Numerical Mathematics (Practical)

Solution of Basic ODE / PDE

PDE's are defined by $u = u(x,y,z)$, $v = v(x,y,z)$, $w = w(x,y,z)$

u, v, w = dependent variable, x, y, z = independent variable. So

in general, $F(x, y, z, u, v, w, u_x, v_x, w_x, u_{xx}, \ldots u_{xy}, \ldots) = 0$

Order → Highest order derivative → $\begin{cases} u_x - bu_y = 0 & (1^{st} \text{ order}) \\ u_{xx} + u_y = 0 & (2^{nd} \text{ order}) \\ u_{xxxx} + u_{yyyy} = 0 & (4^{th} \text{ order}) \end{cases}$

If several independent PDE, then combination to single equation gives the order.

$u_x + v_y = u_z$, $u = w_x$, $v = w_y$ ⇒ $w_{xx} + w_{yy} = w_{z}$ (2^{nd} order)

Linearity → Important to find solution of PDE. for example, consider

$$a(x,y,u,u_x,u_y)\, u_x + b(x,y,u,u_x,u_y)\, u_y = c(x,y,u,u_x,u_y).$$

If $a(x,y,u,u_x,u_y) = a(x,y)$ only (linear) $\quad u_x + bu_y = 0.$
$b(x,y,u,u_x,u_y) = b(x,y)$ only
$c(x,y,u,u_x,u_y) = c(x,y)$ only.

If $a(x,y,u,u_x,u_y) = a(x,y,u)$ only (quasi-linear) → $\quad u_x + uu_y = x^2$
$b(x,y,u,u_x,u_y) = b(x,y,u)$ only
$c(x,y,u,u_x,u_y) = c(x,y,u)$ only

If $a(x,y,u,u_x,u_y) = a(x,y,u,u_x,u_y)$ (nonlinear) $\quad u_x + (u_y)\times(u_y) = 0$
$b(x,y,u,u_x,u_y) = b(x,y,u,u_x,u_y)$
$c(x,y,u,u_x,u_y) = c(x,y,u,u_x,u_y)$

General form 1^{st} order ODE $\dfrac{du}{dx} = f(x,u)$. Given x, u, $\dfrac{du}{dx}$ is uniquely known, while for PDE, given x, y, u gives connection between u_x, u_y but not $u_x = ?$, $u_y = ?$ for 2^{nd} order ODE, point & tangent line on a plane defines the solution while curve, 3D-space & tangent plane defines PDE.

Linear 2^{nd} order PDE

$$\boxed{a u_{xx} + 2b u_{xy} + c u_{yy} + d u_x + e u_y + f u + g = h \text{ (source)} \; = 0} \quad (1)$$

where a, b, c, d, e, f, g are ~~linear~~ constant coefficients. Every linear 2^{nd} order PDE are of canonical forms parabolic, hyperbolic and elliptic.

If $b^2 - ac > 0$, PDE is hyperbolic; $u_{tt} = u_{xx}$; $b^2 - ac = 0 + 1 \times 1 = 1$ (wave equation)

If $b^2 - ac = 0$, PDE is parabolic; $u_t = u_{xx}$; $b^2 - ac = 0 * 1 \times 0 = 0$ (heat equation)

If $b^2 - ac < 0$, PDE is elliptic; $u_{xx} + u_{yy} = 0$; $b^2 - ac = 0 - 1 \times 1 = -1$ (Laplace equation)

Tricomi's equation $y u_{xx} + u_{yy} = 0$, elliptic for $y > 0$, hyperbolic for $y < 0$

Solutions of Elliptic equation (e.g. Laplace eq^n.) can support large gradients as a source/sink term h (in eq^n. (1)). Numerics of linear algebra of diagonally dominant linear equation solvers are a good choice. Parabolic equations (e.g. heat eq^n.) generally have smooth solutions, but often exhibit solutions with evolving regions of high gradients. Matrix factorization with dynamic gridding algorithm (ADI methods) are good. Hyperbolic equations are the most-hardest as they exhibit spurious oscillations at sharp boundary as well as artificial effects. As shown using Octave code in class, artificial diffusion occurs to simulate a wave that can be solved only using 3^{rd} order upwind scheme.

Boundary condition $\quad \alpha(x,y)\, u(x,y) + \beta(x,y)\, u_n(x,y) = \gamma(x,y)$

Dirichlet B.C.	$\beta = 0$,	(Value Specified)
Neumann B.C.	$\alpha = 0$	(Slope specified)
Cauchy B.C.	2 equations $\alpha = 0$ in one $\beta = 0$ in other	(Both slope & value specified)

Robbin B.C. $\alpha \neq \beta \neq 0$ (homogeneous form)

(a) Hyperbolic equations are associated with Cauchy conditions
(wave equation) (2 initial, 2 B.C.) (open region)

(b) Parabolic equations are associated with Dirichlet/Neumann B.C.
(heat equation) (1 initial, 2 B.C.) (open region)

(c) Elliptic equations are associated with Dirichlet/Neumann B.C.
(Laplace equation) (1 B.C.) (closed region)

Finite Difference & Boundary value Problem (BVP)

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2).$$ Consider a simple BVP

$$\frac{d^2y}{dx^2} = 12x^2 \quad \text{with} \quad y(0) = 0, \quad y(1) = 0 \quad \text{(Dirichlet B.C.)}$$

Exact solution $y(x) = x^4 - x$. We divide the 1D interval $[0,1]$ into L subintervals with step size $dx = \frac{1}{L}$ & the points

$$x_i = (i-1)\,dx \quad \text{with} \quad i = 1, 2, 3, \cdots, L+1$$

So in FD form, $y_{i+1} - 2y_i + y_{i+1} = 12x^2 dx^2$, $y_1 = 0 = y_{L+1}$

So we have $L+1$ equations with $L+1$ unknowns

$$\left\{\begin{aligned}
y_1 &= 0 \\
y_1 - 2y_2 + y_3 &= 12x_2^2 dx^2 \\
y_2 - 2y_3 + y_4 &= 12x_3^2 dx^2 \\
&\vdots \\
y_{L-1} - 2y_L + y_{L+1} &= 12x_L^2 dx^2 \\
y_{L+1} &= 0.
\end{aligned}\right.
\Rightarrow
\underbrace{\begin{bmatrix}
1 & 0 & 0 & 0 & \cdots & & 0 \\
1 & -2 & 1 & 0 & \cdots & & 0 \\
0 & 1 & -2 & 1 & 0 & \cdots & \vdots \\
\vdots & & \ddots & \ddots & \ddots & & \vdots \\
0 & 0 & 0 & 0 & 1 & -2 & 1 \\
0 & 0 & 0 & 0 \cdots & 0 & 0 & 1
\end{bmatrix}}_{A}
\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_L \\ y_{L+1} \end{bmatrix}}_{y}
=
\underbrace{\begin{bmatrix} 0 \\ 12x_2^2 dx^2 \\ 12x_3^2 dx^2 \\ \vdots \\ 12x_L^2 dx^2 \\ 0 \end{bmatrix}}_{b}$$

whose solution is $y = A^{-1}b$.

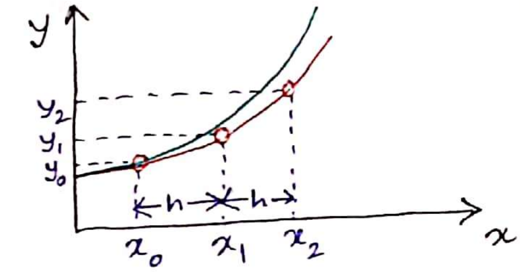
Solution of ODE: Euler, RK2 & RK4 (Explicit Method)

Euler Method Divide the region of interest (a, b) into discrete values of $x = nh$, $n = 0, 1, 2, \cdots, N-1$, spaced at interval $h = \frac{b-a}{N}$.

Use the forward difference approximation for the differential coefficient

$$f(x_n, y_n) = \frac{dy_n}{dx} = y_n' \simeq \frac{y_{n+1} - y_n}{h}$$

$$\therefore\ y_{n+1} \simeq y_n + h f(x_n, y_n).$$



Accuracy Expanding in Taylor series,

$$y_{n+1} = y_n + h y_n' + \frac{h^2}{2!} y_n'' + \cdots = y_n + h f_n + \frac{h^2}{2} y'' + \cdots \simeq y_n + h f_n.$$

$\therefore$ Error per step is $O(h^2)$ and as there are $\frac{b-a}{h}$ steps in the interval, so global error is $O(h)$.

Stability Consider the linear test equation $\frac{dy}{dx} = \lambda y(x)$. The equation
↳ Eigenvalue

is stable if $\text{Real}(\lambda) \le 0$, so that the solution is exponentially decaying $\lim_{x \to \infty} y(x) = 0$. Discretizing of this equation

$$y_{i+1} = y_i + h\lambda y_i = (1 + h\lambda) y_i = (1 + h\lambda)^2 y_{i-1} = \cdots = (1 + h\lambda)^{i+1} y_0$$

The solution is decaying (stable) if $|1 + h\lambda| \le 1$.

Modified-Euler / Midpoint / Heun / Predictor-Corrector's Method

A better way of estimating the slope from (x_n, y_n) to (x_{n+1}, y_{n+1}) would be

$$y_{n+1} \simeq y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_{n+1}, y_{n+1})\right]$$

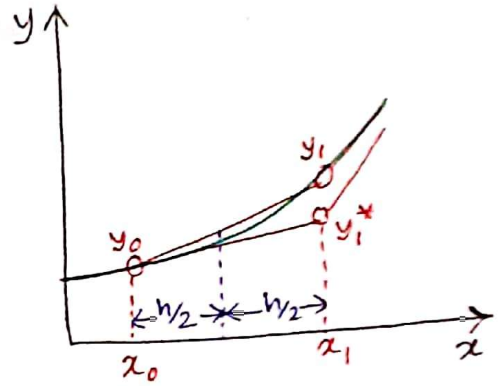
unknown

However we can estimate it by using Euler's method to give a 2-stage predictor-corrector scheme.

(a) Predictor step: $y_{n+1}^* = y_n + h f(x_n, y_n)$

(b) Corrector step: $y_{n+1} \simeq y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^*)\right]$

So the predictor step estimates the slope y' at x_n to predict a guess y^*_{n+1}. The corrector steps correct the value.



Accuracy Expanding f^*_{n+1} in Taylor series

$$f^*_{n+1} = f(x_n + h,\ y_n + hf_n)$$
$$= f(x_n, y_n) + h\frac{\partial f_n}{\partial x} + hf_n\frac{\partial f_n}{\partial y} + O(h^2)$$

So $y_{n+1} = y_n + \frac{h}{2}(f_n + f^*_{n+1}) = y_n + \frac{h}{2}\left(f_n + f_n + h\frac{\partial f_n}{\partial x} + hf_n\frac{\partial f_n}{\partial y} + O(h^2)\right)$

$$= y_n + hf_n + \frac{h^2}{2}\left(\frac{\partial f_n}{\partial x} + f_n\frac{\partial f_n}{\partial y}\right) + O(h^3)$$

So local error per step is $O(h^3)$ and the global error is $O(h^2)$.

Runge Kutta 4 The fourth order RK uses several predictive steps and it's locally $O(h^5)$ and globally $O(h^4)$.

RK4 steps:
$$\left.\begin{aligned} a &= hf(x_n, y_n) \\ b &= hf(x_n + h/2,\ y_n + a/2) \\ c &= hf(x_n + h/2,\ y_n + b/2) \\ d &= hf(x_n + h,\ y_n + c) \end{aligned}\right\} \quad y_{n+1} = y_n + \frac{1}{6}(a + 2b + 2c + d)$$

There are implicit integrators (e.g. Backward Euler, Crank-Nicholson, ADI etc), for which one can take larger h because stiff equations are hard to solve using explicit integrator, because of very small h, they become useless. The backside is implicit integrators are hard to code.

CFL condition Courant-Friedrichs-Lewy condition is a necessary condition for convergence when solving hyperbolic PDEs using explicit integrators. If a wave is moving across a grid & we want to compute its amplitude at discrete timesteps of equal duration then this duration must be less than the time for the wave to travel to next grid point. In 1D, $c = \frac{u \Delta t}{\Delta x}$ = Courant number

In 2D, $c = \frac{u_x \Delta t}{\Delta x} + \frac{u_y \Delta t}{\Delta y}$

Bessel's Equation (Poisson Equation with cylindrical symmetry)

$x^2 y'' + xy' + (x^2 - n^2) y = 0$ vibrations, heat conduction in cylindrical geometry

solution $\Rightarrow y = AJ_n(x) + BJ_{-n}(x)$ → 1st Kind

$$J_n(x) = \sum_{r=0}^{\infty} (-1)^r \left(\frac{x}{2}\right)^{n+2r} \frac{1}{r!\,\Gamma(n+r+1)}, \quad J_{-n}(x) = \sum_{r=0}^{\infty} (-1)^r \left(\frac{x}{2}\right)^{-n+2r} \frac{1}{r!\,\Gamma(-n+r+1)}$$

solution $\Rightarrow y = AJ_n(x) + BY_n(x)$, $Y_n(x) = J_n(x) \int \frac{dx}{x J_n(x)^2}$

→ 2nd Kind (Neumann function)

Generating function $e^{\frac{x}{2}(t - t^{-1})} = \sum_{n=-\infty}^{\infty} t^n J_n(x)$

Legendre's Equation (Poisson Equation with Spherical symmetry H-atom)
Multipole Expansion of 1/r potential

$(1-x^2) y'' - 2xy' + n(n+1) y = 0$, $P_n(x) = \frac{1}{n!\,2^n} \frac{d^n}{dx^n} (x^2-1)^n$ Rodrigue's formula

Generating function $(1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} t^n P_n(x)$

Laguerre's polynomial (Radial part of 1 electron Schrodinger's Eq^n ⇒ H atom)

$xy'' + (1-x) y + ny = 0$, $L_n(x) = e^x \frac{d^n}{dx^n} (x^n e^{-x})$

Generating function $\frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} \frac{L_n(x)}{n!} t^n$

Hermite's polynomial (Eigenstate of Quantum harmonic oscillator)

$y'' - 2xy' + 2ny = 0$, $H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2})$

Generating function $e^{2tx - t^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n$

Chebyshev polynomial (Orr-Sommerfeld Equation) Elliptical coordinates

$(1-x^2) y'' - xy' + n^2 y = 0$, $T_n(x) = \frac{n}{2} \sum_{r=0}^{N} (-1)^r \frac{(n-r-1)!}{r!\,(n-2r)!} (2x)^{n-2r}$,

$N = \frac{n}{2}$, n = even
$= \frac{n-1}{2}$, n = odd

Generating function $\frac{1-xt}{1+2xt+t^2} = \sum_{n=0}^{\infty} T_n(x) t^n$

Univariate Gaussian PDF

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \quad \int f(x)\,dx = 1$$

Limit representations

$$\lim_{\sigma\to 0} f(x) = \delta(x). \quad \lim_{\epsilon\to 0} \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2} = \delta(x) \quad \text{(Lorentzian)}$$

$$\lim_{\epsilon\to 0+} \frac{1}{2\sqrt{\pi\epsilon}} e^{-x^2/4\epsilon} = \delta(x), \quad \lim_{\epsilon\to 0} \frac{1}{2}\epsilon|x|^{\epsilon-1} = \delta(x)$$

$$\lim_{\epsilon\to 0} \frac{1}{\pi x}\sin\left(\frac{x}{\epsilon}\right) = \lim_{\epsilon\to 0} \underbrace{\frac{1}{\epsilon} Ai\left(\frac{x}{\epsilon}\right)}_{\text{Airy function}} = \lim_{\epsilon\to 0} \frac{1}{\epsilon} \underbrace{J_{1/\epsilon}\left(\frac{x+1}{\epsilon}\right)}_{\text{Bessel 1}^{st}\text{ Kind}}$$

$$= \lim_{\epsilon\to 0} \left|\frac{1}{\epsilon} e^{-x^2/\epsilon} \underbrace{L_n\left(\frac{2x}{\epsilon}\right)}_{\text{Laguerre polynomial}}\right| = \delta(x) = \lim_{\epsilon\to 0+} \frac{1}{\sqrt{\pi\epsilon}} e^{-x^2/\epsilon} \left(-\frac{1}{\sqrt{\epsilon}}\right)^n H_n\left(\frac{x}{\sqrt{\epsilon}}\right)$$

$$\lim_{n\to\infty} \frac{1}{2\pi\sin\left(\frac{x}{2}\right)} \sin\left[x\left(n+\tfrac{1}{2}\right)\right] = \lim_{n\to\infty} \log|\coth(nx)| = \lim_{n\to\infty} \frac{n}{\sinh(nx)}$$

$$= \delta(x)$$

Product & Convolution of 2 Univariate Gaussian PDF

$$f(x) = \frac{1}{\sqrt{2\pi\sigma_f^2}} e^{-\frac{(x-\mu_f)^2}{2\sigma_f^2}}, \quad g(x) = \frac{1}{\sqrt{2\pi\sigma_g^2}} e^{-\frac{(x-\mu_g)^2}{2\sigma_g^2}}$$

then $f(x)g(x) = \frac{S_{fg}}{\sqrt{2\pi\sigma_{fg}^2}} e^{-\frac{(x-\mu_{fg})^2}{2\sigma_{fg}^2}}$ where $\sigma_{fg} = \underbrace{\sqrt{\frac{\sigma_f^2\sigma_g^2}{\sigma_f^2+\sigma_g^2}}}_{\text{harmonic mean}}$

$$\mu_{fg} = \frac{\mu_f\sigma_g^2 + \mu_g\sigma_f^2}{\sigma_g^2+\sigma_f^2}$$

individual means weighted by respective variances.

$$\int_0^x f(x-\tau)\,g(\tau)\,d\tau = f \otimes g$$

Convolution

$$P_{f\otimes g}(x) = F^{-1}\left[F(f(x)g(x))\right]$$

Fourier transform; Inverse Fourier transform

$$F(f(x)) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i k x} dx, \quad F^{-1}(f(k)) = \int_{-\infty}^{\infty} f(k) e^{2\pi i k x} dk$$

$$P_{f\otimes g}(x) = \frac{1}{\sqrt{2\pi(\sigma_f^2+\sigma_g^2)}} e^{-\frac{[x-(\mu_f+\mu_g)]^2}{2(\sigma_f^2+\sigma_g^2)}}$$

$$\therefore \boxed{\underbrace{\mu_{f\otimes g} = \mu_f + \mu_g}_{\text{arithmetic mean}}, \quad \sigma_{f\otimes g} = \sqrt{\sigma_f^2+\sigma_g^2}}$$

Fourier Series

Sawtooth Wave

$$f(t) = t \text{ for } -\overset{T}{\text{period}} < t < +\overset{T}{\text{period}}$$

$$f(t + 2n\,\text{period}) = f(t)$$

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\omega t) + \sum_{n=1}^{\infty} b_n \sin(n\omega t) \quad \text{with}$$

$$a_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\cos n\omega t\, dt, \quad b_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\sin n\omega t\, dt$$

As $f(t) \neq + f(-t)$ [odd function], (so $a_n = 0$)

$$b_n = \frac{2}{n\pi}(-1)^{n+1}, \quad f(t) = \sum_{n=\text{odd}}^{\infty} \frac{2}{n\pi}(-1)^{n+1}\sin(n\omega t), \quad \omega = \frac{2\pi n}{T}$$

Analytic form $\Rightarrow$ $\boxed{f(t) = 2\left[\frac{t}{\text{period}} - \left\lfloor \frac{1}{2} + \frac{t}{\text{period}} \right\rfloor\right]}$ (floor)

Triangular Wave

Analytic form $\Rightarrow$ $\boxed{f(t) = \frac{2A}{\pi}\sin^{-1}\left(\sin\frac{\pi t}{\text{period}}\right)}$ [odd function] ($a_n = 0$)

$$= \sum_{n=\text{odd}}^{\infty} \frac{8A}{n^2\pi^2}(-1)^{\frac{n-1}{2}}\sin(n\omega t)$$

Square Wave

Analytic form $\Rightarrow$ $\boxed{f(t) = A\,\text{sgn}\left(\sin\frac{2\pi t}{\text{period}}\right)}$. [odd function] ($a_n = 0$)

$$= \sum_{n=\text{odd}}^{\infty} \frac{4A}{n\pi}\sin(n\omega t)$$

18% overshoot at discontinuities $\rightarrow$ donot change by incorporating more harmonics $\rightarrow$ Gibb's phenomena.

$$f(t) = \sqrt{(2L - t)t}, \quad a_0 = \frac{\pi L}{2}, \quad a_n = \frac{(-1)^n L J_1(n\pi)}{n}, \quad b_n = 0$$

so that $f(t) = L\left[\frac{\pi}{4} + \sum_{n=1}^{\infty}\frac{(-1)^n J_1(n\pi)}{n}\cos\left(\frac{n\pi t}{L}\right)\right]$

(Semicircle)