Numerical Solution of ODE Systems

1. Extensions of single ODE methods
2. ODE system stiffness
3. Implicit solution methods
4. In-class exercise

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Numerical Solution of ODE Systems

Extension of Single ODE Methods

Nonlinear ODE Systems

- Background
  - » Many chemical engineering models consist of coupled nonlinear ODEs
  - » Numerical solution usually is the only option
- Initial value problem

$$\begin{aligned} \frac{dy_1}{dx} &= f_1(x, y_1, \ldots, y_m) \quad y_1(x_0) = y_{10} \\ &\vdots \\ \frac{dy_m}{dx} &= f_m(x, y_1, \ldots, y_m) \quad y_m(x_0) = y_{m0} \end{aligned} \quad \Rightarrow \quad \frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}) \quad \mathbf{y}(x_0) = \mathbf{y}_0$$

- Methods also applicable to second-order ODEs by conversion to first-order ODEs

$$\frac{d^2y}{dx^2} = f_1\left(x, y, \frac{dy}{dx}\right)$$

Extensions of Single Equation Methods

- Methods developed for numerical solution of single ODEs can be extended directly to ODE systems
- Forward Euler

$$\left.\begin{array}{l} y_{1,n+1} = y_{1,n} + hf_1(x, y_{1,n}, \ldots, y_{m,n}) \quad y_{1,0} = y_{10} \\ \vdots \\ y_{m,n+1} = y_{m,n} + hf_m(x, y_{1,n}, \ldots, y_{m,n}) \quad y_{m,0} = y_{m0} \end{array}\right. \Rightarrow \quad \mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(x_n, \mathbf{y}_n)$$

- Runge-Kutta

$$\mathbf{k}_1 = h\mathbf{f}(x_n, \mathbf{y}_n) \quad \mathbf{k}_2 = h\mathbf{f}(x_n + \tfrac{1}{2}h, \mathbf{y}_n + \tfrac{1}{2}\mathbf{k}_1)$$

$$\mathbf{k}_3 = h\mathbf{f}(x_n + \tfrac{1}{2}h, \mathbf{y}_n + \tfrac{1}{2}\mathbf{k}_2) \quad \mathbf{k}_4 = h\mathbf{f}(x_n + h, \mathbf{y}_n + \mathbf{k}_3)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \tfrac{1}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

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Chemical Reactor Example

- Van de Vusse reaction scheme

$$A \xrightarrow{r_1} B \xrightarrow{r_2} C \qquad r_1 = k_1 C_A \qquad r_2 = k_2 C_B$$

$$2A \xrightarrow{r_3} D \qquad\qquad r_3 = k_3 C_A^2$$

- Chemical reactor model

$$\frac{dC_A}{dt} = \frac{q}{V}(C_{Ai} - C_A) - k_1 C_A - 2k_3 C_A^2 = f_1(C_A) \qquad C_A(0) = C_{A0}$$

$$\frac{dC_B}{dt} = -\frac{q}{V} C_B + k_1 C_A - k_2 C_B = f_2(C_A, C_B) \qquad C_B(0) = C_{B0}$$

- Forward Euler equations

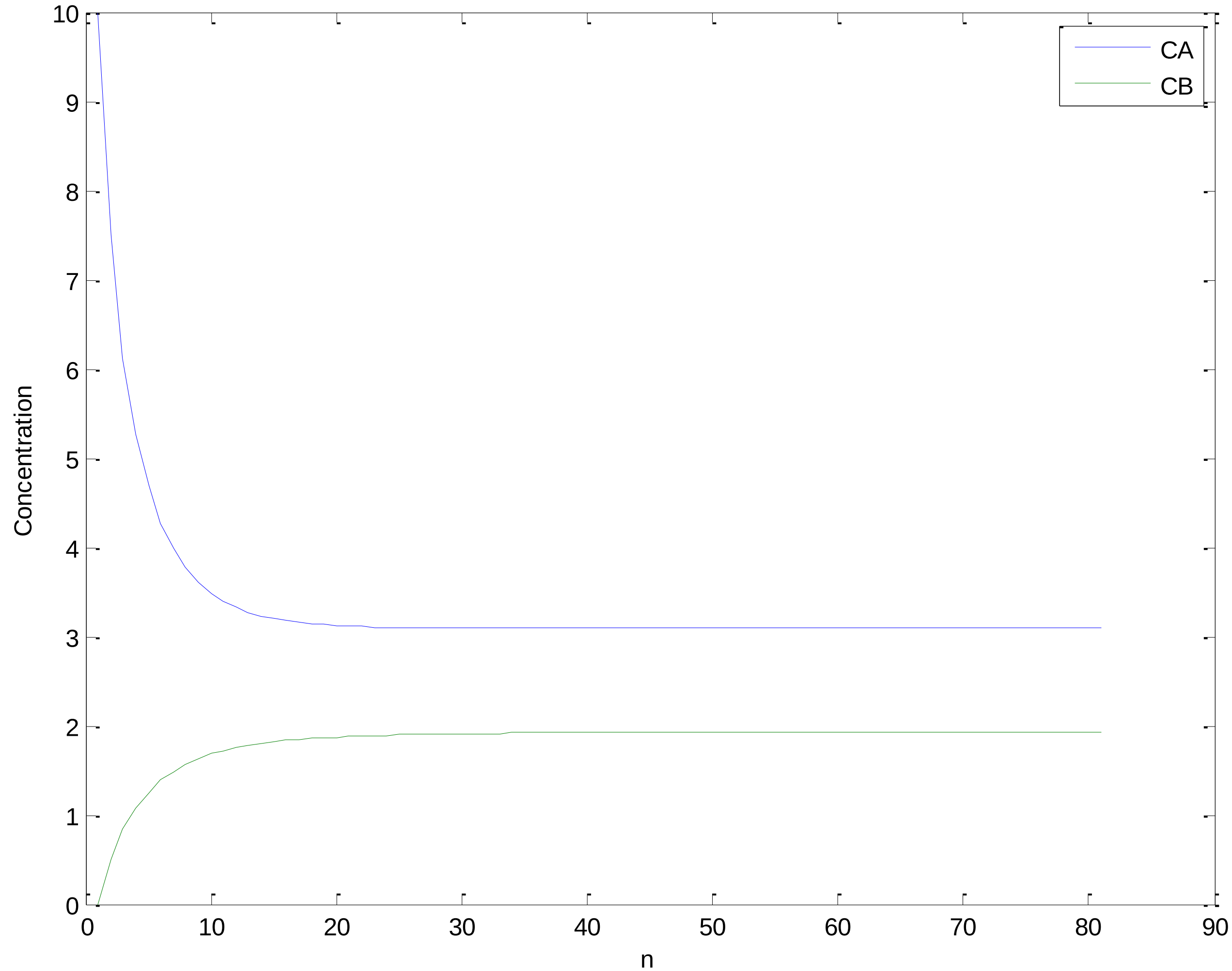
$$C_{A,n+1} = C_{A,n} + hf_1(C_{A,n}) = C_{A,n} + h\left[\frac{q}{V}(C_{Ai} - C_{A,n}) - k_1 C_{A,n} - 2k_3 C_{A,n}^2\right] \qquad C_{A,0} = C_{A0}$$

$$C_{B,n+1} = C_{B,n} + hf_2(C_{A,n}, C_{B,n}) = C_{B,n} + h\left[-\frac{q}{V} C_{B,n} + k_1 C_{A,n} - k_2 C_{B,n}\right] \qquad C_{B,0} = C_{B0}$$

Chemical Reactor Example

$$C_{Ai} = 10,\ q = 5,\ V = 1,\ k_1 = 5,\ k_2 = 3,\ k_3 = 1,\ h = 0.01$$

n	C_A	C_B
0	10	0
1	7.5	0.5
2	6.125	0.835
3	5.262	1.074
4	4.682	1.252
5	4.276	1.386
10	3.394	1.721
20	3.114	1.877
30	3.092	1.911
50	3.090	1.928
80	3.090	1.931



Numerical Solution of ODE Systems

ODE System Stiffness

Stiff Linear ODE Systems

- Large difference in magnitudes of the smallest and largest eigenvalues
- Necessitates small step size to maintain numerical stability
- Example

$$\frac{d\mathbf{y}}{dt} = \begin{bmatrix} 0 & 1 \\ -1000 & -1001 \end{bmatrix} \mathbf{y} = \mathbf{A}\mathbf{y}$$

$$\lambda(\mathbf{A}) = \begin{vmatrix} -\lambda & 1 \\ -1000 & -1001-\lambda \end{vmatrix} = \lambda^2 + 1001\lambda + 1000 = (\lambda+1)(\lambda+1000) = 0$$

$$\text{Stiffness ratio}: \frac{|-1000|}{|-1|} = 1000$$

Stiff Nonlinear ODE Systems

- Separation of time scales

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}, \mathbf{z}) \qquad \varepsilon \frac{d\mathbf{z}}{dx} = \mathbf{g}(x, \mathbf{y}, \mathbf{z})$$

  - » $\varepsilon \ll 1$
  - » **y** are "slow" variables
  - » **z** are "fast" variables

- Slow and fast physicochemical phenomenon
- Common in models of chemical engineering systems
- ODEs are not always in a form where stiffness is easily deduced
- Can investigate stiffness by computing the eigenvalues of the linearized system

Stiff Nonlinear ODE Example

- Metabolic reaction sequence: S →M →P
- Reaction kinetics

$$v_1 = \frac{v_{1m} S}{K_1 + S} \qquad v_2 = \frac{v_{2m} M}{K_2 + M}$$

- Mass balances

$$\frac{dS}{dt} = -v_1 = -\frac{v_{1m} S}{K_1 + S} = f_1(S)$$

$$\frac{dM}{dt} = v_1 - v_2 = \frac{v_{1m} S}{K_1 + S} - \frac{v_{2m} M}{K_2 + M} = f_1(S, M)$$

Stiff Nonlinear ODE Example

- Linearize ODEs about steady state

$$0 = -v_1 = -\frac{v_{1m}\bar{S}}{K_1 + \bar{S}} \quad \Rightarrow \quad \bar{S} = 0$$

$$0 = v_1 - v_2 = \frac{v_{1m}\bar{S}}{K_1 + \bar{S}} - \frac{v_{2m}\bar{M}}{K_2 + \bar{M}} \quad \Rightarrow \quad \bar{M} = 0$$

- Linearize first equation

$$\frac{dS'}{dt} = f_1(\bar{S}) + \left.\frac{\partial f_1}{\partial S}\right|_{\bar{S},\bar{M}} S' + \left.\frac{\partial f_1}{\partial M}\right|_{\bar{S},\bar{M}} M' = \left.\frac{\partial f_1}{\partial S}\right|_{\bar{S},\bar{M}} S'$$

$$\frac{dS'}{dt} = \frac{-(K_1 + \bar{S})v_{1m} - v_{1m}\bar{S}(1)}{(K_1 + \bar{S})^2} S' = -\frac{K_1 v_{1m}}{K_1^2} S' = -\frac{v_{1m}}{K_1} S'$$

Stiff Nonlinear ODE Example

- Linearize second equation

$$\frac{dM'}{dt} = f_2(\bar{S}) + \left.\frac{\partial f_2}{\partial S}\right|_{\bar{S},\bar{M}} S' + \left.\frac{\partial f_2}{\partial M}\right|_{\bar{S},\bar{M}} M' = \left.\frac{\partial f_2}{\partial S}\right|_{\bar{S},\bar{M}} S' + \left.\frac{\partial f_2}{\partial M}\right|_{\bar{S},\bar{M}} M'$$

$$\frac{dM'}{dt} = \frac{v_{1m}}{K_1} S' - \frac{v_{2m}}{K_2} M'$$

- Compute eigenvalues

$$\frac{d}{dt}\begin{bmatrix} S' \\ M' \end{bmatrix} = \begin{bmatrix} -\frac{v_{1m}}{K_1} & 0 \\ \frac{v_{1m}}{K_1} & -\frac{v_{2m}}{K_2} \end{bmatrix} \begin{bmatrix} S' \\ M' \end{bmatrix} \Rightarrow \quad \lambda_1 = -\frac{v_{1m}}{K_1}, \lambda_2 = -\frac{v_{2m}}{K_2}$$

Stiff Nonlinear ODE Example

- Reaction rate parameters

$$\lambda_1 = -\frac{v_{1m}}{K_1} = -\frac{10}{5} = -2 \qquad \lambda_2 = -\frac{v_{2m}}{K_2} = -\frac{2000}{10} = -200$$

- The ODE system is stiff

$$\text{Stiffness ratio}: \frac{|-200|}{|-2|} = 100$$

Numerical Solution of ODE Systems

Implicit Solution Methods

Implicit Solution Methods

- Motivation
  - » Implicit methods offer better stability and speed than explicit methods for stiff ODE systems
  - » Often do not know if a particular ODE model is stiff
  - » Most large ODE systems are stiff
- Backward Euler
  - » Simplest implicit method

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(x_{n+1}, \mathbf{y}_{n+1})$$

  - » Requires repeated solution of nonlinear algebraic system
  - » Better stability properties but more computationally demanding than forward Euler

Stiff ODE System Example

- Chemical reactor: A → B → C

$$\frac{dC_A}{dt} = \frac{q}{V}(C_{Ai} - C_A) - k_1 C_A \qquad \frac{dC_B}{dt} = -\frac{q}{V}C_B + k_1 C_A - k_2 C_B$$

- This ODE system is not homogeneous unless $C_{Ai} = 0$
- Can be converted into a homogeneous ODE system by the introduction of deviation variables

$$0 = \frac{q}{V}(C_{Ai} - \overline{C}_A) - k_1 \overline{C}_A \qquad 0 = -\frac{q}{V}\overline{C}_B + k_1 \overline{C}_A - k_2 \overline{C}_B$$

$$C_A^{'}(t) \equiv C_A(t) - \overline{C}_A \qquad C_B^{'}(t) \equiv C_B(t) - \overline{C}_B$$

Stiff ODE System Example

- Homogeneous system

$$\frac{dC_A'}{dt} = \frac{dC_A}{dt} - \underbrace{\frac{d\overline{C}_A}{dt}}_{=0} = \frac{dC_A}{dt}$$

$$\frac{dC_A'}{dt} = \frac{q}{V}(C_{Ai} - C_A) - k_1 C_A - \left[\frac{q}{V}(C_{Ai} - \overline{C}_A) - k_1 \overline{C}_A\right] = -\frac{q}{V}C_A' - k_1 C_A'$$

$$\frac{dC_B'}{dt} = -\frac{q}{V}C_B' + k_1 C_A' - k_2 C_B'$$

- Parameter values: $q/V = 1$, $k_1 = 1$, $k_2 = 200$

$$\frac{dC_A'}{dt} = -2C_A' \qquad \frac{dC_B'}{dt} = C_A' - 201C_B'$$

Stiff ODE System Example

- Eigenvalue analysis

$$\frac{dC_A'}{dt} = -2C_A' \quad \frac{dC_B'}{dt} = C_A' - 201C_B'$$

$$y'(t) \equiv \begin{bmatrix} C_A'(t) \\ C_B'(t) \end{bmatrix} \quad \frac{dy'}{dt} = \begin{bmatrix} -2 & 0 \\ 1 & -201 \end{bmatrix} y' = \mathbf{A}y'$$

$$\lambda_1 = -2 \quad \lambda_2 = -201$$

- This ODE system is stiff due to large difference in the two reaction rate constants

Stiff ODE System Example

- Forward Euler (explicit method)

$$\frac{dC'_A}{dt} = -2C'_A \quad \Rightarrow \quad C'_{A,n+1} = C'_{A,n} + h(-2C'_{A,n})$$

$$\frac{dC'_B}{dt} = C'_A - 201C'_B \quad \Rightarrow \quad C'_{B,n+1} = C'_{B,n} + h(C'_{A,n} - 201C'_{B,n})$$

- First iterative equation

$$C'_{A,n+1} = C'_{A,n} + h(-2C'_{A,n}) = (1-2h)C'_{A,n} \quad \Rightarrow \quad C'_{A,n} = (1-2h)^n C'_{A,0}$$

$$0 < h < \tfrac{1}{2} \quad \Rightarrow \quad \text{well behaved}$$

$$\tfrac{1}{2} < h < 1 \quad \Rightarrow \quad \text{oscillatory but stable}$$

$$h > 1 \quad \Rightarrow \quad \text{oscillatory and unstable}$$

Stiff ODE System Example

- Second iterative equation

$$C'_{B,n+1} = C'_{B,n} + h(C'_{A,n} - 201C'_{B,n}) \quad \Rightarrow \quad C'_{B,n} = (1-2h)^n hC'_{A,0} + (1-201h)^n C'_{B,0}$$

$$0 < h < \tfrac{1}{201} \quad \Rightarrow \quad \text{well behaved}$$

$$\tfrac{1}{201} < h < \tfrac{2}{201} \quad \Rightarrow \quad \text{oscillatory but stable}$$

$$h > \tfrac{2}{201} \quad \Rightarrow \quad \text{oscillatory and unstable}$$

- The forward Euler method is conditionally stable
- Backward Euler (implicit method)

$$\frac{dC'_A}{dt} = -2C'_A \quad \Rightarrow \quad C'_{A,n+1} = C'_{A,n} + h(-2C'_{A,n+1})$$

$$\frac{dC'_B}{dt} = C'_A - 201C'_B \quad \Rightarrow \quad C'_{B,n+1} = C'_{B,n} + h(C'_{A,n+1} - 201C'_{B,n+1})$$

Stiff ODE System Example

- First iterative equation

$$C'_{A,n+1} = C'_{A,n} + h(-2C'_{A,n+1}) \quad \Rightarrow \quad C'_{A,n} = \frac{1}{(1+2h)^n} C'_{A,0}$$

$$h > 0 \quad \Rightarrow \quad \text{well behaved}$$

- Second iterative equation

$$C'_{B,n+1} = C'_{B,n} + h(C'_{A,n+1} - 201C'_{B,n+1}) \quad \Rightarrow \quad C'_{B,n} = \frac{1}{(1+2h)^{n+1}} hC'_{A,0} + \frac{1}{(1+201h)^n} C'_{B,0}$$

$$h > 0 \quad \Rightarrow \quad \text{well behaved}$$

- The backward Euler method is unconditionally stable

Numerical Solution of ODE Systems

In-class Exercise