Numerical solution of ODE & PDE

A first order ordinary differential equation (ODE), with initial value(s) given, can generically be written as

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

dy/dx is a tangent to the solution curve $y = y(x)$ at point x and initial condition states at $x = x_0$, $y = y_0$.

Often possible to rewrite second-order ODE in terms of two coupled first order ODE,

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

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

Taylor expand the function $f(x_0 + h)$ about x_0 assuming h is small

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

Consider $x_1 = x_0 + h$ a small h step away from x_0, then Forward Euler gives the solution at x_1 as

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

Take the next step from x_1 to $x_2 = x_1 + h$, then to $x_3 = x_2 + h$ and so on. At the n-th step, the solution of the ODE is,

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

where $\kappa_1 = hf(y(x_n), x_n)$ generically implies slope or tangent at the beginning of the interval boundary.

Forward Euler depends on tangent dy/dx calculated at earlier point x_n *i.e.* beginning of the interval, to obtain solution at the end of interval $x_n + h$. It is Forward because

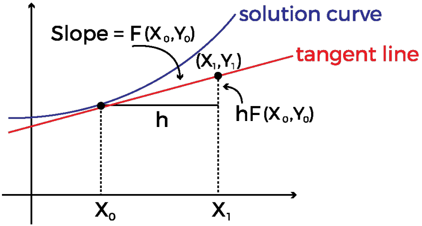
$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \to 0} \frac{y(x + \Delta x) - y(x)}{\Delta x} = f(y(x), x)$$

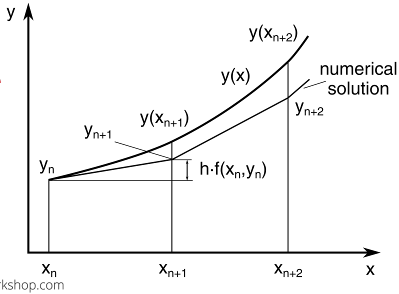
$$\Rightarrow \qquad y(x + \Delta x) \approx y(x) + \Delta x\, f(y(x), x)$$

Forward Euler often returns fairly good approximation to the actual solution $y = y(x)$.

But it is extremely slow – h has to be quite small to achieve some desired accuracy.

Forward Euler also has stability problem and can easily veer away from the solution.





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

Backward (implicit) Euler

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

$$\frac{\Delta y}{\Delta x} \approx \frac{y(x) - y(x-\Delta x)}{\Delta x} = f(y(x), x) \Rightarrow y(x) = y(x-\Delta x) + \Delta x\, f(y(x), x)$$

$$\Rightarrow \quad y(x+\Delta x) = y(x) + f(y(x+\Delta x), x+\Delta x)$$

$$\equiv \quad y(x_n + h) = y(x_n) + h\, f(y(x_n+h), x_n + h)$$

The $y(x_n + h)$ 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,

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

Hence, solving the differential equation by

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

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

Predictor-Corrector method

The method `predicts` $y^p(x_n + h)$ using Forward Euler and estimate the slope $f(y^p(x_n + h), x_n + h)$

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

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

$$y^c(x_n + h) = y(x_n) + \frac{h}{2}\Big[f(y(x_n), x_n) + f(y^p(x_n + h), x_n + h)\Big] \equiv y(x_n) + \frac{1}{2}\Big[\kappa_1 + \kappa_2\Big]$$

where, we have defined

$$\kappa_1 = hf(y(x_n), x_n) \quad \kappa_2 = hf(y^p(x_n + h), x_n + h)$$

Here κ_2 typically denotes the predicted slope or tangent at the end of interval boundary.

Hence, the Predictor-Corrector algorithm is

1. Compute slope $\kappa_1 = hf(y(x_n), x_n)$ at x_n.
2. Calculate the predicted $y^p(x_n + h) = y(x_n) + \kappa_1$, hence compute $\kappa_2 = hf(y^p(x_n + h), x_n + h) = h\, f(y(x_n) + \kappa_1, x_n + h)$.
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,

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

The last step above is Forward Euler. This 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,

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

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

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

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

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

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.

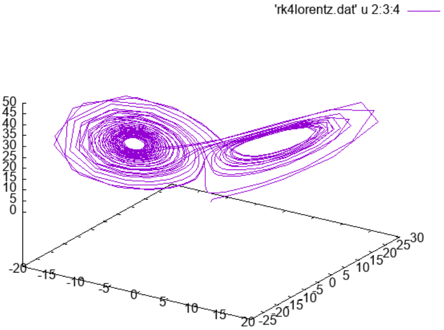
The *RK4* for damped SHO takes the following appearance

```
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 Lorentz attractor



Generalizing RK4 to n coupled first order ODE

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

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

$$\begin{aligned}
\vec{\kappa}_1 &= h\,\vec{f}(\vec{y}_i, x_i) \\
\vec{\kappa}_2 &= h\,\vec{f}(\vec{y}_i + \vec{\kappa}_1/2, x_i + h/2) \\
\vec{\kappa}_3 &= h\,\vec{f}(\vec{y}_i + \vec{\kappa}_2/2, x_i + h/2) \\
\vec{\kappa}_4 &= h\,\vec{f}(\vec{y}_i + \vec{\kappa}_3, x_i + h) \\
\vec{y}_{i+h} &= \vec{y}_i + \frac{1}{6}\left[\vec{\kappa}_1 + 2\vec{\kappa}_2 + 2\vec{\kappa}_3 + \vec{\kappa}_4\right]
\end{aligned}$$

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 :

$$\begin{aligned}
\dot{x} &= -5x + 5y & \qquad \dot{x} &= -2y \\
\dot{y} &= 14x - 2y - zx & \qquad \dot{y} &= x + z^2 \\
\dot{z} &= -3z + xy & \qquad \dot{z} &= 1 + y - 2z
\end{aligned}$$

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	$y'(x_N) = Y'_N$

$$\frac{d^2y}{dx^2} = f(x, y, y') \quad \text{where} \quad a \leq x \leq b \quad \text{and} \quad y(a) = \alpha,\ y(b) = \beta$$

$$\Rightarrow \qquad \frac{dy}{dx} = z \quad \text{with} \quad y(a) = \alpha$$

$$\frac{dz}{dx} = \frac{d^2y}{dx^2} = f(x, y, z) \quad \text{with} \quad z(a) = \zeta_h \quad (guess)$$

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 $\zeta_h \to \zeta_l$ 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 $z(a) = \zeta$

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

$z(a) = \zeta$ 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

$$y(x) = c_1 \, e^{\sqrt{2}\,x} + C_2 \, e^{-\sqrt{2}\,x}, \quad \text{where} \quad C_1 = 0.157, \; C_2 = 1.043$$

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

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

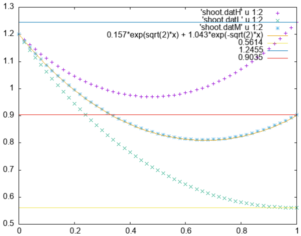
Next try $z(x = 0.0) = -1.0$,

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

Use Lagrange's linear interpolating formula,

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

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.

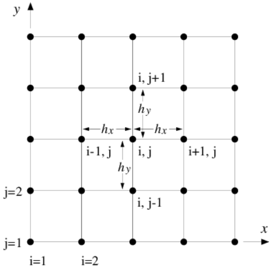
Consider explicit scheme in $1{+}1$ dimension diffusion or heat equation,

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

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

$$\begin{aligned} u(x,0) &= g(x) \quad \text{for } 0<x<L \\ u(0,t) &= a(t) \quad \text{for } t \geq 0 \\ u(L,t) &= b(t) \quad \text{for } t \geq 0 \end{aligned}$$

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

$$u_t \approx \frac{u(x, t+h_t) - u(x,t)}{h_t} \equiv \frac{u(x_i, t_j + h_t) - u(x_i, t_j)}{h_t} = \frac{u_{i,j+1} - u_{i,j}}{h_t}$$

$$u_{xx} \approx \frac{u(x+h_x, t) + u(x-h_x, t) - 2u(x,t)}{h_x^2}$$

$$\equiv \frac{u(x_i + h_x, t_j) + u(x_i - h_x, t_j) - 2u(x_i, t_j)}{h_x^2} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h_x^2}$$

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

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

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

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

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

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

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

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

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.

$$\begin{aligned} u_t &\approx \frac{u_{i,j} - u_{i,j-1}}{h_t} \\ u_{i,j-1} &= -\alpha\left(u_{i+1,j} + u_{i-1,j}\right) + (1+2\alpha)\, u_{i,j} \end{aligned}$$

The corresponding evolution equation for implicit scheme is

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

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

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

$$u(0,t) = 0^oC = u(2,t) \qquad \text{for} \quad 0 \le t \le 4$$
$$u(x,0) = 20\,|\sin(\pi x)|^oC \qquad \text{for} \quad 0 \le x \le 2$$

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