

Fourier

Normal mode analysis of advection-dispersion: $u_t + Vu_x = Du_{xx}$

Set $u(x,t) = u_k(x,t) = a(k) e^{i[kx - \omega t]}$

$$u_t = -i\omega u_k, \quad u_x = ik u_k, \quad u_{xx} = (ik)^2 u_k = -ik^3 u_k$$

Dispersion relation: $-i\omega + V ik = -ik^3 D \Rightarrow \omega(k) = -\frac{ik^3 D}{-i} - \frac{ikV}{-i} = Dk^3 + V k$

$$\Rightarrow \text{Im } \omega(k) = 0 \quad \forall k \stackrel{\Omega=0}{\Rightarrow} \text{and normal modes are } u_k(x,t) = a(k) e^{ik[x - (V + Dk^2)t]}$$

Cauchy problem is well-posed and neutrally stable

Normal modes are harmonic waves, which do not decay,

with speed $V + Dk^2$, so modes of smaller wavelengths $\lambda = \frac{2\pi}{k}$ propagate with much higher speed.

$\omega''(k) \neq 0$, so PDE is dispersive. (phase speed $c_p = \frac{dx}{dt} = \frac{\omega(k)}{k} = V + Dk^2$)

Fourier analysis of ^{linear} FDEs: $U_j^{n+1} = U_j^n + \sum (\text{terms with } U_{j-1}^n, U_j^n, U_{j+1}^n)$

Now $x = x_j = j \Delta x$, $t = t_n = n \Delta t$

Normal modes $U_j^n = a e^{i[kx_j - \omega t_n]} = a e^{i[kj \Delta x - \omega n \Delta t]} = a (e^{-i\omega \Delta t})^n \cdot e^{ikj \Delta x}$
set $\lambda = e^{-i\omega \Delta t}$, $\xi = k \Delta x$
 $= a(n) \lambda^n e^{ik \Delta x j} = a(k) \lambda^n e^{i\xi j}$

Substituting into the FDE, we determine $\lambda = \lambda(k)$ and the FDE will be

stable if $|\lambda(k)| \leq 1 \quad \forall k \in \mathbb{R}$

In fact, for a ^{linear} homogeneous PDE and FDE, $a(k)$ will factor out, so may just use

$$U_j^n = \lambda^n e^{ikj \Delta x} = \lambda_j^n e^{i\xi_j j}, \quad j = 1, 2, \dots, M, \quad \text{any } \xi_j \in [-n, n]$$

This is commonly known as von Neumann stability analysis.

For linear FDE, $U_{j+1}^n = U_j^n \cdot e^{i\xi_j}$, so FDE $\Rightarrow U_j^{n+1} = Q(-\lambda, \xi_j) U_j^n$
amplification factor per timestep
scheme is stable if $|Q| \leq 1$

Semi-discretization: "method of lines" for PDEs $u_t = \mathcal{L}u + f$

yields system of ODEs in time

Instead of space and time discretization, we can discretize only in space,

thus replacing the space derivatives by a discrete operator A_h for space mesh $h = \Delta x, \dots$
(advection-diffusion)

Thus we get a system of ODEs: for $\vec{y}(t) \approx \begin{bmatrix} u(x_1, t) \\ u(x_2, t) \\ \vdots \\ u(x_M, t) \end{bmatrix}, \vec{y} = \begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_M(t) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$

$$\vec{y}'(t) = A_h \vec{y} + \vec{S}(x_h, t, \vec{y}), \text{ an ODE for each node, so } M \times M$$

which we can solve with any ODE integrator, e.g. θ-schemes, RK, multistep, ...

for which there are excellent packages available, very convenient (VODE, rksuite, ...)

1. Many full discretizations can be obtained via semidiscretizations, but not all,

2. So, time discretizations can be viewed as ODE systems $\vec{y}' = \vec{F}(t, \vec{y})$
and can employ any ODE solver

3. If the PDE is linear, then the ODE is linear: $\vec{y}' = A\vec{y} + g(t)$

else nonlinear $\vec{y}' = \vec{F}(t, \vec{y})$

e.g. Semidiscrete upwind scheme: for linear advection: $u_t + V u_x = 0, a < x < b, t > 0, V > 0$

$$u_t + F_x = 0 \Rightarrow \frac{d}{dt} U_i = - \int_{x_{i-1}}^{x_{i+1}} F_x dv = \frac{V}{\Delta x} [F_{i+1/2} - F_{i-1/2}] \quad | \quad u(x, 0) = f(x), \text{ periodic BCs: } u(a, t) = u(b, t)$$

Here advection flux $F = Vu$,

$$\text{upwind flux: } F_{i-1/2} = Vu_{i-1} \Rightarrow \frac{d}{dt} U_i(t) = \frac{V}{\Delta x} [U_{i-1} - U_i], i=1, 2, \dots, M, U_0(t) = U_M(t)$$

$$\text{Set } \vec{y} = \begin{bmatrix} U_1 \\ \vdots \\ U_M \end{bmatrix} \Rightarrow \begin{cases} \vec{y}' = A\vec{y} = \frac{V}{\Delta x} \begin{bmatrix} -1 & 0 & \cdots & 1 \\ 1 & -1 & 0 & \vdots \\ 0 & \ddots & \ddots & 0 \\ \vdots & & -1 & -1 \end{bmatrix} \begin{bmatrix} U_1 \\ \vdots \\ U_M \end{bmatrix} \\ \vec{y}(0) = f(x_i) \end{cases}_{M \times M}$$

4. Solution of $\vec{y}' = A\vec{y}; \vec{y}(t) = e^{tA} \vec{y}(0), e^{tA} = I + tA + \frac{t^2 A^2}{2!} + \dots$ (always converges)

$\Sigma(t) = e^{tA}$ is the propagator of initial data to time t , $\{\Sigma(t)\}_{t \geq 0}$ is a semigroup of operators; $\Sigma(0) = I$

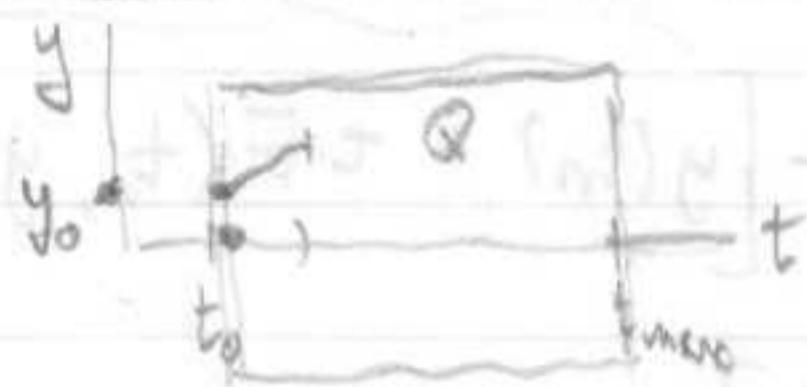
meaning of e^{tA} has been extended to nonlinear operators A in 1970's,

$$\Sigma(b+s) = \Sigma(b)\Sigma(s)$$

Numerical ODEs for (IVP) $\begin{cases} \vec{y}' = \vec{F}(t, \vec{y}), t_0 < t < t_{\max} \\ \vec{y}(t_0) = \vec{y}_0, \text{ given} \end{cases}$

Well-posedness. Then for the (IVP): 1. If $\vec{F}(t, y)$ is continuous on \bar{Q}

then the IVP has a sol near t_0 , i.e. for $t_0 \leq t \leq \bar{t}$



$$Q = \{(t, y) : 0 < t < t_{\max}, \|y - y_0\| < K_0\}$$

$\|\cdot\|$ some vector norm

3. If \vec{F} is Lipschitz w.r.t. y in Q , i.e.

$$\|\vec{F}(t, z) - \vec{F}(t, w)\| \leq L \cdot \|z - w\| \quad \forall (t, z), (t, w) \in \bar{Q}$$

then solution is unique.

Thus, \vec{F} cont's, bdd, Lip in $y \Rightarrow$ IVP well-posed locally (near the initial pt)

Note: $\left\| \frac{\partial \vec{F}}{\partial y} \right\| \leq L \Rightarrow F$ is Lip with const. $\geq L$
Jacobian

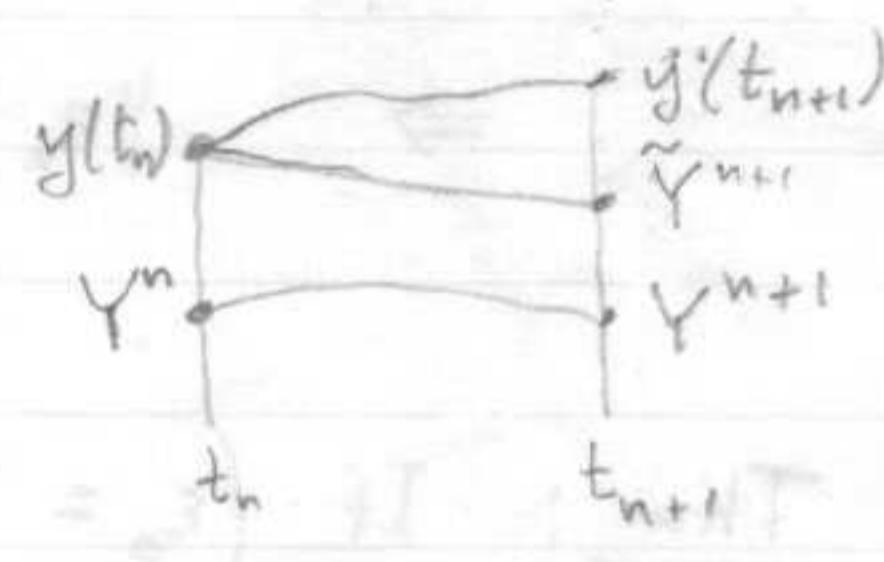
Most basic, fundamental method is Euler Method: $\vec{Y}^n \approx \vec{y}(t_n)$

$$\vec{Y}^0 = \vec{y}_0$$

$$(1) \quad \vec{Y}^{n+1} = \vec{Y}^n + \Delta t \cdot \vec{F}(t_n, \vec{Y}^n) \quad \left| \begin{array}{l} Y^{n+1} = Y^n + \Delta t [(1-\theta) F(t_n, Y^n) + \theta F(t_{n+1}, Y^{n+1})] \\ FDE[\vec{Y}] = \frac{Y^{n+1} - Y^n}{\Delta t} - F(t_n, Y^n) \end{array} \right.$$

$$(2) \quad FDE[\vec{Y}] = \frac{Y^{n+1} - Y^n}{\Delta t} - F(t_n, Y^n)$$

$$\text{Consistency error (local truncation error)}: \rho_n = FDE[\vec{y}(t_n)] - ODE[y] \\ = \frac{y(t_{n+1}) - y(t_n)}{\Delta t} - F(t_n, y^n) \\ = \frac{\Delta t}{2} y''(t_n) + O(\Delta t^2)$$



Proof: By Taylor expansion of $y(t_n + \Delta t)$ about t_n : $y(t_{n+1}) = y(t_n) + \Delta t \cdot y'(t_n) + \frac{\Delta t^2}{2} y''(t_n) + O(\Delta t^3)$

$$\rho_n = \frac{y(t_{n+1}) - y(t_n)}{\Delta t} - F(t_n, y(t_n)) = \frac{\Delta t}{2} y''(t_n) + O(\Delta t^2)$$

$$\text{For } 0 \leq \theta \leq 1: \rho_n = \frac{\Delta t}{2} (1-2\theta) y'' + \frac{\Delta t^2}{6} (1-3\theta) y''' + O(\Delta t^3)$$

(3) If $y \in C^2[0, t_{\max}]$ (with $\|y''(t)\| \leq M_2$) then $\|\rho_n\| \leq \frac{\Delta t}{2} \cdot \max_{t_n \leq t \leq t_{n+1}} \|y''(t)\| = O(\Delta t)$ 1st order

$$= \frac{\Delta t}{2} \cdot M_2 \quad \rightarrow 0 \text{ as } \Delta t \rightarrow 0$$

i consistent method

(4) Hence, $\Delta t \cdot \rho_n = y(t_{n+1}) - y(t_n) - \Delta t \cdot F(t_n, y(t_n))$

$$\Rightarrow y(t_{n+1}) = [\text{apply scheme to } y(t_n)] + \Delta t \cdot \rho_n$$

If $\rho_n = O(\Delta t^p)$ then

scheme is of order p

Discretization error: $\varepsilon_n = Y^n - y(t_n)$ (at ∞ precision!)

$$\text{Estimate: } (1) - (4) \Rightarrow \varepsilon_{n+1} = Y^{n+1} - y(t_{n+1}) = \underbrace{Y^n + \tau F(t_n, Y^n)}_{Y^n} - \left[\underbrace{y(t_n) + \tau F(t_n, y(t_n))}_{y(t_n)} + \tau p_n \right] \\ = \varepsilon_n + \tau [F(t_n, Y^n) - F(t_n, y(t_n))] - \tau \cdot p_n$$

$$\text{Using the Lip condition: } |F - F| \leq L \cdot |Y^n - y(t_n)| = \tau L$$

$$\Rightarrow \|\varepsilon_{n+1}\| \leq \|\varepsilon_n\| \cdot \underbrace{[1 + \tau L]}_{=: \kappa} + \tau \|p_n\| \\ \Rightarrow \|\varepsilon_n\| \leq \kappa \|\varepsilon_{n-1}\| + \tau \|p_{n-1}\| \leq \kappa \cdot (\kappa \|\varepsilon_{n-2}\| + \tau \|p_{n-2}\|) + \tau \|p_{n-1}\| \\ = \kappa^2 \|\varepsilon_{n-2}\| + \tau (\|p_{n-1}\| + \kappa \|p_{n-2}\|)$$

$$\Rightarrow \|\varepsilon_n\| \leq \kappa^n \|\varepsilon_0\| + \sum_{j=0}^{n-1} \kappa^j \tau \|p_{n-1-j}\| \leq \kappa^n \|\varepsilon_0\| + \tau \cdot \max_{0 \leq j \leq n} \|p_j\| \cdot \frac{\kappa^n - 1}{\kappa - 1}$$

$$\text{Using } \kappa = 1 + \tau L < 1 + \tau L + (\tau L)^2 + \dots = e^{\tau L}, \quad \|p_j\| \leq \frac{\tau}{2} M_2$$

$$\leq e^{L \cdot n \tau} \|\varepsilon_0\| + \tau \cdot \frac{e^{L \cdot n \tau} - 1}{\tau L} \frac{\tau}{2} M_2, \quad M_2 = \max_{0 \leq t \leq t_n} \|y''(t)\|$$

$$\Rightarrow \|\varepsilon_n\| = e^{L \cdot t_n} \|\varepsilon_0\| + \frac{\tau}{2} K \cdot \max_{0 \leq t \leq t_n} \|y''(t)\|, \quad K = \frac{e^{L \cdot t_n} - 1}{L}$$

Thm: If $(\varepsilon_0 = Y^0 - y_0 = 0)$, $y \in C^2[0, t_{\max}]$, F is Lip with const. L

$$\text{then } \|Y^n - y(t_n)\| \leq \frac{\Delta t}{2} \cdot \max_{[0, t_{\max}]} \|y''(t)\| \cdot \frac{e^{L t_{\max}} - 1}{L} = O(\Delta t) \rightarrow 0 \text{ as } \Delta t \rightarrow 0$$

\therefore convergent, of 1st order

$$+ e^{L \cdot t_n} \|Y^0 - y_0\|$$

initial error will grow exponentially! try to avoid...
up to $e^{L t_{\max}}$