STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (1)

- System of first-order ODEs:

$$\frac{d\mathbf{y}}{dt} = \frac{d}{dt}\begin{pmatrix} y^1 \\ \vdots \\ y^n \end{pmatrix} = \mathbf{y}' := \mathbf{f}(\mathbf{y},\, t) = \begin{pmatrix} f^1 \\ \vdots \\ f^n \end{pmatrix}$$

  where $y^i = i^{\text{th}}$ component of $\mathbf{y}$

- Linearize:

$$\mathbf{f}(\mathbf{y},\, t) \approx \mathbf{f}(\mathbf{y}_0,\, t) + \mathbf{J}(\mathbf{f},\, \mathbf{y}_0)(\mathbf{y} - \mathbf{y}_0)$$

  $\mathbf{J}(\mathbf{f},\, \mathbf{y}) = N \times N$ Jacobian matrix, $J^i_j = \partial f^i / \partial y^j$

- Why study a linearized system?
  - ▷ A numerical method for a system of nonlinear ODEs must at least be stable and accurate for the linearized system
  - ▷ The linearized system has the same local behavior as the nonlinear system
  - ▷ **The eigenvalues of $\mathbf{J}(\mathbf{f},\, \mathbf{y})$ determine which methods are locally most stable and accurate for a given ODE**

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (2)

References

1. C. W. Gear, *Numerical Initial Value Problems in Ordinary Differential Equations,* Prentice-Hall, 1974
2. L. Lapidus and J. H. Seinfeld, *Numerical Solutions of Ordinary Differential Equations,* Academic Press, 1971
3. G. Dahlquist and A. Björck, *Numerical Methods,* Prentice-Hall, 1974
4. R. W. Hamming, *Digital Filters,* Third Edition, Prentice-Hall, 1989

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (3)

- For stability analysis, approximate a system of nonlinear ODEs locally by

$$\frac{d\mathbf{y}}{dt} = \mathbf{M}\mathbf{y}$$

  ▷ $\mathbf{M}$ is constant or slowly varying in t

- Assume that $\mathbf{M}$ is a normal matrix (and therefore has an orthonormal basis of eigenvectors):

$$\mathbf{M}\mathbf{v}_j = \lambda_j \mathbf{v}_j$$

  ▷ $\mathbf{v}_j$ = dressed state if $\mathbf{M} = -i\mathbf{H}$

  ▷ $\mathbf{v}_i^* \cdot \mathbf{v}_j = \delta_{ij}$

  ▷ m^{th} component of $\mathbf{y}_n = y_n^m$

  ▷ 1-component vector is denoted y_n

- Exact solution of $d\mathbf{y}/dt = \mathbf{M}\mathbf{y}$ for constant $\mathbf{M}$:

$$\mathbf{y}(t) = \sum_{j=1}^{N} c_j \, e^{\lambda_j t} \, \mathbf{v}_j$$

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (4)

- Discretize by sampling at points $t = nh$
  - ▹ $\mathbf{y}_n := \mathbf{y}(nh)$
- Linear, multistep **difference equation** which approximates $d\mathbf{y}/dt = \mathbf{f}(\mathbf{y}, t) = \mathbf{y}'$:

$$\begin{aligned}\mathbf{y}_{n+1} = &\alpha_1 \mathbf{y}_n + \alpha_2 \mathbf{y}_{n-1} + \cdots + \alpha_k \mathbf{y}_{n-k+1} \\ &+ h[\beta_0 \mathbf{y}'_{n+1} + \beta_1 \mathbf{y}'_n + \cdots + \beta_k \mathbf{y}'_{n-k+1}]\end{aligned}$$

  - ▹ $\beta_0 \neq 0 \Rightarrow$ **implicit** method $\Rightarrow$ iterative solution if $\mathbf{y}'$ is nonlinear in $\mathbf{y}$
  - ▹ $\beta_0 = 0 \Rightarrow$ **explicit** method
- The difference equation above is a recursive digital filter
  - ▹ output vector = $\mathbf{y}_n$
  - ▹ input vector = $\mathbf{y}'_n$
  - ▹ Digital filtering & windowing may help ensure stability & accuracy

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (5)

- Solution of the difference equation for $\mathbf{y}' = \mathbf{M}\mathbf{y}$:

$$\mathbf{y}_n = \sum_{j=1}^{N} \{ d_1^{(j)} [\xi_1^{(j)}]^n + \cdots + d_k^{(j)} [\xi_k^{(j)}]^n \} \mathbf{v}_j$$

  ▷ $d_1^{(j)}, \ldots, d_k^{(j)}$ = real or complex constants

  ▷ $\xi_1^{(j)}, \ldots, \xi_k^{(j)}$ = roots of the **characteristic equation**

$$\begin{aligned}[\xi^{(j)}]^k =& \alpha_1 [\xi^{(j)}]^k + \alpha_2 [\xi^{(j)}]^{k-1} + \cdots + \alpha_k \\ &+ h\lambda_j \{ \beta_0 [\xi^{(j)}]^k + \beta_1 [\xi^{(j)}]^{k-1} + \cdots + \beta_k \}\end{aligned}$$

  ▷ If root $\xi_l^{(j)}$ is repeated r times: add a linear combination of $n[\xi_l^{(j)}]^n \mathbf{v}_j, \ldots, n^{r-1}[\xi_l^{(j)}]^n \mathbf{v}_j$ to above solution for $\mathbf{y}_n$

- **The characteristic roots determine the local stability and accuracy of the finite-difference method**

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (6)

- The k initial vectors $\mathbf{y}_0$, $\mathbf{y}_1$, . . . , $\mathbf{y}_{k-1}$ determine the constants $d_l^{(j)}$ which appear in the analytical solution of the difference equation
- Assume that:
  - ▷ The characteristic equation has k distinct roots
  - ▷ We are given (by some other method) $\mathbf{y}_n = \kappa_n^{(j)} \mathbf{v}_j$ for $n = 0, \ . \ . \ . \ , k - 1$ (usually we want the principal root $\Rightarrow j = 1$)
- The k equations

$$\kappa_n^{(j)} = \sum_{l=1}^{k} d_l^{(j)} [\xi_l^{(j)}]^n$$

for $n = 0, \ldots, k - 1$ are a non-singular linear system which can be solved for $d_l^{(j)}$ in terms of $\kappa_n^{(j)}$

- In practice one just computes $\mathbf{y}_0$, $\mathbf{y}_1$, . . . , $\mathbf{y}_{k-1}$ by a one-step method

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (7)

- Basic concepts of stability of a finite-difference method
  - ▷ The **principal characteristic root** approximates the exact solution:
    $$[\xi_1^{(j)}]^n \approx e^{nh\lambda_j}$$
  - ▷ $\xi_2^{(j)}, \ldots, \xi_k^{(j)}$, which occur whenever $k > 1$, are **parasitic roots**
  - ▷ **Relative stability:**
    $$|\xi_1| \geq |\xi_l|$$
    for $l = 2, \ldots, k \Rightarrow$ the parasitic part of the solution never exceeds the principal part
  - ▷ **Absolute stability,**
    $$|\xi_l| \leq 1 \quad (l = 1, \ldots, k),$$
    is necessary when the exact solution of the ODE is damped or has a constant norm

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (8)

- Basic concepts pertaining to the accuracy of a finite-difference method:
  - ▷ **Local truncation error:**

    $$T(\{\alpha\};\{\beta\};h\lambda) = \xi_1 - e^{h\lambda}$$

  - ▷ The **order** of the **local discretization error**

    $$L_h[y(t)] = \sum_{l=0}^{k} \left[\alpha_l y(t - lh) + h\beta_l y'(t - lh)\right]$$

    (where $\alpha_0 = -1$) is the largest r such that

    $$L_h[y(t)] \sim O(h^{r+1})$$

    for every y with $r + 1$ continuous derivatives
  - ▷ A finite-difference method is **consistent** with an ODE of order p if the order of L_h is at least p.
  - ▷ Consistency $\Rightarrow$ L_h approaches the correct differential operator as $h \to 0$.

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (9)

- A quantitative expression for the effect of the finite-difference operator:
  - ▷ Apply Taylor's theorem to $L_h[y(t)]$:

$$L_h[y(t)] = \sum_{q=0}^{r+1} C_q h^q y^{[q]}(t) + O(h^{r+2})$$

$$C_0 = \sum_{l=0}^{k} \alpha_l$$

$$C_q = \sum_{l=0}^{k} \left[\frac{(-l)^q}{q!} \alpha_l + \frac{(-l)^{q-1}}{(q-1)!} \beta_l \right] \quad (q > 0)$$

  - ▷ If the method is consistent with a first-order ODE, then

$$C_0 = 0, \quad C_1 = 0$$

  - ▷ If the order of the finite-difference operator L_h is r, then

$$C_0 = C_1 = \cdots = C_r = 0$$

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (10)

- A quantitative expression for the local truncation error:
  - ▷ If $y' = \lambda y$ ($\Rightarrow$ exact solution is $e^{\lambda t}$) and if L_h is of order r, then

$$\begin{aligned} L_h[e^{\lambda t}] &= e^{\lambda(t-hk)}\phi(e^{h\lambda}) \\ &= C_{r+1}(h\lambda)^{r+1} + O(h^{r+2}) \end{aligned}$$

$$\phi(e^{h\lambda}) = \sum_{l=0}^{k} (\alpha_l + h\lambda\beta_l) \left[e^{h\lambda}\right]^{k-l}$$

$$\Rightarrow \phi(e^{h\lambda}) = C_{r+1}(h\lambda)^{r+1} + O(h^{r+2})$$

$$\Rightarrow \xi_1 = e^{h\lambda} - \frac{C_{r+1}(h\lambda)^{r+1}}{\sum_{l=0}^{k} \beta_l}$$

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (11)

- Common methods for ODEs which are *not* discretized PDEs:

Method	k	E	Type	Stiff Eqs?
Runge-Kutta	1	≥ 4	ex.	no
Adams-Bashforth (P)	≥ 4	1	ex.	no
Adams-Moulton (C)	≥ 4	1	im.	no
Gear	≥ 4	1	im.	yes

k = no. of steps, E = no. of evaluations of right-hand side per step, "Type" = explicit or implicit

- Common methods for discretized PDEs:

Method	k	E	Type	Stiff Eqs?
Midpoint (P)	2	1	ex.	no
Trapezoidal (C)	1	1	im.	no
Backward Euler	1	1	im.	yes

- In the above, P means a predictor method and C means a corrector method. The usual usage of a predictor-corrector set is PECE (predict, evaluate y', correct, evaluate y').

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (12)

- The **minimax approach** to designing a finite-difference method:
  - ▷ The **maximum local truncation error** is

    $$T_{\max}(\{\alpha\};\{\beta\};S) = \max_{h\lambda\in S} |T(\{\alpha\};\{\beta\};h\lambda)|$$

    where S is the region of stability (or some useful subset)
  - ▷ Choose the coefficients $\{\alpha\};\{\beta\}$ in L_h to minimize $T_{\max}(\{\alpha\};\{\beta\};S)$:

    $$T_{\text{minimax}}(S) = \min_{\{\alpha\};\{\beta\}} T_{\max}(\{\alpha\};\{\beta\};S)$$
  - ▷ Implementation of the minimax principle:
    - ◦ Expand the local truncation error in Chebyshev polynomials and make the first N Chebyshev coefficients vanish
    - ◦ Perform a numerical minimization