solution.

Coupled ODE

Numerical methods like Euler and Runge-Kutta are all applied to first order ODE.

To solve higher order ODE : convert to coupled first order ODE. For instance, SHO

$$\begin{aligned}\frac{d^2x}{dt^2} &= -\mu \frac{dx}{dt} - \omega^2 x, \text{ with } x(t=0) = x_0, \quad v(t=0) = \left. \frac{dx}{dt} \right|_{t=0} = v_0 \\ \Rightarrow v &= \frac{dx}{dt} \text{ with } v(t=0) = v_0 \\ \frac{dv}{dt} &= -\mu v - \omega^2 x \text{ with } x(t=0) = x_0\end{aligned}$$

In addition, there can be just a set of coupled first order ODEs. For instance, Lorentz equations,

$$\frac{dx}{dt} = \sigma(y - x), \quad \frac{dy}{dt} = x(\rho - z) - y, \quad \frac{dz}{dt} = xy - \beta z$$

The equations relate the properties of a two-dimensional fluid layer uniformly warmed from below and cooled from above, and σ, ρ, β are three parameters whose certain values give rise to chaotic behavior.

The *RK4* for damped SHO takes the following appearance

```
k1x = dt*dxdt(x,v,t);
k1v = dt*dvdt(x,v,t);

k2x = dt*dxdt(x+k1x/2,v+k1v/2,t+dt/2);
k2v = dt*dvdt(x+k1x/2,v+k1v/2,t+dt/2);

⋮ = ⋮
x += (k1x + 2*k2x + 2*k3x + k4x)/6;
v += (k1v + 2*k2v + 2*k3v + k4v)/6;
t += dt;
```

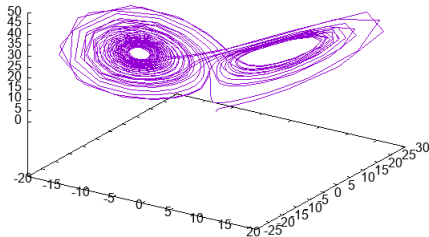
For Lorentz equations, the expressions are similar to SHO

```
k1x = dt*dxdt(x,y,z,t);
k1y = dt*dydt(x,y,z,t);
k1z = dt*dzdt(x,y,z,t);

k2x = dt*dxdt(x+k1x/2,y+k1y/2,z+k1z/2,t+dt/2);
k2y = dt*dydt(x+k1x/2,y+k1y/2,z+k1z/2,t+dt/2);
k2z = dt*dzdt(x+k1x/2,y+k1y/2,z+k1z/2,t+dt/2);
etc.
```

Just for fun : for $\sigma = 10, \rho = 28, \beta = 8/3$, the 3-dim plot of the solution shows the famous Lorenz attractor

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Generalizing RK4 to n coupled first order ODE

$$\left. \begin{aligned} \frac{dy_1}{dx} &= f_1(y_1, y_2, \dots, y_n, x) \\ \frac{dy_2}{dx} &= f_2(y_1, y_2, \dots, y_n, x) \\ &\vdots \\ \frac{dy_n}{dx} &= f_n(y_1, y_2, \dots, y_n, x) \end{aligned} \right\} \equiv \frac{d\vec{y}}{dx} = \vec{f}(\vec{y}, x)$$

where $\vec{y} = (y_1, y_2, \dots, y_n)$ and $\vec{f} = (f_1, f_2, \dots, f_n)$. Vector sign simply implies collection of variables. In such case the RK4 equations take the forms,

$$\vec{\kappa}_1 = h \vec{f}(\vec{y}_i, x_i)$$

$$\vec{\kappa}_2 = h \vec{f}(\vec{y}_i + \vec{\kappa}_1/2, x_i + h/2)$$

$$\vec{\kappa}_3 = h \vec{f}(\vec{y}_i + \vec{\kappa}_2/2, x_i + h/2)$$

$$\vec{\kappa}_4 = h \vec{f}(\vec{y}_i + \vec{\kappa}_3, x_i + h)$$

$$\vec{y}_{i+h} = \vec{y}_i + \frac{1}{6} [\vec{\kappa}_1 + 2\vec{\kappa}_2 + 2\vec{\kappa}_3 + \vec{\kappa}_4]$$

where \vec{y}_i are the values at the i -th interval boundary. Above set of equations have to be read only in terms of components and not as vector equations.

Use RK4 to solve the following :

$$\dot{x} = -5x + 5y$$

$$\dot{y} = 14x - 2y - zx$$

$$\dot{z} = -3z + xy$$

$$\dot{x} = -2y$$

$$\dot{y} = x + z^2$$

$$\dot{z} = 1 + y - 2z$$

Boundary Value Problem : Shooting method

Many problems in physics are **boundary value problems**. Like Laplace equation in electrostatics or, more famously, Schrödinger equations.

In boundary value problems, we have conditions specified at two different space (and/or time) points. We can have either

Dirichlet condition : $y(x_0) = Y_0$ and $y(x_N) = Y_n$

Neumann condition : $y'(x_0) = Y'_0$ and $y'(x_N) = Y'_N$

$$\begin{aligned} & \frac{d^2 y}{dx^2} = f(x, y, y') \quad \text{where } a \leq x \leq b \quad \text{and } y(a) = \alpha, y(b) = \beta \\ \Rightarrow & \frac{dy}{dx} = z \quad \text{with } y(a) = \alpha \\ & \frac{dz}{dx} = \frac{d^2 y}{dx^2} = f(x, y, z) \quad \text{with } z(a) = \zeta_h \text{ (guess)} \end{aligned}$$

the slope $z(a) = \zeta_h$ at $x = a$ is a guess. Solve the coupled ODEs with initial values $y(a) = \alpha$ and $z(a) = \zeta_h$.

Solution obtained at end point x_N is compared with the boundary condition $y(b) = \beta$. If $y_{\zeta_h}(b) = \beta$ within tolerance then the ODE is solved.

Suppose $y_{\zeta_h}(b) \neq \beta$ but $y_{\zeta_h}(b) > \beta$. Change the guess initial value $\zeta_h \rightarrow \zeta_l$ of course and solve it again.

Unless the choice lands bang on the solution, choose ζ_l such that $y_{\zeta_l}(b) < \beta$ implying

$$\zeta_l < z(a) < \zeta_h$$

Use Lagrange's interpolation formula to choose the next $z(a) = \zeta$

$$\zeta = \zeta_l + \frac{\zeta_h - \zeta_l}{y_{\zeta_h}(b) - y_{\zeta_l}(b)} (y(b) - y_{\zeta_l}(b))$$

$z(a) = \zeta$ is our new guess value for initial slope and chances are this choice will lead us to the solution of the ODE i.e. $y_{\zeta}(b) \approx \beta$.

If not, go through the above procedure until $y_{\zeta}(b)$ converges to β .

Let us study the following example,

$$\frac{d^2y}{dx^2} = 2y \quad \text{with} \quad y(x = 0.0) = \alpha = 1.2, \quad y(x = 1.0) = \beta = 0.9$$

Analytical solution of the above ODE is

$$y(x) = c_1 e^{\sqrt{2}x} + c_2 e^{-\sqrt{2}x}, \quad \text{where} \quad c_1 = 0.157, \quad c_2 = 1.043$$

Let our initial guess slope is $z(x = 0.0) = -1.5$. RK4 returns

$$y(x = 1.0) = 0.5614 < \beta = 0.9 \Rightarrow \zeta_l = -1.5, y_{\zeta_l}(1.0) = 0.5614$$

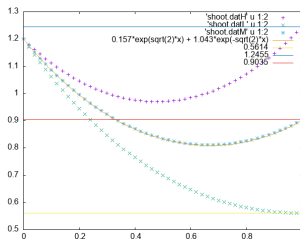
Next try $z(x = 0.0) = -1.0$,

$$y(x = 1.0) = 1.2455 > \beta = 0.9 \Rightarrow \zeta_h = -1.0, y_{\zeta_h}(1.0) = 1.2455$$

Use Lagrange's linear interpolating formula,

$$\zeta = -1.5 + \frac{-1.0 - (-1.5)}{1.2455 - 0.5614} \times (0.9 - 0.5614) = -1.2525$$

Using $z(x = 0.0) = -1.2525$, we obtain $y_{\zeta}(x = 1.0) = 0.9035 \approx \beta = 0.9$ thus solving the ODE. A graphical view of the process



Partial differential equations

Many equations in physics are partial differential equations – Maxwell equations, Laplace and Poisson equations, wave equations, Schrödinger equation, diffusion equation and so on.

A general linear partial differential equation in 2-dimension *i.e.* second-order in two independent variables reads,

$$A(x, y) \frac{\partial^2 u}{\partial x^2} + B(x, y) \frac{\partial^2 u}{\partial x \partial y} + C(x, y) \frac{\partial^2 u}{\partial y^2} = F\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$$

Most common method employed to solve PDE is *finite difference*, converting *derivatives to differences*.

Two categories of method exist – *explicit* and *implicit*.

Consider *explicit* scheme in **1+1** dimension diffusion or heat equation,

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{\partial u(x, t)}{\partial t} \quad \equiv \quad u_{xx} = u_t$$

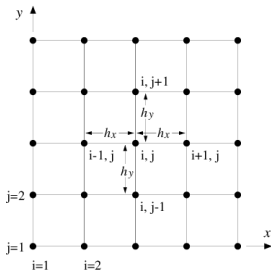
initial conditions at $t = 0$ and boundary conditions at later time $t > 0$,

$$u(x, 0) = g(x) \quad \text{for } 0 < x < L$$

$$u(0, t) = a(t) \quad \text{for } t \geq 0$$

$$u(L, t) = b(t) \quad \text{for } t \geq 0$$

Discretize space and time such that $\Delta x = h_x$, $\Delta t = h_t$ are differences between two space and time points respectively. (Take $y \equiv t$, $h_y \equiv h_t$)



Position after i steps and time at j step are given by

$$\begin{cases} x_i = ih_x & 0 \leq i \leq n+1 \\ t_j = jh_t & j \geq 0 \end{cases}$$

Discretized forward derivatives for explicit scheme are

$$\begin{aligned} u_t &\approx \frac{u(x, t + h_t) - u(x, t)}{h_t} \equiv \frac{u(x_i, t_j + h_t) - u(x_i, t_j)}{h_t} = \frac{u_{i,j+1} - u_{i,j}}{h_t} \\ u_{xx} &\approx \frac{u(x + h_x, t) + u(x - h_x, t) - 2u(x, t)}{h_x^2} \\ &\equiv \frac{u(x_i + h_x, t_j) + u(x_i - h_x, t_j) - 2u(x_i, t_j)}{h_x^2} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h_x^2} \end{aligned}$$

Define $\alpha = h_t/h_x^2$, results in explicit scheme

$$\begin{aligned}\frac{u_{i,j+1} - u_{i,j}}{h_t} &= \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h_x^2} \\ u_{i,j+1} &= \alpha (u_{i+1,j} + u_{i-1,j}) + (1 - 2\alpha) u_{i,j}\end{aligned}$$

Given initial values $u_{i,0} = g(x_i)$, after one time step we get $u_{i,1}$,

$$\begin{aligned}u_{i,1} &= \alpha (u_{i+1,0} + u_{i-1,0}) + (1 - 2\alpha) u_{i,0} \\ &= \alpha (g(x_{i+1,0}) + g(x_{i-1,0})) + (1 - 2\alpha) g(x_{i,0})\end{aligned}$$

For simplicity and without loss of generality, consider $a(t) = b(t) = 0$ implying $u_{0,j} = u_{L=n+1,j} = 0$ where the interval $[0, L]$ is divided in n parts.

Then a vector V_j at the time $t_j = j h_t$ is defined as,

$$V_j = \begin{pmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{n,j} \end{pmatrix}$$

with $V_0 \equiv u_{i,0} = g(x_i)$.

Therefore, the solution at a given time slice V_{j+1} proceeds as

$$V_{j+1} = A V_j \quad \text{where} \quad A = \begin{pmatrix} 1-2\alpha & \alpha & 0 & 0 & \cdots \\ \alpha & 1-2\alpha & \alpha & 0 & \cdots \\ 0 & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \alpha & 1-2\alpha \end{pmatrix}$$

This implies that the solution is evolving in time using **matrix-vector** multiplication till the end of time, say $u_{i,T}$

$$V_{j+1} = A V_j = A^2 V_{j-1} = \cdots = A^{j+1} V_0$$

Like explicit Euler, it too has weak stability condition given by $\alpha = h_t/h_x^2 \leq 0.5$ and is overcome by implicit scheme using backward derivative in time, keeping second derivative unchanged.

$$u_t \approx \frac{u_{i,j} - u_{i,j-1}}{h_t}$$

$$u_{i,j-1} = -\alpha (u_{i+1,j} + u_{i-1,j}) + (1 + 2\alpha) u_{i,j}$$

The corresponding evolution equation for implicit scheme is

$$V_{j-1} = A V_j \text{ where } A = \begin{pmatrix} 1+2\alpha & -\alpha & 0 & 0 & \cdots \\ -\alpha & 1+2\alpha & -\alpha & 0 & \cdots \\ 0 & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -\alpha & 1+2\alpha \end{pmatrix}$$

$$V_j = A^{-1} V_{j-1} = A^{-2} V_{j-2} = \cdots = A^{-j} V_0$$

Problem : Solve the 1-dimension heat equation $u_{xx} = u_t$ over a metal rod of length 2 units, with the initial conditions,

$$u(0, t) = 0^\circ\text{C} = u(2, t) \quad \text{for } 0 \leq t \leq 4$$

$$u(x, 0) = 20 |\sin(\pi x)|^\circ\text{C} \quad \text{for } 0 \leq x \leq 2$$

Use *explicit scheme* taking number of position grid $nx = 20$ and time grid $nt = 5000$. Show the temperature profile across the length of the rod at time steps 0, 10, 20, 50, 100, 200, 500 and 1000 in a plot. It should look something like

