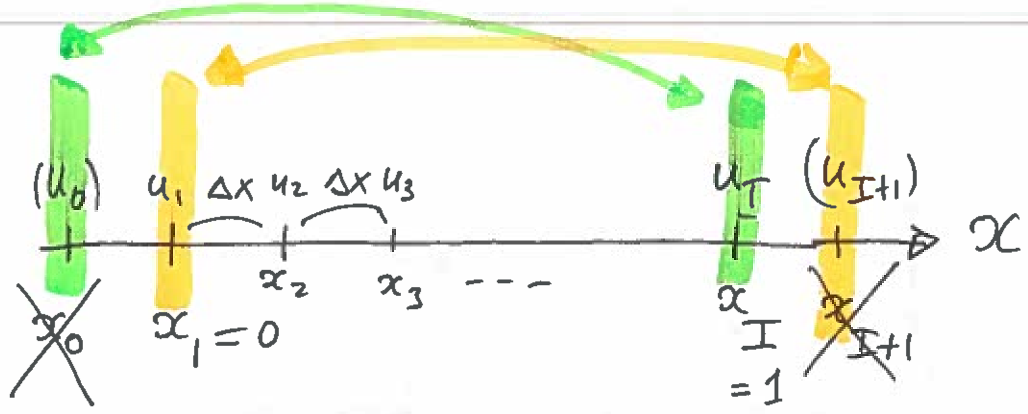
Finite Difference Matrices (FD)



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 $x = x_i$:

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

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

$i=1 \to u_0$ X

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

Define the solution vector:

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

$\frac{u_2 - u_I}{2\Delta x}$

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

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

skew-symmetric $\Rightarrow$ eigenvalues $\lambda \in i\mathbb{R} \subset \mathbb{C}$

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

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

D_{1-}: $\dfrac{u_i - u_{i-1}}{\Delta x}$ "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!

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

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

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matrix $D_3 = D_2 D_{1c} = D_{1+} D_{1-} D_{1c} = \dfrac{1}{(\Delta x)^3}\begin{pmatrix} \cdots \end{pmatrix}$

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

check! (exercise/Matlab)

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

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matrix $D_4 = D_2^2 = D_{1+} D_{1-} D_{1+} D_{1-} = \dfrac{1}{(\Delta x)^4}\begin{pmatrix} \cdots \end{pmatrix}$

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

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

etcetera!!!

Square roots of matrices

Definition:

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

A matrix can have several (many) square roots

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

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

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

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matrix variant of this iteration method:

$\boxed{X^2 - A = \mathbb{O}}$ $\longrightarrow$ $\begin{cases} X_0 = A \\ \boxed{X_{k+1} = \frac{1}{2}\left(X_k + X_k^{-1} A\right)} \end{cases}$

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

$$\mathbb{O} = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \Theta & \vdots \\ 0 & \cdots & 0 \end{pmatrix}$$

"matrix_Newton" for square roots of matrices.

<u>Theorem</u> : 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)

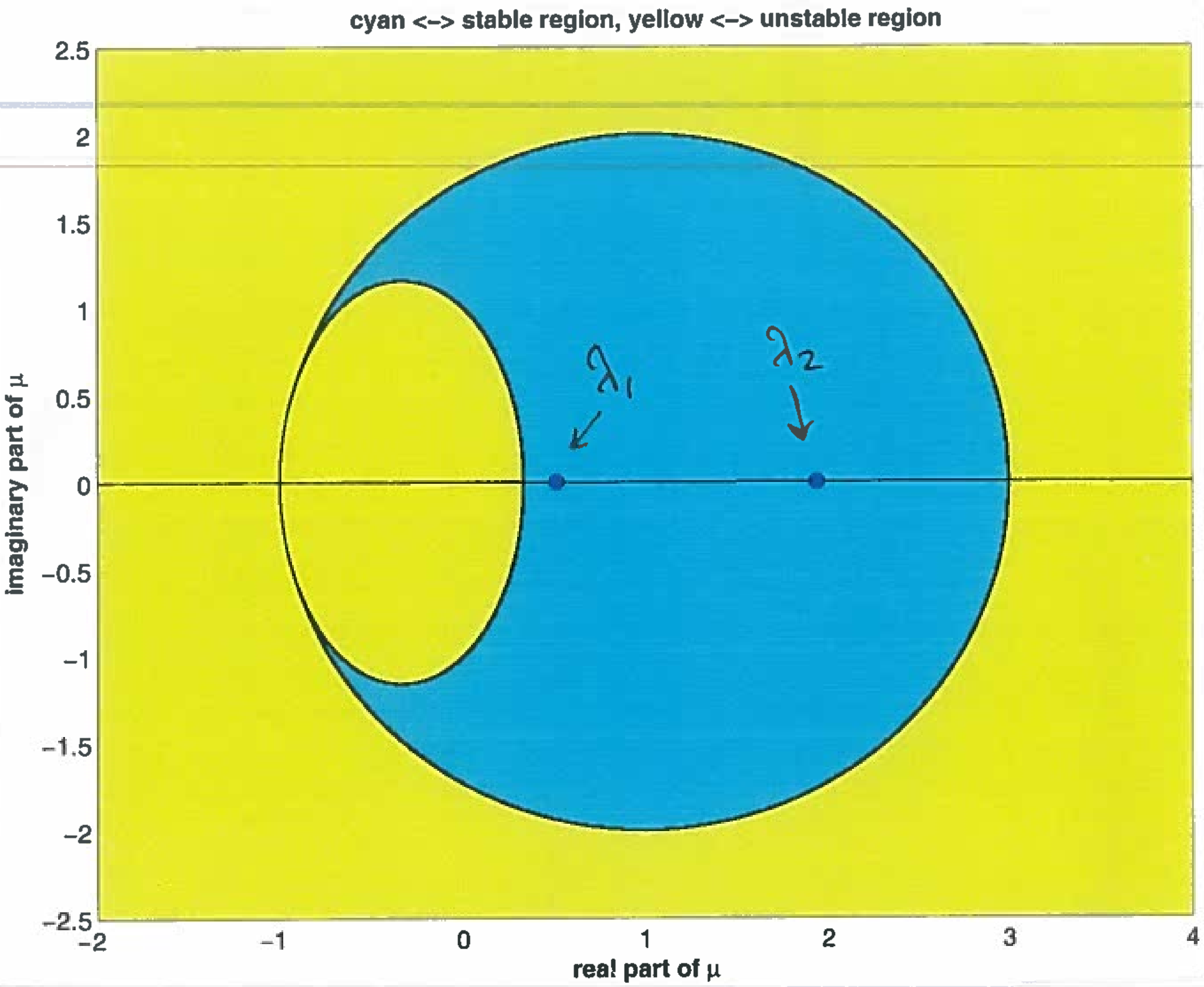
[λ's are eigenvalues of A]

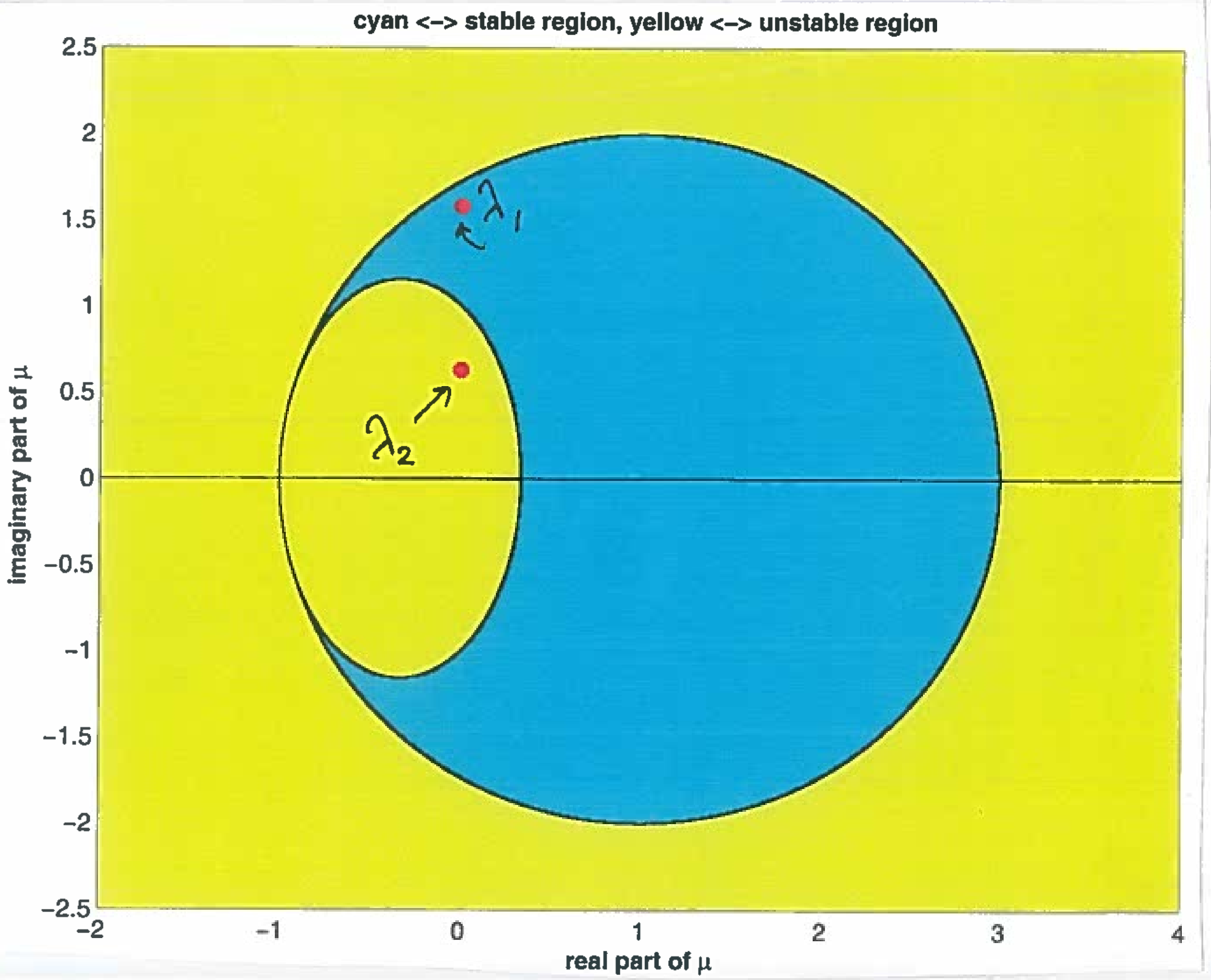
then matrix_Newton is <u>stable</u>

(small roundoff errors won't be amplified)

(otherwise, it <u>may</u> be unstable)

for a 2x2 matrix this condition can be visualized:





Stabilizing matrix Newton → "Denman-Beavers"

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

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

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

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

6)
$$= A^{-\frac{1}{2}} \cdot \frac{1}{2}\left(X_k + Y_k^{-1}\right) A^{-\frac{1}{2}}$$

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

4)
$$A^{\frac{1}{2}} Y_k = X_k A^{-\frac{1}{2}}$$
$$A^{\frac{1}{2}} Y_k A^{\frac{1}{2}} = X_k$$
$$\Rightarrow X_k^{-1} = \left(A^{\frac{1}{2}} Y_k A^{\frac{1}{2}}\right)^{-1}$$
$$= A^{-\frac{1}{2}} Y_k^{-1} A^{-\frac{1}{2}}$$

7)

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

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) $\underbrace{A^{\frac{1}{2}} I A^{\frac{1}{2}}}_{A} \overset{?}{=} A^{\frac{1}{2}} A^{-\frac{1}{2}} A A^{-\frac{1}{2}} A^{\frac{1}{2}}$

$$= I A I$$
$$= A$$

$\Rightarrow$ Denman-Beavers, 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)].