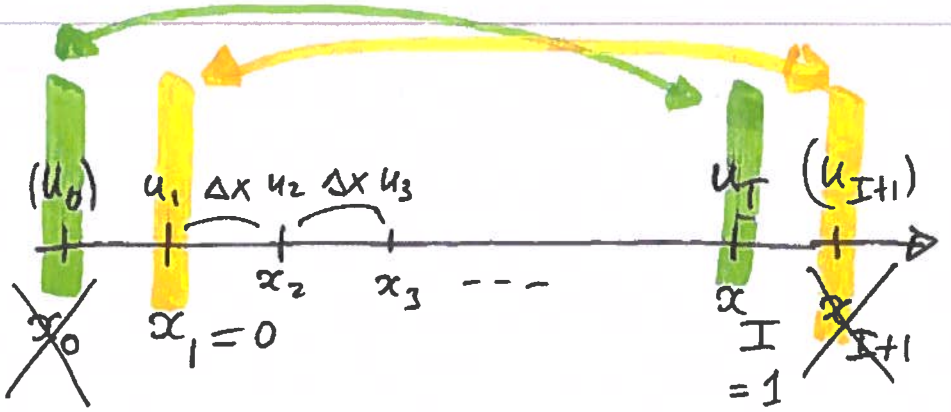
Finite Difference Matrices (FD)



periodic boundary conditions

Identify: $\boxed{u_0 = u_I}$ and $\boxed{u_{I+1} = u_1}$

A central approximation for $\frac{\partial u}{\partial x}$ at $x = x_i$:

$$\boxed{\frac{u_{i+1} - u_{i-1}}{2\Delta x}}$$

$i = 2, 3, \ldots, I-1$

$i=1 \rightarrow u_0$ X

$i=I \rightarrow u_{I+1}$ X

Define the solution vector:

$$\vec{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{I-1} \\ u_I \end{pmatrix} \Big\} \text{length } I$$

$$\frac{u_2 - u_I}{2\Delta x} \qquad (-1) \cdot u_I$$

$$\frac{u_{I+1} - u_{I-1}}{2\Delta x} \qquad (1) \cdot u_1$$

$$\Rightarrow \text{matrix } D_{1c} = \frac{1}{2\Delta x} \begin{pmatrix} 0 & 1 & & & & -1 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{pmatrix}$$

$I \times I$ matrix

$\left(A^T = A \text{ symm.}\right)$

skew-symmetric $\left(A^T = -A\right)$ $\Rightarrow$ eigenvalues $\lambda \in i\mathbb{R} \subset \mathbb{C}$

property

$$D_{1c} = \frac{1}{2}\left(D_{1+} + D_{1-}\right) = \frac{1}{2\Delta x}\left\{\begin{pmatrix} -1 & 1 & & 0 \\ & -1 & 1 & \\ & & \ddots & \ddots \\ & 0 & & -1 & 1 \\ 1 & & & & -1 \end{pmatrix} + \begin{pmatrix} 1 & & & & -1 \\ -1 & 1 & & 0 & \\ & -1 & 1 & & \\ & 0 & \ddots & \ddots & \\ 0 & & & -1 & 1 \end{pmatrix}\right\}$$

"upwind" $\dfrac{u_{i+1} - u_i}{\Delta x} \sim \left.\dfrac{\partial u}{\partial x}\right|_{x=x_i}$

$\dfrac{u_i - u_{i-1}}{\Delta x}$ "downwind" $\sim \left.\dfrac{\partial u}{\partial x}\right|_{x=x_i}$

periodic boundary condition(s)

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matrix $D_2 = D_{1+} D_{1-}$ CHECK!

$$= \frac{1}{(\Delta x)^2}\begin{pmatrix} \circ & & & \circ \\ & 1\,-2\,1 & 0 & \\ & 0 & \ddots & \\ & & 1\,-2\,1 & \\ \circ & & & \circ \end{pmatrix} \sim \frac{\partial^2 u}{\partial x^2} \text{ at } x = x_i$$

eigenvalues $\lambda \in \mathbb{R}^- \subset \mathbb{C}$

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matrix $D_3 = D_2 D_{1c} = D_{1+} D_{1-} D_{1c} = \dfrac{1}{(\Delta x)^3}\left(\; - - - \;\right)$

$\sim \dfrac{\partial^3 u}{\partial x^3}$ at $x = x_i$

check! (exercise/Matlab)

eigenvalues $\lambda \in i\mathbb{R} \subset \mathbb{C}$

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matrix $D_4 = D_2^2 = D_{1+} D_{1-} D_{1+} D_{1-} = \dfrac{1}{(\Delta x)^4}\left(\; - - - \;\right)$

$\sim \dfrac{\partial^4 u}{\partial x^4}$ at $x = x_i$

eigenvalues $\lambda \in \mathbb{R}^+ \subset \mathbb{C}$

etcetera!!!

Square roots of matrices

Definition:

matrix A , $B = \sqrt{A}$ if $B.B = \sqrt{A}\sqrt{A} = A$

A matrix can have several (many) square roots

Examples 1) $A = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ (identity matrix)

has infinitely many square roots:

$$\begin{pmatrix} 1 & 0 \\ 0 & \pm 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & \pm 1 \end{pmatrix}, \frac{1}{c}\begin{pmatrix} b & a \\ a & -b \end{pmatrix}, \frac{1}{c}\begin{pmatrix} b & -a \\ -a & -b \end{pmatrix},$$

$$\frac{1}{c}\begin{pmatrix} -b & a \\ a & b \end{pmatrix}, \frac{1}{c}\begin{pmatrix} -b & -a \\ -a & b \end{pmatrix}$$

!

with $a^2 + b^2 = c^2$

2) a positive semi-definite matrix ($\overset{\text{eigenvalues}}{\lambda \geq 0}$)
has only one positive semi-definite square root:
"principal square root"

3) a 2×2 matrix with eigenvalues $\lambda_1 \neq 0$, $\lambda_2 \neq 0$
and $\lambda_1 \neq \lambda_2$
has four square roots

4) a general $n \times n$ matrix with $\lambda_1 \neq \lambda_2 \neq \cdots \neq \lambda_n \neq 0$
has 2^n square roots

5) $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ has no square roots .... ETCETERA!

Matrix - Newton

remember : $\boxed{x^2 - a = 0} \longrightarrow \begin{cases} x_0 = a \\ x_{k+1} = \frac{1}{2}\left(x_k + \frac{a}{x_k}\right), \quad k = 0, 1, 2, \ldots \\ \quad\;\;\; = \frac{1}{2}\left(x_k + x_k^{-1} a\right) \end{cases}$

check $\rightarrow$ $= x_k - \dfrac{x_k^2 - a}{2x_k}$

Newton-Raphson to find $\pm\sqrt{a}$

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matrix variant of this iteration method :

$$\boxed{X^2 - A = 0} \rightarrow \begin{cases} X_0 = A \\ \boxed{X_{k+1} = \frac{1}{2}\left(X_k + X_k^{-1} A\right)} \end{cases} \quad k = 0, 1, 2, \ldots$$

$$0 = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ominus & \vdots \\ 0 & \cdots & 0 \end{pmatrix}$$

"matrix_Newton" for square roots of matrices.

Theorem : if $\boxed{\frac{1}{2}\left|1 - \left(\frac{\lambda_j}{\lambda_i}\right)^{1/2}\right| \leq 1 \quad \forall i, j}$ ($n \times n$ matrix)

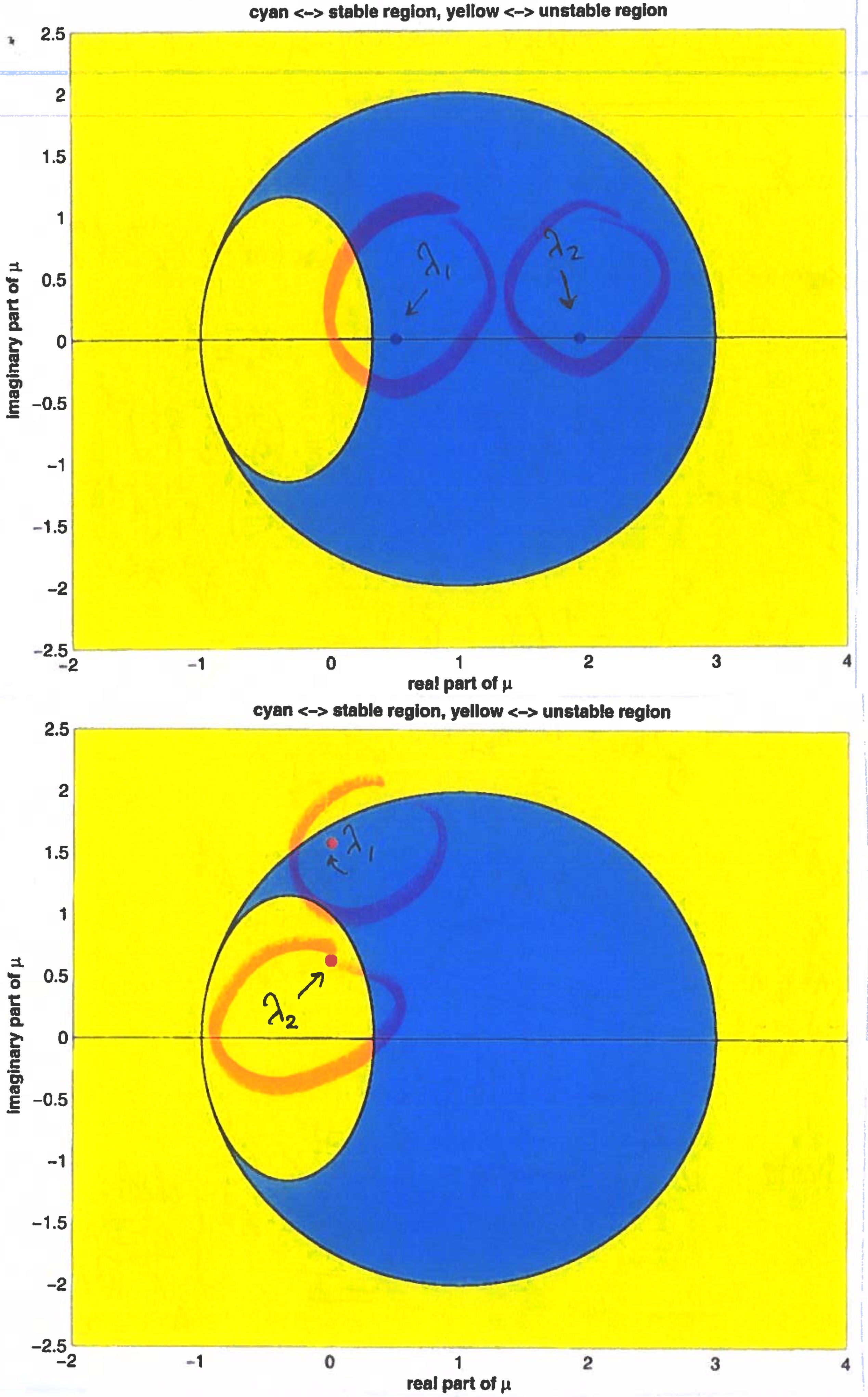
(Higham, 1986)

λ's are eigenvalues of A

then matrix_Newton is stable (small roundoff errors won't be amplified)

(otherwise, it may be unstable)

for a 2x2 matrix this condition can be visualized:



Stabilizing matrix Newton → "Denman-Beaver"

$$X_{k+1} = \frac{1}{2}\left(X_k + \underline{X_k^{-1} A}\right), \quad X_0 = A$$

"symmetrize" the iteration : ? or $A X_k^{-1}$? (may be different!)

1) $$X_{k+1} = \frac{1}{2}\left(X_k + \underline{A^{\frac{1}{2}} X_k^{-1} A^{\frac{1}{2}}}\right), \quad X_0 = A$$

Define : 2) $Y_k = A^{-\frac{1}{2}} X_k A^{-\frac{1}{2}}$ $\Rightarrow$ $Y_k^{-1} = \left(A^{-\frac{1}{2}} X_k A^{-\frac{1}{2}}\right)^{-1}$ 3)

$$= \left(A^{-\frac{1}{2}}\right)^{-1} X_k^{-1} \left(A^{-\frac{1}{2}}\right)^{-1}$$

$$= A^{\frac{1}{2}} X_k^{-1} A^{\frac{1}{2}}$$

5) then : $X_{k+1} = \frac{1}{2}\left(X_k + Y_k^{-1}\right)$

and 6) $Y_{k+1} = A^{-\frac{1}{2}} X_{k+1} A^{-\frac{1}{2}}$

$$= A^{-\frac{1}{2}} \cdot \frac{1}{2}\left(X_k + Y_k^{-1}\right) A^{-\frac{1}{2}}$$

$$= \frac{1}{2} \underbrace{A^{-\frac{1}{2}} X_k A^{-\frac{1}{2}}}_{= Y_k} + \frac{1}{2} \underbrace{A^{-\frac{1}{2}} Y_k^{-1} A^{-\frac{1}{2}}}_{= X_k^{-1}}$$

7)

$$= \frac{1}{2}\left(Y_k + X_k^{-1}\right)$$

1)

$A^{\frac{1}{2}} Y_k = X_k A^{-\frac{1}{2}}$

$A^{\frac{1}{2}} Y_k A^{\frac{1}{2}} = X_k \underbrace{A^{-\frac{1}{2}} A^{\frac{1}{2}}}_{= I}$

$\Rightarrow X_k^{-1} = \left(A^{\frac{1}{2}} Y_k A^{\frac{1}{2}}\right)^{-1}$

$= A^{-\frac{1}{2}} Y_k^{-1} A^{-\frac{1}{2}}$

Note : 8) $Y_0 \overset{?}{=} I$ satisfies : $Y_0 = A^{-\frac{1}{2}} X_0 A^{-\frac{1}{2}}$

$= A^{-\frac{1}{2}} A A^{-\frac{1}{2}}$

9) $= I$

check : 10) $A^{\frac{1}{2}} I A^{\frac{1}{2}} \overset{?}{=} A$

$A^{\frac{1}{2}} A^{-\frac{1}{2}} A A^{-\frac{1}{2}} A^{\frac{1}{2}}$

$= I A I$

$= A$

$\Rightarrow$ Denman-Beaver, 1976

(stable iterations, but twice as expensive)

$$\begin{cases} X_{k+1} = \frac{1}{2}(X_k + Y_k^{-1}), & X_0 = A \\ Y_{k+1} = \frac{1}{2}(Y_k + X_k^{-1}), & Y_0 = I \end{cases}$$

$k = 0, 1, 2, \ldots$

For checking the convergence, one could use the Frobenius-norm of a matrix: $\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} |a_{ij}|^2}$

(in Matlab: norm(A, 'fro'))

and check $\|X_{k+1} - X_k\|_F$, for example.

[Matlab $\sqrt{A}$: sqrtm.m $\rightsquigarrow$ sqrt(A)].