Algorithms for matrix sector function

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(the joint work with Beata Laszkiewicz)

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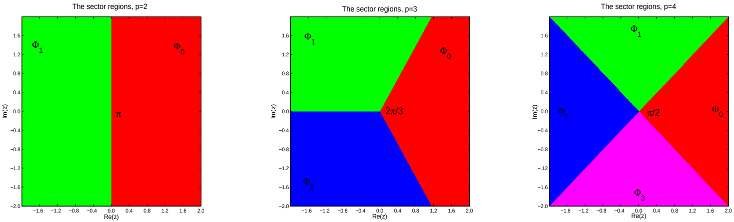
Outline

The sector regions

$$\Phi_k = \left\{ z \in \mathbb{C} : \frac{2k\pi}{p} - \frac{\pi}{p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{p} \right\}$$

$k = 0, \ldots, p-1$



The scalar p-sector function

- $s_p(\lambda)$ is the pth root of unity which lies in the same sector Φ_k in which λ is.

Representation

$$s_p(\lambda) = \frac{\lambda}{\sqrt[p]{\lambda^p}}$$

- $\sqrt[p]{a}$ principal pth root of $a \notin \mathbb{R}^-$, $\sqrt[p]{a}$ lies in Φ_0
- $s_p(\lambda)$ is not defined for the pth roots of nonpositive real numbers.

Principal matrix pth root

Let nonsingular complex matrix A have no negative eigenvalue. There is a unique pth root of A:

$$X = A^{1/p}$$

all of whose eigenvalues lie in the region Φ_0.

$$X^p = A, \qquad \arg \lambda_j(X) \in \left(-\frac{\pi}{p}, \frac{\pi}{p}\right)$$

N.J. Higham, *Functions of Matrices: Theory and Computation*, SIAM 2008

The scalar p-sector function

Let $\lambda = |\lambda| e^{i\varphi} \in \mathbb{C}, \quad \lambda \neq 0,$

$$\varphi = \arg(\lambda) \neq \frac{2k\pi}{p} + \frac{\pi}{p}, \quad k \in \{0, 1, \ldots, p-1\}$$

Then

$$s_p(\lambda) = e^{i2\pi q/p}$$

where $q \in \{0, 1, \ldots, p-1\}$ such that

$$\frac{2q\pi}{p} - \frac{\pi}{p} < \varphi < \frac{2q\pi}{p} + \frac{\pi}{p}$$

Matrix sector function of $A \in \mathbb{C}^{n\times n}$

$$\mathrm{sect}_p(A) = A\left(\sqrt[p]{A^p}\right)^{-1}$$

$$\lambda_j(A) \neq 0, \quad arg(\lambda_j) \neq 2\pi(q+\tfrac{1}{2})/p$$

$$q \in \{0, \ldots, p-1\}$$

Matrix sector function is some *pth* root of identity I.

Matrix sector function

$$\mathrm{sect}_p(A) = Z \mathrm{diag}\left(s_p(\lambda_j) I_{r_j}\right) Z^{-1}$$

$$A = Z \mathrm{diag}\left(J_1, J_2, \ldots, J_m\right) Z^{-1},$$

Jordan canonical form

Jordan block $J_k(\lambda)$

Matrix sign function

Let

$$A = Z\mathrm{diag}(J_1, J_2)Z^{-1},$$

eigenvalues of J_1 lie in the open left half-plane, those of J_2 in open right half-plane. Then

$$\mathrm{sign}(A) = Z\mathrm{diag}(-I_1, I_2)Z^{-1}$$

Algorithms for matrix sign function: Schur method, Newton's method, Pade family of iterations,...

Fréchet derivative and condition numbers of matrix function

Let $F = F(X)$ be a matrix function. The Fréchet derivative of F at X in the direction E is a linear mapping such that

$$F(X+E) - F(X) = L(X,E) = o(||E||).$$

Absolute and relative condition numbers of $F(X)$

$$\mathrm{cond}_{\mathrm{abs}}(F,X) = \lim_{\varepsilon\to 0} \sup_{||E||\le\varepsilon} \frac{||F(X+E)-F(X)||}{\varepsilon} = ||L(X)||$$

$$\mathrm{cond}_{\mathrm{rel}}(F,X) = \frac{||L(X)||\ ||X||}{||F(X)||}$$

Fréchet derivative of matrix sign function

Matrix sign decomposition - Higham

$$A = SN, \quad S = \mathrm{sign}(A), \quad N = (A^2)^{1/2}$$
$$S^2 = I, \qquad S^{-1} = S$$

$$S + \Delta_S = \mathrm{sign}(A + \Delta_A)$$

$L = L(A, \Delta_A)$ Fréchet derivative of matrix sign function of A in direction Δ_A

$$\Delta_S - L = o(||\Delta_A||)$$

Kenney-Laub

L satisfies $\quad NL + LN = \Delta_A - S\Delta_A S.$

Fréchet derivative of matrix sector function

$$\mathrm{sect}_p(A) + \Delta_S = \mathrm{sect}_p(A + \Delta_A)$$

Matrix sector decomposition $A = SN$,

$S = \mathrm{sect}_p(A), \quad N = (A^p)^{1/p}, \qquad S^{-1} = S^{p-1}$

The Fréchet derivative $L = L(A, \Delta_A)$ of matrix sector function is the unique solution of

$$NL + \sum_{k=0}^{p-2} S^k L S^{-k} N = \Delta_A - S^{-1}\Delta_A S$$

Real Schur algorithm for $f(A)$

$A \in \mathbb{R}^{n\times n}$, $A = QRQ^T$ real Schur decomposition

R upper quasi-triangular and block, Q orthogonal

Matrix function f of R has the same block structure as R

Parlett 1976

Main blocks of R are 1×1 or 2×2.

Recurrence relations between blocks of R and $f(R)$ lead to real Schur algorithm for f.

Schur algorithm for matrix *p*th root

Schur algorithms

Higham 1987 - square root
Smith 2003 - *p*th root

Stability of Schur algorithm - Smith 2003

Let $A = QRQ^T$ be real Schur decomposition, $U = (R)^{1/p}$.

$$\beta(U) = \frac{||U||_F^p}{||R||_F} \geq 1$$

Schur algorithm for *p*th root stable provided $\beta(U)$ is sufficiently small.

Algorithms for matrix sector function

$$\mathrm{sect}_p(A) = A(A^p)^{-1/p}$$

$$\mathrm{sect}_p(A) = A\exp(-\log(A^p)/p)$$

MATLAB: `expm`, `logm`

- real Schur algorithm
- Newton's iterations
- Halley's method

Real Schur algorithm for sector

$$A = QRQ^T \qquad \text{real Schur decomposition}$$

$$U = \mathrm{sect}_p(R), \qquad \mathrm{sect}_p(A) = QUQ^T.$$

$$RU = UR, \qquad U^p = I$$

Recurrence relations between blocks of R and U and some Sylvester equations for the blocks lead to real Schur algorithm for sector.

Remark. If A has multiple complex eigenvalues in the sectors different from $\Phi_{p/2}$ (if p even) and Φ_0 then real Schur algorithm does not work.

Newton's method for sector

Shieh, Tsay, Wang, 1984

$$X_0 = A$$

$$X_{k+1} = \left((p-1)X_k^p + I\right) pX_k^{1-p}$$

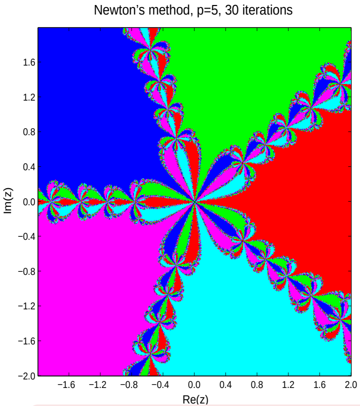
Newton's method is applied to the scalar equation

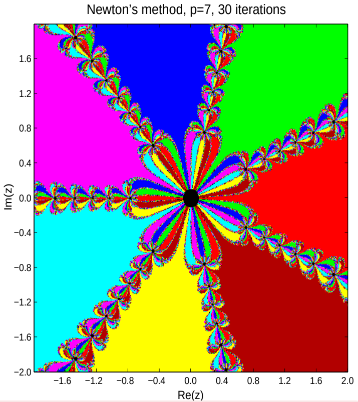
$$x^p - 1 = 0; \quad x_0 = \lambda_j(A)$$

Convergence regions for matrix sector function follow from the results of Higham and Iannazzo for matrix pth roots.

Regions of convergence of Newton for sector

determined experimentally





ω_j pth root of unity

color: $|x_{30} - \omega_j| < 10^{-5}$

Convergence of Newton for sector

If all eigenvalues of A lie in

$$\bigcup_{k=0}^{p-1}(\mathbb{B}_k \cup \mathbb{C}_k \cup \mathbb{R}_k^+)$$

$$\mathbb{B}_k = \left\{ z \in \mathbb{C} : \ |z| \geq 1, \ \frac{2k\pi}{p} - \frac{\pi}{2p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{2p} \right\}$$

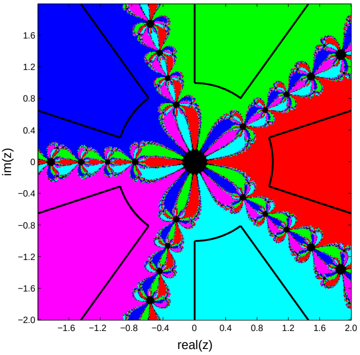
$$\mathbb{C}_k = \left\{ z \in \mathbb{C} : \frac{1}{2^{1/p}} \leq |z| \leq 1, \frac{2k\pi}{p} - \frac{\pi}{2p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{2p} \right\}$$

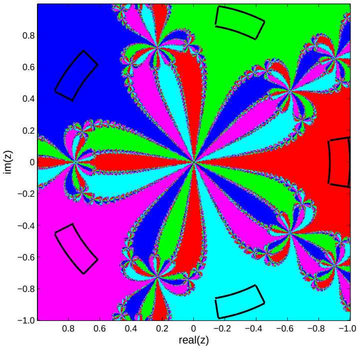
$$\mathbb{R}_k^+ = \left\{ z : \mathbb{C} : \ \mathrm{Re}\ z > 0 \text{ and } \frac{2k\pi}{p} - \frac{\pi}{2p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{2p} \right\}$$

then Newton is convergent

Convergence regions of Newton

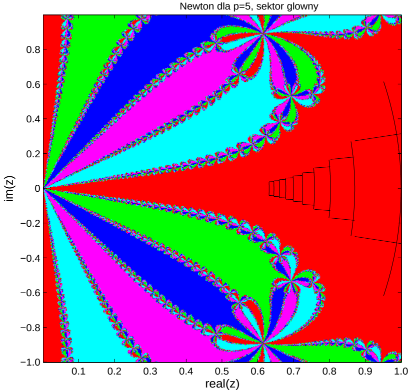
Region $\mathbb{B}_k$ and Region $\mathbb{C}_k$

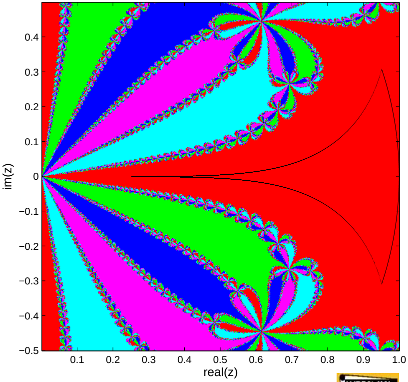




Convergence regions of Newton

Additional regions





Halley's method for sector

Bakkaloğlu, Koç, 1995

$$X_0 = A$$

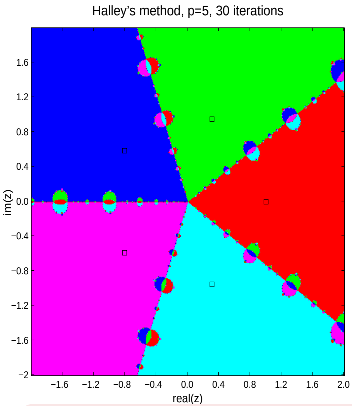
$$X_{k+1} = X_k \left[(p-1)X_k^p + (p+1)I\right] \times \left[(p+1)X_k^p - (p-1)I\right]^{-1}$$

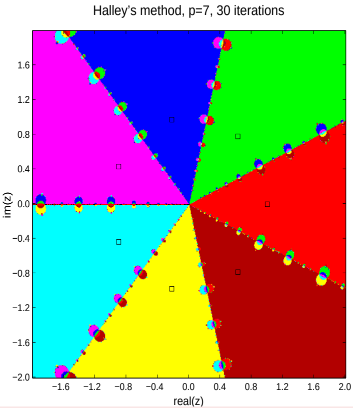
Halley's method is applied to the scalar equation

$$x^p - 1 = 0; \quad x_0 = \lambda_j(A)$$

Regions of convergence of Halley for sector

determined experimentally





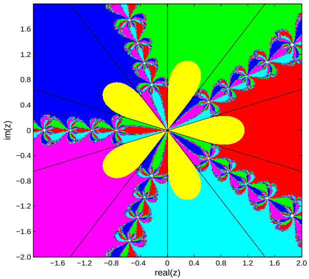
ω_j pth root of unity

color: $|z_{30} - \omega_j| < 10^{-5}$

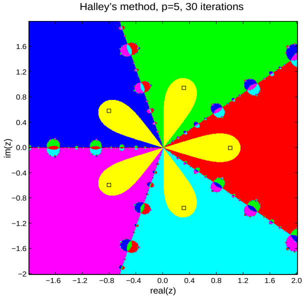
Halley for sector

"yellow flowers" - conjecture for Pade

Newton and $\mathbb{B}_p^{\mathrm{hall}}$



Halley and Pade



If all eigenvalues of A lie in

$$\mathbb{B}_p^{\mathrm{hall}} = \bigcup_{k=0}^{p-1} \left\{ z \in \mathbb{C} : \frac{2k\pi}{p} - \frac{\pi}{2p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{2p} \right\}$$

then Halley is convergent to sector.

Stability of Newton's and Halley's methods for matrix sector function

- Matrix sector function is idempotent, i.e. $\mathrm{sect}_p(\mathrm{sect}_p(A)) = \mathrm{sect}_p(A)$.
- From the theorem of Higham we deduce that Newton's and Halley's iterations are stable, i.e. Fréchet derivatives of the functions, generating iterations, have bounded powers.

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Fréchet derivative

Let $A \in \mathbb{C}^{n\times n}$ be such that $\mathrm{sect}_p(A)$ exists and the Newton iterates X_k are convergent to $\mathrm{sect}_p(A)$. Let

$$Y_{k+1} = \frac{1}{p}\left((p-1)Y_k - X_k^{1-p}\left(\sum_{j=0}^{p-2} X_k^{p-2-j} Y_k X_k^j\right) X_k^{1-p}\right),$$

$$Y_0 = \Delta_A, \qquad X_0 = A.$$

Then the sequence Y_k tends to the Fréchet derivative $L(A, \Delta_A)$ of $\mathrm{sect}_p(A)$: $\lim_{k\to\infty} Y_k = L(A, \Delta_A)$.

Matrix sign ($p = 2$) Kenney-Laub

$$Y_{k+1} = \tfrac{1}{2}(Y_k - X_k^{-1} Y_k X_k^{-1})$$

Implementation

Newton

$$X_{k+1} = \left[(p-1)X_k^p + I\right]\left(X_k^{-1}\right)^{p-1}$$

Halley

$$X_{k+1} = X_k\left[(p-1)X_k^p + (p+1)I\right] \times \left[(p+1)X_k^p - (p-1)I\right]^{-1}$$

Example 1- test matrix

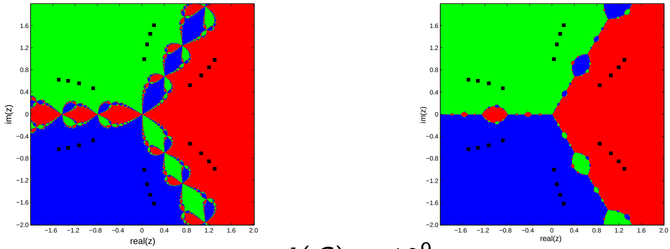
$$A \in \mathbb{C}^{n\times n}, \qquad Y = A^{1/p}$$

$$C = \begin{bmatrix} 0 & I & & & \\ & 0 & I & & \\ & & \ddots & \ddots & \\ & & & \ddots & I \\ A & & & & 0 \end{bmatrix} \in \mathbb{C}^{pn\times pn}.$$

$$\mathrm{sect}_p(C) = \begin{bmatrix} 0 & Y^{-1} & & 0 \\ \vdots & 0 & \ddots & \\ 0 & \ddots & \ddots & Y^{-1} \\ AY^{-1} & 0 & \cdots & 0 \end{bmatrix}.$$

eigenvalues of $A \in \mathbb{R}^{8\times 8}$: $\frac{-k^2}{10} \pm ik, \qquad k = 1, 2, 3, 4$

black boxes - eigenvalues of C for $p = 3$, convergence regions



$$\mathrm{cond}(C) \approx 10^9$$

C has 4 groups of eigen. with $2p$ eigenvalues
with the same module in each group

for $p = 3$: $\beta(U) \approx \mathbf{10^{16}}$

for $p = 6$: $\beta(U) \approx \mathbf{10^{35}}$

$U = \mathrm{sect}(R)$, R quasi-triang. from Schur decomp. of C

Table: Results for C

$n = 24, \quad p = 3, \quad \|\hat{X}\| = 1.71 \times 10^6, \quad iter_{\text{Newt}} = 8, \quad iter_{\text{Hall}} = 5$

$alg.$	$\|\hat{X}^p - I\|$	$\|C\hat{X} - \hat{X}C\|$	$\frac{\|C\hat{X}-\hat{X}C\|}{\|\hat{X}\|\|C\|}$
Newt	$1.32e-09$	$1.50e-09$	$1.94e-18$
Hall	$1.88e-09$	$3.12e-09$	$4.03e-18$
r − Sch	**2.76e − 06**	$8.91e-08$	$1.15e-16$

$n = 48, \quad p = 6, \quad \|\hat{X}\| = 8.76 \times 10^5, \quad iter_{\text{Newt}} = 9, \quad iter_{\text{Hall}} = 5$

$alg.$	$\|\hat{X}^p - I\|$	$\|C\hat{X} - \hat{X}C\|$	$\frac{\|C\hat{X}-\hat{X}C\|}{\|\hat{X}\|\|C\|}$
Newt	$5.07e-09$	$3.21e-09$	$8.10e-18$
Hall	$4.00e-09$	$3.57e-09$	$9.03e-18$
r − Sch	**8.81e − 04**	$5.81e-08$	$1.47e-16$

for $p = 6$ $\qquad max_j|\lambda_j^{\text{schur}} - \lambda_j^A| \approx 10^{-10}$

Example 2

$$A = D + T, \qquad D = \mathrm{diag}(\lambda_j), \quad \text{complex}$$

T triangular real, $\quad n = 40$

Table: Results for A

$$p = 5, \quad \|\hat{X}\| = 1.1, \quad iter_{\mathrm{Newt}} = 28, \quad iter_{\mathrm{Hall}} = 16$$

alg.	$\|\hat{X}^p - I\|$	$\|A\hat{X} - \hat{X}A\|$	$\frac{\|A\hat{X}-\hat{X}A\|}{\|\hat{X}\|\|A\|}$
Newt	$6.40e-16$	$5.57e-15$	$4.13e-17$
Hall	$1.45e-15$	$\mathbf{1.65e-11}$	$1.22e-13$

Example 3

A as in the previous example, $n = 10$

$$p = 4, \quad \|\hat{X}\| = 1.01, \quad iter_{\mathrm{Newt}} = 22, \quad iter_{\mathrm{Hall}} = 13$$

$alg.$	$\|\hat{X}^p - I\|$	$\frac{\|\hat{X}^p - I\|}{\|\hat{X}\|^p}$	$\|A\hat{X} - \hat{X}A\|$	$\frac{\|A\hat{X} - \hat{X}A\|}{\|\hat{X}\|\|A\|}$
Newt	$2.68e-18$	$2.54e-18$	$1.47e-15$	$1.52e-17$
Hall	$4.44e-16$	$4.22e-16$	$4.32e-15$	$4.46e-17$
c − Sch	$2.68e-18$	$2.55e-18$	$3.57e-16$	$3.69e-18$

slow convergence of Newton

$$p = 10, \quad \|\hat{X}\| = 1.02, \quad \mathbf{iter}_{\mathrm{Newt}} = \mathbf{51}, \quad iter_{\mathrm{Hall}} = 28$$

$alg.$	$\|\hat{X}^p - I\|$	$\frac{\|\hat{X}^p - I\|}{\|\hat{X}\|^p}$	$\|A\hat{X} - \hat{X}A\|$	$\frac{\|A\hat{X} - \hat{X}A\|}{\|\hat{X}\|\|A\|}$
Newt	$1.32e-15$	$1.08e-15$	$1.75e-15$	$1.47e-17$
Hall	$1.94e-15$	$1.59e-15$	$\mathbf{3.29e-08}$	$2.76e-10$
c − Sch	$1.28e-15$	$1.05e-15$	$4.11e-16$	$3.45e-18$

Summary

- Real Schur algorithm for the matrix sector function was proposed.
- Some convergence regions of Newton's and Halley's iterations were given.
- Conditioning and stability of the algorithms were discussed.
- Numerical experiments were presented.
  - the commutativity condition was not well satisfied by Halley in some cases,
  - accuracy of Schur algorithm for A with multiple eigenvalues was bad.

Other results in PhD of Beata Laszkiewicz, in preparation.

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Thank you for your attention!

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