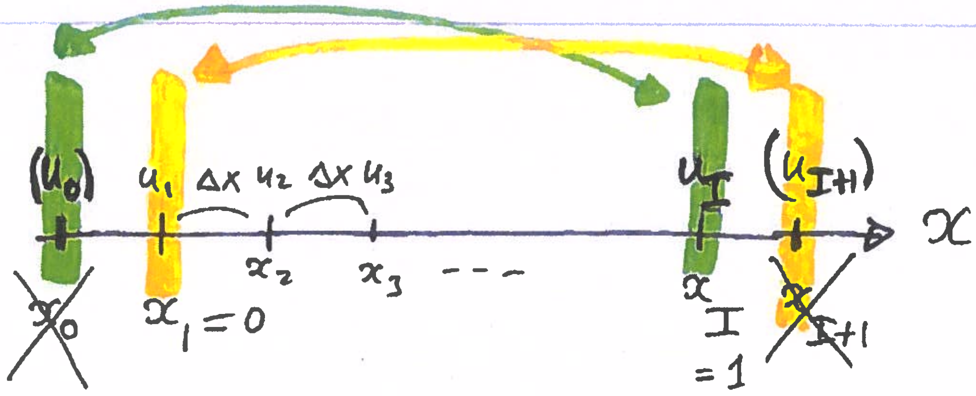
Finite Difference Matrices (FD)



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 $x = x_i$:

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

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

$i=1 \to u_0$ ✗

$i=I \to u_{I+1}$ ✗

Define the solution vector:

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

$\frac{u_2 - u_I}{2\Delta x}$ $\quad (-1)\, u_I$

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

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

$I \times I$ matrix

($A^T = A$ symm.)

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

property

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

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

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

periodic boundary condition(s)

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

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

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

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

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

check! (exercise/Matlab)

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

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

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

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

etcetera!!!

Square roots of matrices

<u>Definition:</u>

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

A matrix can have <u>several (many)</u> square roots

<u>Example</u> 1) $A = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ (identity matrix)

has <u>infinitely many</u> 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 <u>semi</u>-definite matrix (eigenvalues $\lambda \geq 0$)
<u>has only one</u> positive semi-definite square root:
<u>"principal square root"</u>

3) a 2×2 matrix with eigenvalues $\lambda_1 \neq 0$, $\lambda_2 \neq 0$ and $\lambda_1 \neq \lambda_2$
has <u>four</u> 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 <u>no</u> square roots ... ETCETERA!

Matrix-Newton

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

check

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

matrix variant of this iteration method:

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

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

"matrix-Newton" for square roots of matrices.

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

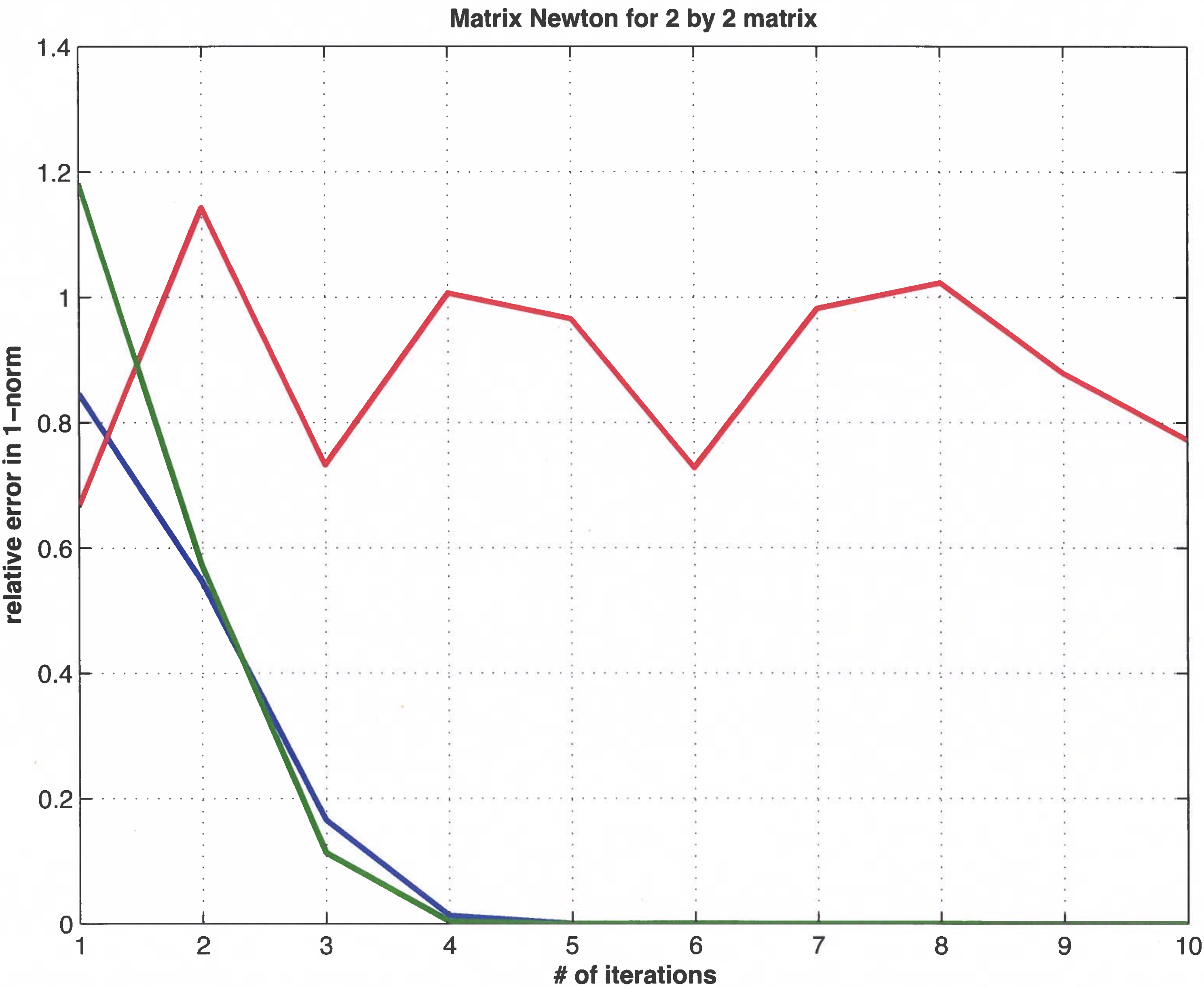
(Higham, 1986)

then matrix-Newton is stable

(small roundoff errors won't be amplified)

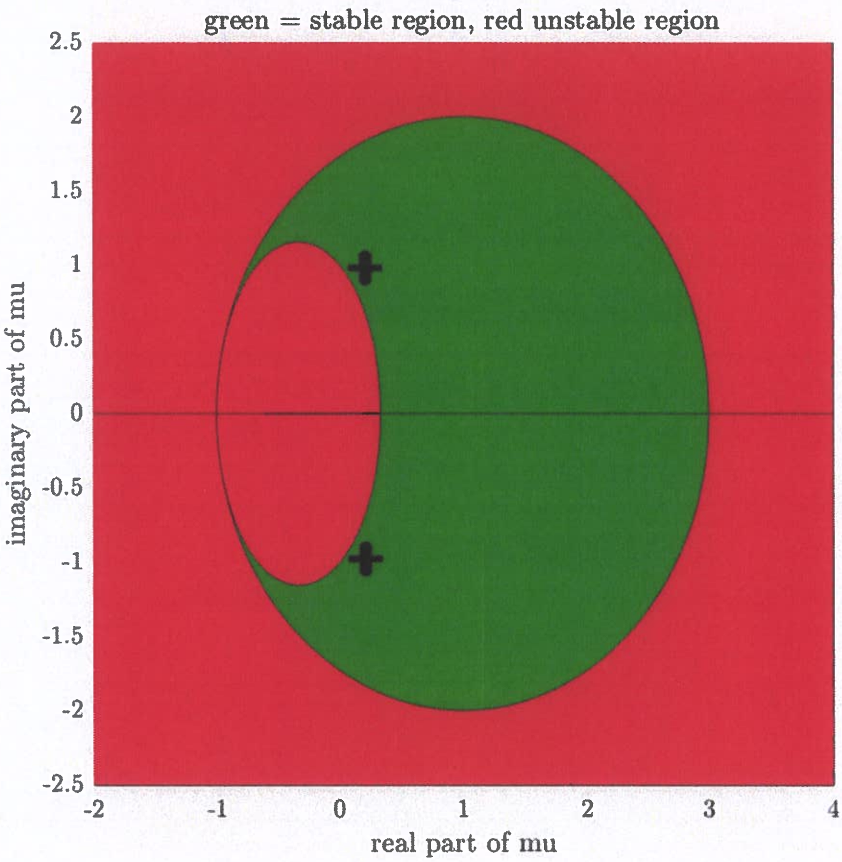
(otherwise, it may be unstable)

[λ's are eigenvalues of A]

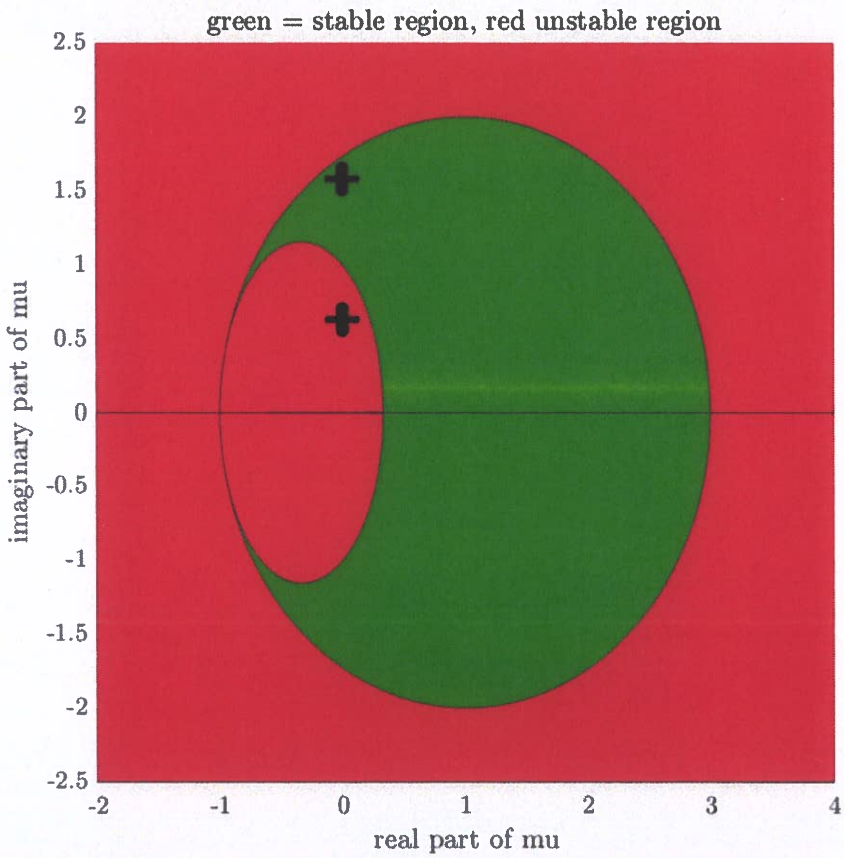


Matrix Newton for 2 by 2 matrix
relative error in 1−norm
# of iterations
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1
2
3
4
5
6
7
8
9
10

6



green = stable region, red unstable region
imaginary part of mu
real part of mu
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-2
-1
0
1
2
3
4



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real part of mu
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2
1.5
1
0.5
0
-0.5
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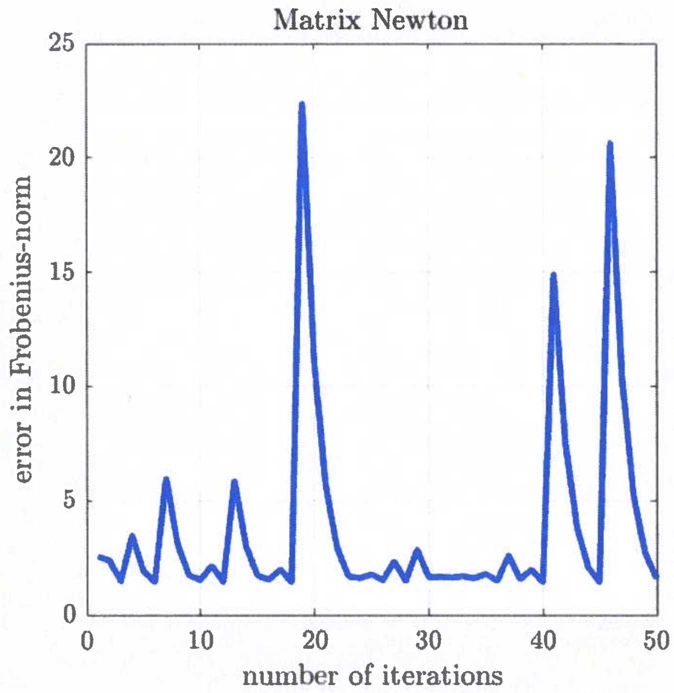
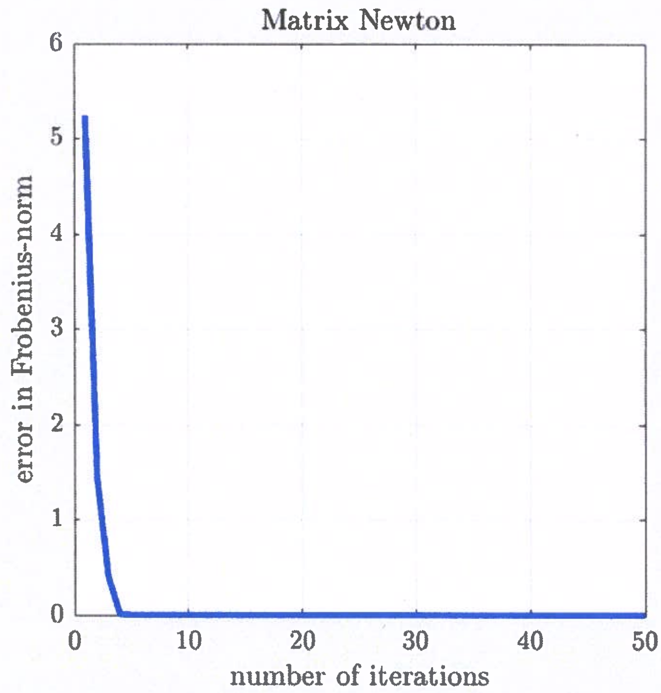
-1.5
-2
-2.5
-2
-1
0
1
2
3
4

7



Matrix Newton
error in Frobenius-norm
number of iterations



Matrix Newton
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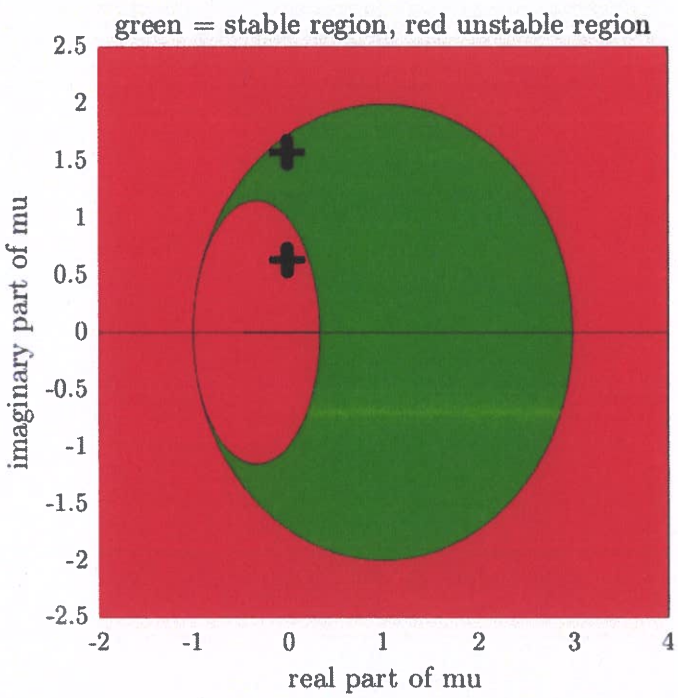
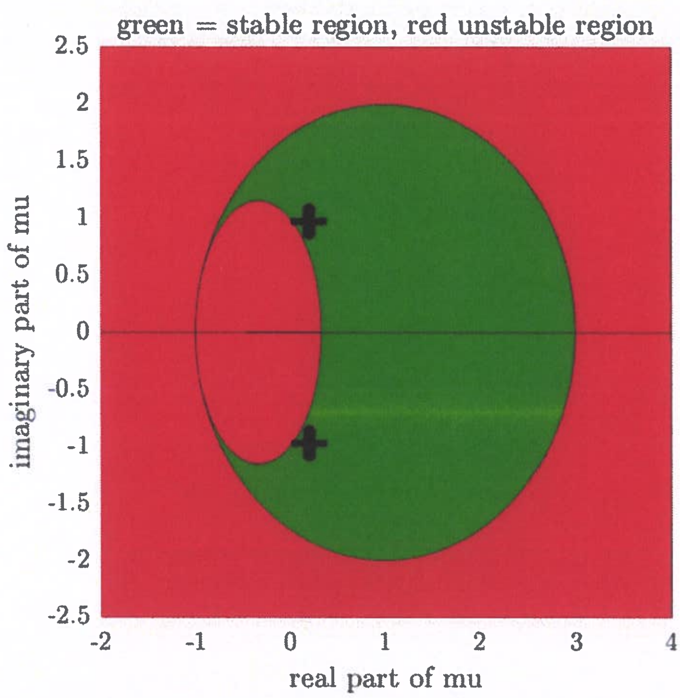


green = stable region, red unstable region
imaginary part of mu
real part of mu



green = stable region, red unstable region
imaginary part of mu
real part of mu

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Matrix-Newton:

instead of A, to explain the difference

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

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

if A symmetric positive-definite, then 1) & 2) are equivalent

if A not symmetric, but positive-definite, then:

> 1) and 2) have different stability properties, different error-propagation, different iteration steps.

Example: $A = \begin{pmatrix} 4 & 1 \\ 0 & 1 \end{pmatrix}$, $X_0 = I$ (not symmetric, positive-definite!)

1), 2) $\rightarrow X_1 = \frac{1}{2}(I + A) = \begin{pmatrix} \frac{5}{2} & \frac{1}{2} \\ 0 & 1 \end{pmatrix}$

$X_1^{-1} = \begin{pmatrix} \frac{2}{5} & -\frac{1}{5} \\ 0 & 1 \end{pmatrix}$

1) $\rightarrow X_1^{-1} A = \begin{pmatrix} \frac{8}{5} & \frac{1}{5} \\ 0 & 1 \end{pmatrix} \Rightarrow X_2 = \begin{pmatrix} \frac{205}{100} & \frac{35}{100} \\ 0 & 1 \end{pmatrix}$

2) $\rightarrow A X_1^{-1} = \begin{pmatrix} \frac{8}{5} & \frac{3}{5} \\ 0 & 1 \end{pmatrix} \Rightarrow X_2 = \begin{pmatrix} \frac{205}{100} & \frac{55}{100} \\ 0 & 1 \end{pmatrix}$

$\Rightarrow X_2^{(1)} \neq X_2^{(2)}$

etcetera for $X_3, X_4, \ldots$ (in the limit $\rightarrow \sqrt{A}$)

Stabilizing matrix-Newton ⇝ "Denman-Beavers"

$$\begin{cases} X_0 = A \\ X_{k+1} = \frac{1}{2}(X_k + X_k^{-1}A), \; k=0,1,2,\dots \end{cases}$$

1) "symmetrize" the iterations: $\begin{cases} X_0 = A \\ X_{k+1} = \frac{1}{2}(X_k + A^{\frac{1}{2}} X_k^{-1} A^{\frac{1}{2}}), \; k=0,1,2,\dots \end{cases}$

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

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

$$\Rightarrow X_{k+1} = \frac{1}{2}(X_k + Y_k^{-1}) \quad \boxed{*}$$

$$Y_{k+1} = A^{-\frac{1}{2}} \frac{1}{2}(X_k + Y_k^{-1}) A^{-\frac{1}{2}} = \frac{1}{2} \underbrace{A^{-\frac{1}{2}} X_k A^{-\frac{1}{2}}}_{=Y_k} + \frac{1}{2} \underbrace{A^{-\frac{1}{2}} Y_k^{-1} A^{-\frac{1}{2}}}_{=X_k^{-1}} = \frac{1}{2}(Y_k + X_k^{-1}) \quad \boxed{**}$$

3) note: $A^{\frac{1}{2}} Y_k = X_k A^{-\frac{1}{2}} \Rightarrow A^{\frac{1}{2}} Y_k A^{\frac{1}{2}} = X_k$

$$\Downarrow$$

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

4) note: $Y_0 = I$, since $Y_0 = A^{-\frac{1}{2}} X_0 A^{-\frac{1}{2}} = A^{-\frac{1}{2}} A A^{-\frac{1}{2}} = I$

check: $A = A^{\frac{1}{2}} I A^{\frac{1}{2}}$

and $A = IAI = A^{\frac{1}{2}} \underbrace{A^{-\frac{1}{2}} A A^{-\frac{1}{2}}}_{} A^{\frac{1}{2}}$ ($=I$, $=I$)

⇒ **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')) help norm

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

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

help sqrtm

! sqrt(A) takes square roots of each element of A ("componentwise")
↑ ↑ matrix

Let A be a $n \times n$ symmetric positive-definite matrix

Then a) $\exists!$ symmetric positive-definite matrix X such that $X^2 = A$ $\quad (X = \sqrt{A})$

b) $\begin{cases} X_0 = I \\ X_{k+1} = \frac{1}{2}\left(X_k + A X_k^{-1}\right), k = 0, 1, 2, \dots \end{cases}$

$\Rightarrow \lim_{k\to\infty} X_k \to \sqrt{A}$

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

matrix-ODE : $\begin{cases} \ddot{X}(t) + A X(t) = 0, t > 0 \\ X(0) = C_1, \dot{X}(0) = C_2 \end{cases}$

element-wise!

If A is symmetric positive-definite, then:

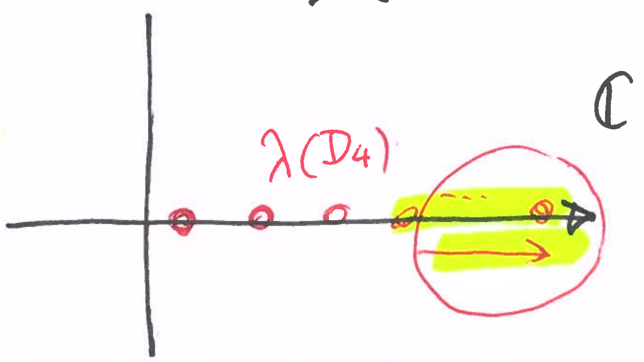
$$X(t) = C_1 \cos(t\sqrt{A}) + C_2 \sqrt{A}^{-1} \sin(t\sqrt{A})$$

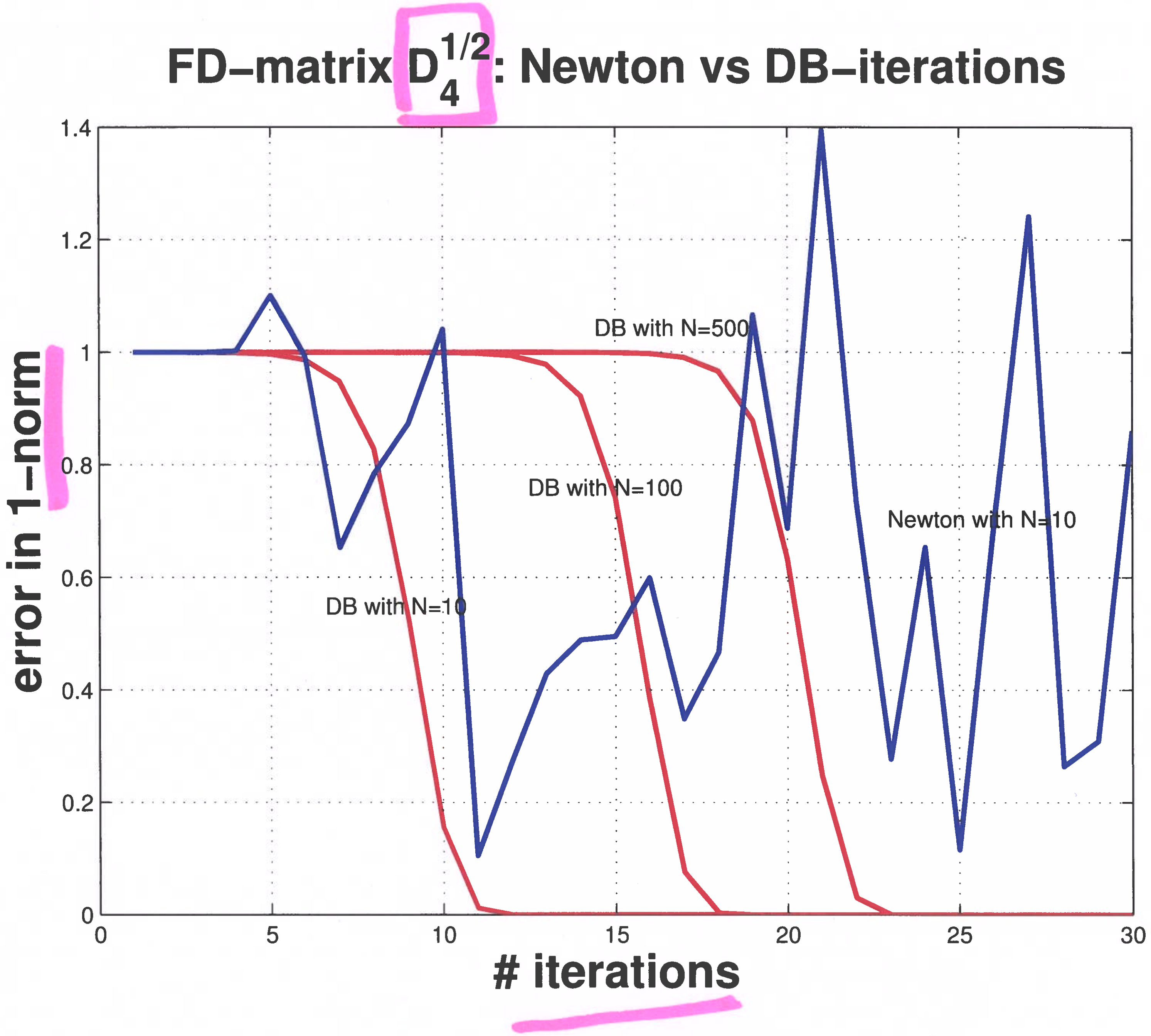
$\boxed{\text{matrix } D_4} \sim \frac{d^4}{dx^4}$: $D_4 = D_2^2 = \frac{1}{(\Delta x)^4}\left(\quad \cdots \quad \right)$

symmetric positive-definite (λ's >0)

Exercise 5a

$\sqrt{D_4}$?
- matrix-Newton (convergence ....?)
- Denman-Beavers (dependence on Δx?)




FD–matrix $D_4^{1/2}$: Newton vs DB–iterations
error in 1–norm
iterations
DB with N=500
DB with N=100
DB with N=10
Newton with N=10
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
5
10
15
20
25
30