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Convergence and Stability of Iterations for Matrix Functions

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THE NUMERICAL STABILITY
OF
TWO MATRIX NEWTON ITERATIONS

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Numerical Analysis Report available on request.

Iteration (I)

$$Y_{k+1} = \frac{1}{2}\left(Y_k + Y_k^{-1}A\right); \quad Y_0 = A \text{ nonsingular.}$$

Assume: $\lambda_i(A) \notin \mathbb{R}^-$ and $\det(Y_k) \neq 0$ for all k.

Then $Y_k \to A^{\frac{1}{2}}$ quadratically as $k \to \infty$ where $A^{\frac{1}{2}}$ = unique square root of A for which every eigenvalue has positive real part.

Overview

Iterations $X_{k+1} = g(X_k)$ for computing $\sqrt{A}$, $\mathrm{sign}(A)$, $\sqrt[p]{A}$ (+ unitary polar factor).

- **Avoid Jordan form** in convergence proofs.
  Reduce to: **Does G^k tend to zero?**
- Can reduce stability to: **Is H^k bounded?**
- **Connections**: **matrix sign** and **matrix square root**.
- **Role of commutativity**.
- **Rule of thumb** for deriving stable iterations.

10 Digit Algorithm

```
%cuberootA2    Cube root of matrix  by Newton iteration.
%              Cf. cuberootA, Ten Digit Algorithms, LNT.

p = 3; % p'th root.  p can be arbitrary.
n = 4;
A = rand(n)/sqrt(n) + 3*eye(n)
X = eye(n); M = A;
for i=1:10
    W = ((p-1)*eye(n) + M)/p;
    X = X*W;
    M = W^(-p)*M;
end
X
res = norm(A-X^p)/norm(A)
```

```
res =
  3.4719e-016
```

Matrix Square Root

- X is a square root of $A \in \mathbb{C}^{n \times n} \iff X^2 = A$.
- Number of square roots may be zero, finite or infinite.

For A with no eigenvalues on $\mathbb{R}^- = \{x \in \mathbb{R} : x \le 0\}$, denote by $A^{1/2}$ the **principal square root**: unique square root with spectrum in open right half-plane.

Matrix Sign Function

Let $A \in \mathbb{C}^{n\times n}$ have **no pure imaginary eigenvalues** and let $A = ZJZ^{-1}$ be a Jordan canonical form with

$$J = \begin{array}{c} \\ p \\ q \end{array}\!\!\begin{array}{c} \begin{array}{cc} p & q \end{array} \\ \begin{bmatrix} J_1 & 0 \\ 0 & J_2 \end{bmatrix} \end{array}, \qquad \Lambda(J_1) \in \text{LHP}, \quad \Lambda(J_2) \in \text{RHP}.$$

$$\operatorname{sign}(A) = Z \begin{bmatrix} -I_p & 0 \\ 0 & I_q \end{bmatrix} Z^{-1}.$$

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$$\operatorname{sign}(A) = Z \begin{bmatrix} -I_p & 0 \\ 0 & I_q \end{bmatrix} Z^{-1}.$$

$$\operatorname{sign}(A) = A(A^2)^{-1/2}.$$

$$\operatorname{sign}(A) = \frac{2}{\pi} A \int_0^\infty (t^2 I + A^2)^{-1}\, dt.$$

Newton's Method for Sign

$$X_{k+1} = \tfrac{1}{2}(X_k + X_k^{-1}), \qquad X_0 = A.$$

Convergence

- Let $S := \mathrm{sign}(A)$, $G := (A - S)(A + S)^{-1}$. Then

$$X_k = (I - G^{2^k})^{-1}(I + G^{2^k})S,$$

Ei'vals of G are $(\lambda_i - \mathrm{sign}(\lambda_i))/(\lambda_i + \mathrm{sign}(\lambda_i))$.

Hence $\rho(G) < 1$ and $G^k \to 0$.

- Easy to show

$$\|X_{k+1} - S\| \le \frac{1}{2}\|X_k^{-1}\|\,\|X_k - S\|^2.$$

Frechét Derivative

The **Fréchet derivative** of a matrix function $f : \mathbb{C}^{n\times n} \rightarrow \mathbb{C}^{n\times n}$ at a point $X \in \mathbb{C}^{n\times n}$ is a linear mapping $L_X : \mathbb{C}^{n\times n} \rightarrow \mathbb{C}^{n\times n}$ such that for all $E \in \mathbb{C}^{n\times n}$

$$f(X+E) - f(X) - L_X(E) = o(\|E\|).$$

Example For $f(X) = X^2$ we have

$$f(X+E) - f(X) = XE + EX + E^2,$$

so $L_X(E) = XE + EX$.

Newton's Method for Square Root

Newton's method: X_0 given,

Solve $$\left.\begin{aligned} X_k E_k + E_k X_k &= A - X_k^2 \\ X_{k+1} &= X_k + E_k \end{aligned}\right\} \quad k = 0, 1, 2, \ldots$$

Newton's Method for Square Root

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$$\left.\begin{aligned} \text{Solve}\ \ X_k E_k + E_k X_k &= A - X_k^2 \\ X_{k+1} &= X_k + E_k \end{aligned}\right\} \quad k = 0, 1, 2, \dots$$

Assume $AX_0 = X_0 A$. Then can show

$$X_{k+1} = \tfrac{1}{2}(X_k + X_k^{-1} A). \qquad (*)$$

- For nonsingular A, **local quadratic cgce** of full Newton to a primary square root.
- To **which square root** do the iterations converge?
- $(*)$ can converge when full Newton breaks down.
- **Lack of symmetry** in $(*)$.

Convergence (Jordan)

Assume $X_0 = p(A)$ for some poly p. Let $Z^{-1}AZ = J$ be Jordan canonical form and set $Z^{-1}X_kZ = Y_k$. Then

$$Y_{k+1} = \tfrac{1}{2}(Y_k + Y_k^{-1}J), \qquad Y_0 = J.$$

- Convergence of diagonal of Y_k reduces to scalar case:

Heron: $$y_{k+1} = \tfrac{1}{2}\left(y_k + \frac{\lambda}{y_k}\right), \qquad y_0 = \lambda.$$

- Can show that off-diagonal converges.

Problem: analysis does not generalize to $X_0A = AX_0$!
X_0 not necessarily a polynomial in A.

Convergence (via Sign)

Theorem 1 *Let $A \in \mathbb{C}^{n\times n}$ have no eigenvalues on $\mathbb{R}^-$. The Newton* ***square root iterates*** *X_k with $X_0 A = A X_0$ are related to the Newton* ***sign iterates***

$$S_{k+1} = \frac{1}{2}(S_k + S_k^{-1}), \qquad S_0 = A^{-1/2} X_0$$

by $X_k \equiv A^{1/2} S_k$. Hence, provided that $A^{-1/2} X_0$ has no pure imaginary eigenvalues, the X_k are defined and $X_k \to A^{1/2} \mathrm{sign}(S_0)$ quadratically.

Conclude: $X_k \to A^{1/2}$ if spectrum of $A^{-1/2} X_0$ is in RHP, e.g., if $X_0 = A$.

Convergence: Singular Case

$$X_{k+1} = \frac{1}{2}(X_k + X_k^{-1}A), \qquad X_0 = A.$$

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Notice that $X_1 = \frac{1}{2}(A + I)$.

Convergence: Singular Case

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Notice that $X_1 = \frac{1}{2}(A + I)$.

Theorem 4 *Let singular* $A \in \mathbb{C}^{n\times n}$ *have semisimple zero eigenvalues and nonzero eigenvalues lying off* $\mathbb{R}^-$. *The Newton iterates* X_k *started with* $X_1 = \frac{1}{2}(I + A)$ *are nonsingular and converge linearly to* $A^{1/2}$, *with*

$$\|X_k - A^{1/2}\| = O(2^{-k}).$$

Proof JCF: $A = Z\mathrm{diag}(J_1, 0)Z^{-1}$. Then
$X_1 = Z\mathrm{diag}((J_1 + I)/2, I/2)Z^{-1}, \ldots,$
$X_k = Z\mathrm{diag}(J_1^{(k)}, 2^{-k}I)Z^{-1}.$

Numerical Example

Positive definite *Wilson matrix:* $A = \begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix}, \quad \kappa_2(A) \approx 2984.$

	Sign		Square root	
	$\|I - X_k\|_2$	$(X_k)_{11}$	$\frac{\|A^{1/2} - X_k\|_2}{\|A^{1/2}\|_2}$	$(X_k)_{11}$
2	2.36e1	8.90e0	5.97e-1	3.36e0
3	1.13e1	4.67e0	1.12e-1	2.57e0
4	5.21e0	2.61e0	5.61e-3	2.40e0
5	2.19e0	1.63e0	4.57e-3	2.40e0
6	7.50e-1	1.20e0	1.22e-1	2.21e0
7	1.61e-1	1.04e0	3.26e0	7.20e0
8	1.11e-2	1.00e0	8.74e1	-1.26e2
9	6.12e-5	1.00e0	2.33e3	3.41e3
10	9.78e-10	1.00e0	1.91e4	2.79e4
11	0	1.00e0	1.97e4	-2.87e4

History of Newton Sqrt Instability

- Instability of Newton noted by **Laasonen (1958)**:

  "Newton's method if carried out indefinitely, is not stable whenever the ratio of the largest to the smallest eigenvalue of A exceeds the value 9."

- Described informally by **Blackwell (1985)** in *Mathematical People: Profiles and Interviews*.
- Analyzed by **H (1986)** for diagonalizable A by deriving "error amplification factors".

Stability

Definition 1 ***The iteration $X_{k+1} = g(X_k)$ is stable in a nbhd of a fixed point X if the Fréchet derivative dg_X has bounded powers.***

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- Stability is trivial for scalars, since $g'(x) = 0$!
  For matrices, $dg_X \neq 0$.

Stability

Definition 1 ***The iteration $X_{k+1} = g(X_k)$ is stable in a nbhd of a fixed point X if the Fréchet derivative dg_X has bounded powers.***

Let $X_0 = X + E_0$, $E_k := X_k - X$. Then

$$X_{k+1} = g(X_k) = g(X + E_k) = g(X) + dg_X(E_k) + o(\|E_k\|).$$

So, since $g(X) = X$,

$$E_{k+1} = dg_X(E_k) + o(\|E_k\|).$$

If $\|dg_X^i(E)\| \le c$, then recurring leads to

$$\|E_k\| \le c\|E_0\| + kc \cdot o(\|E_0\|).$$

Stability of Newton Square Root

- $g(X) = \frac{1}{2}(X + X^{-1}A)$.
- $dg_X(E) = \frac{1}{2}(E - X^{-1}EX^{-1}A)$.
- Relevant fixed point: $X = A^{1/2}$.
- $dg_{A^{1/2}}(E) = \frac{1}{2}(E - A^{-1/2}EA^{1/2})$.
- Ei'vals of $dg_{A^{1/2}}$ are

$$\frac{1}{2}(1 - \lambda_i^{-1/2}\lambda_j^{1/2}), \qquad i,j = 1\colon n.$$

- For stability we need

$$\max_{i,j} \tfrac{1}{2}\left|1 - \lambda_i^{-1/2}\lambda_j^{1/2}\right| < 1.$$

- For hpd A, need $\kappa_2(A) < 9$.

Advantages

- Uses only Fréchet derivative of g.
- No additional assumptions on A.
- Perturbation analysis is all in the definition.
- General, unifying approach.
- Facilitates analysis of families of iterations.

Stabilizing Newton

$$X_{k+1} = \frac{1}{2}(X_k + X_k^{-1}A), \qquad X_0 = A.$$

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"Symmetrize":

$$X_{k+1} = \frac{1}{2}\big(X_k + A^{1/2}X_k^{-1}A^{1/2}\big), \qquad X_0 = A.$$

Let $Y_k = A^{-1/2}X_kA^{-1/2}$. Then

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

$$Y_{k+1} = \frac{1}{2}\left(Y_k + X_k^{-1}\right), \qquad Y_0 = I.$$

The iteration of Denman & Beavers (1976).

Class of Square Root Iterations

Theorem 5 *Suppose the iteration* $X_{k+1} = X_k h(X_k^2)$, $X_0 = A$ *converges to* $\mathrm{sign}(A)$ *with order* m. *If* $\Lambda(A) \cap \mathbb{R}^- = \emptyset$ *and*

$$\begin{aligned} Y_{k+1} &= Y_k h(Z_k Y_k), & Y_0 &= A, \\ Z_{k+1} &= h(Z_k Y_k) Z_k, & Z_0 &= I, \end{aligned}$$

then $Y_k \to A^{1/2}$ *and* $Z_k \to A^{-1/2}$ *as* $k \to \infty$ *with order* m.

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then $Y_k \to A^{1/2}$ *and* $Z_k \to A^{-1/2}$ *as* $k \to \infty$ *with order* m.

- Proof makes use of $\operatorname{sign}\left(\begin{bmatrix} 0 & A \\ I & 0 \end{bmatrix}\right) = \begin{bmatrix} 0 & A^{1/2} \\ A^{-1/2} & 0 \end{bmatrix}.$
- Newton sign leads to DB iteration.
  Sign: $X_{k+1} = X_k \cdot \frac{1}{2}(I + (X_k^2)^{-1}) \equiv X_k h(X_k^2), \quad X_0 = A$.
  DB: $Y_{k+1} = \frac{1}{2} Y_k (I + (Z_k Y_k)^{-1}) = \frac{1}{2}(Y_k + Z_k^{-1}), \quad Y_0 = A$.

Stability of Sign Iterations

Theorem 6 *Let* $X_{k+1} = g(X_k)$ *be* ***any superlinearly convergent*** *iteration for* $S = \mathrm{sign}(X_0)$.

Then $dg_S(E) = L_S(E) = \frac{1}{2}(E - SES)$ *, where* L_S *is the Fréchet derivative of the matrix sign function at* S*.*
Hence dg_S *is* ***idempotent*** ($dg_S \circ dg_S = dg_S$) *and the* ***iteration is stable****.*

"All" sign iterations are automatically stable.

Implication

Theorem 7 *Consider the iteration function*

$$G(Y,Z) = \begin{bmatrix} Y h(ZY) \\ h(ZY)Z \end{bmatrix},$$

where $X_{k+1} = X_k h(X_k^2)$ *is any superlinearly convergent iteration for* $\mathrm{sign}(X_0)$. *Any pair* $P = (B, B^{-1})$ *is a fixed point for* G, *and the Fréchet derivative of* G *at* P *is*

$$dG_P(E,F) = \frac{1}{2}\begin{bmatrix} E - BFB \\ F - B^{-1}EB^{-1} \end{bmatrix}.$$

dG_P *is* ***idempotent*** *and hence the iteration is* ***stable***.

- In particular: DB iteration is stable.

Stability is Subtle

$$G_1(Y, Z) = \begin{bmatrix} Y h(ZY) \\ h(ZY) Z \end{bmatrix}$$

gives a **stable** iteration.

$$G_2(Y, Z) = \begin{bmatrix} Y h(ZY) \\ Z h(ZY) \end{bmatrix}$$

gives an **unstable** iteration.

Avoid using commutativity when deriving iterations.

$f(AB)$ and $f(BA)$

For any polynomial, $Ap(BA) = p(AB)A$.

Theorem 8 ***Let $A \in \mathbb{C}^{m\times n}$ and $B \in \mathbb{C}^{n\times m}$ and let f be defined on the spectra of both AB and BA. Then***

$$Af(BA) = f(AB)A. \qquad (*)$$

E.g., $A(BA)^{1/2} = (AB)^{1/2}A$.

Previous slide:

$$h(ZY)Z \Rightarrow Zh(ZY) \qquad \times$$

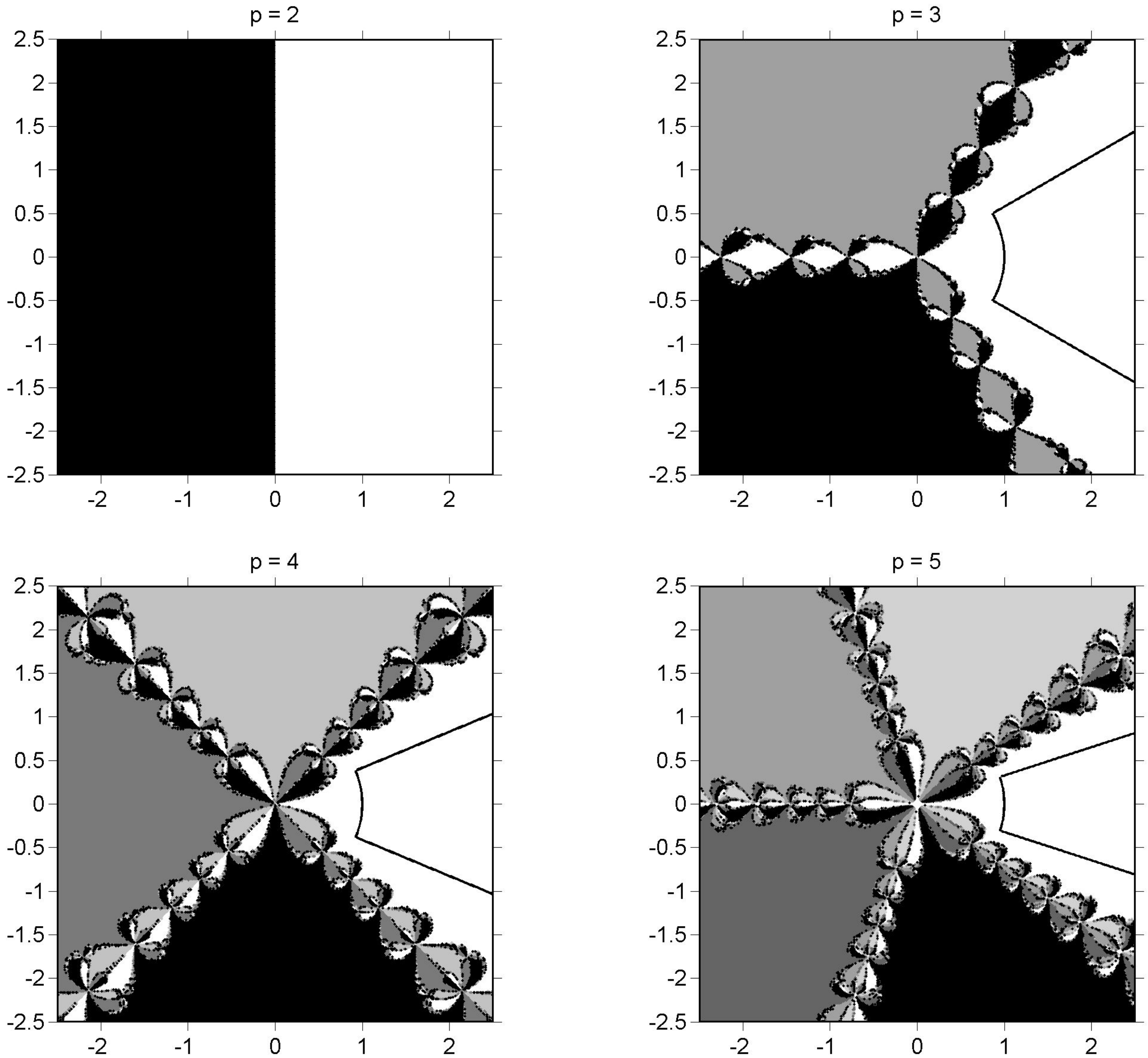
$$h(ZY)Z \Rightarrow Zh(YZ) \qquad \surd$$

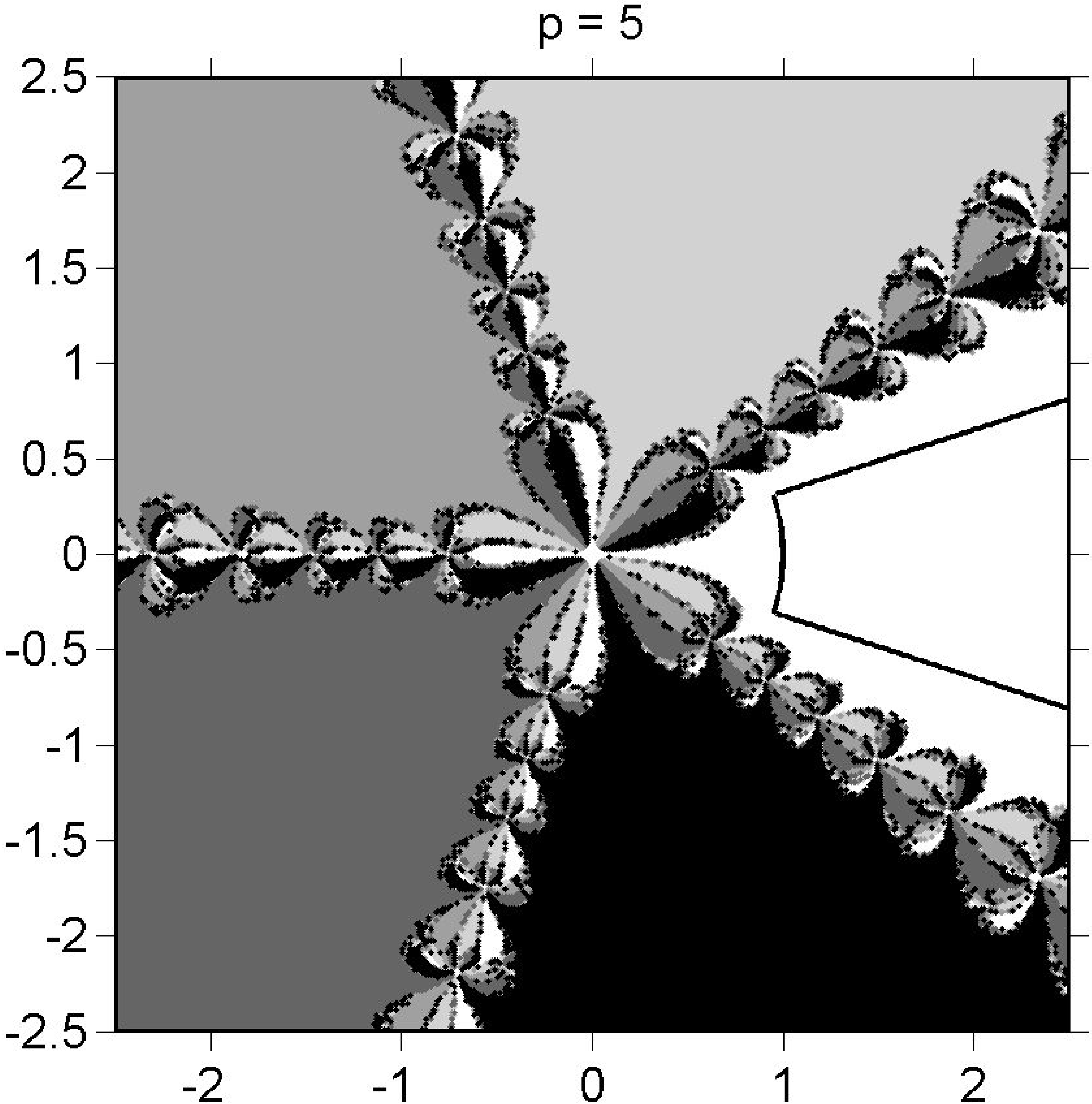
Rule of Thumb

Use $(*)$ instead of commutativity when deriving iterations.

Matrix pth Root

Newton's method: $X_{k+1} = \frac{1}{p}\left((p-1)X_k + X_k^{1-p}A\right)$




p = 5
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-2
-1
0
1
2

Newton Convergence

Theorem 9 (Iannazzo, 2005) *For all $p > 1$, the iteration*

$$x_{k+1} = \frac{1}{p}\big((p-1)x_k + x_k^{1-p}a\big), \qquad x_0 = 1,$$

converges quadratically to $a^{1/p}$ if a belongs to

$$S := a \in \{\, z \in \mathbb{C} : \mathrm{Re}\, z > 0 \text{ and } |z| \le 1 \,\} \cup \mathbb{R}^+.$$

Corollary 1 *Let $A \in \mathbb{C}^{n\times n}$ have no eigenvalues on $\mathbb{R}^-$. For all $p > 1$, the Newton iteration with $X_0 = I$ converges quadratically to $A^{1/p}$ if all the ei'vals of A belong to S.*

Algorithm for $A^{1/p}$

Algorithm 1 (Iannazzo, 2005) *Given $A \in \mathbb{C}^{n\times n}$ having no ei'vals on $\mathbb{R}^-$ this alg. computes $A^{1/p}$.*

1 $B = A^{1/2}$

2 $C = B/\|B\|$ (any norm)

3 Use Newton to compute $Y = \begin{cases} C^{2/p}, & p \text{ even}, \\ \left(C^{1/p}\right)^2, & p \text{ odd}. \end{cases}$

4 $X = \|B\|^{2/p} Y$

C satisfies conditions of corollary, since $\Lambda(C) \in$ RHP, and $\rho(C) \le \|C\| = 1$.

Algorithm for $A^{1/p}$

Algorithm 2 (Iannazzo, 2005) *Given* $A \in \mathbb{C}^{n\times n}$ *having no ei'vals on* $\mathbb{R}^-$ *this alg. computes* $A^{1/p}$*.*

1 $B = A^{1/2}$
2 $C = B/\|B\|$ (any norm)
3 Use Newton to compute $Y = \begin{cases} C^{2/p}, & p \text{ even}, \\ \left(C^{1/p}\right)^2, & p \text{ odd}. \end{cases}$
4 $X = \|B\|^{2/p}Y$

C satisfies conditions of corollary, since $\Lambda(C) \in$ RHP, and $\rho(C) \le \|C\| = 1$.

Problem: Newton is unstable!

Algorithm for $A^{1/p}$

Define $M_k = X_k^{-p} A$. Then obtain (Iannazzo, 2005)

$$X_{k+1} = X_k \left(\frac{(p-1)I + M_k}{p} \right), \qquad X_0 = I,$$
$$M_{k+1} = \left(\frac{(p-1)I + M_k}{p} \right)^{-p} M_k, \qquad M_0 = A.$$

Can show

$$dG_{(X,I)}(E,F) = \begin{bmatrix} I & -\frac{X}{p} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}.$$

Hence $dG_{(A^{1/p},I)}$ is idempotent and iteration is stable.

Other iterations for $A^{1/p}$: Bini, H & Meini (Num. Alg., 2005).

$f(AB)$ and $f(BA)$ Again

Recall $Af(BA) = f(AB)A$.

Theorem 10 *Let* $A \in \mathbb{C}^{m\times n}$, $B \in \mathbb{C}^{n\times m}$, *with* $m \ge n$, *assume* BA *nonsingular, and let* f *be defined on spectrum of* $\alpha I_m + AB$. *Then*

$$f(\alpha I_m + \underbrace{AB}_{m\times m}) = f(\alpha)I_m + A\underbrace{(BA)^{-1}\big(f(\alpha I_n + BA) - f(\alpha)I_n\big)}_{n\times n}B.$$

$n = 1$: $f(\alpha I + uv^*) = f(\alpha)I + f[\alpha + v^*u, \alpha]uv^*$.

$f(x) = x^{-1}$: Sherman–Morrison–Woodbury, after $A + UV^* = A(I + A^{-1}U \cdot V^*)$.

Conclusions

- Stability equivalent to **matrix power boundedness**.
- Better understanding of **convergence analysis** (prefer matrix powers to Jordan form.)
- **Matrix sign function is fundamental** and connections with **sqrt** can be exploited.
- **Rule of thumb**: don't use commutativity, use $Af(BA) = f(AB)A.$
- More to say about structured A: **preservation of structure** in $f(A)$ and in iterates X_k (H, Mackey, Mackey, Tisseur, 2004, 2005—SIMAX).

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