Ralph, the Matrix Sign Function, and the Polar Decomposition

Nick Higham
School of Mathematics
The University of Manchester

higham@ma.man.ac.uk
http://www.ma.man.ac.uk/~higham/

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Matrix Sign Function

Let $A \in \mathbb{C}^{n\times n}$ have no pure imaginary eigenvalues. Given Jordan form

$$A = Z \begin{bmatrix} J_1 & 0 \\ 0 & J_2 \end{bmatrix} Z^{-1},$$

where $\Lambda(J_1) \in$ open LHP, $\Lambda(J_2) \in$ open RHP,

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

Alternative definition:

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

Introduced by Roberts (1971).

Polar Decomposition

Autonne (1902): for $A \in \mathbb{C}^{m\times n}$, $m \geq n$, $A = UH$, where $U \in \mathbb{C}^{m\times n}$ has orthonormal columns and $H \in \mathbb{C}^{n\times n}$ is Hermitian positive semidefinite.

- $H = (A^*A)^{1/2}$ is unique.
- U is unique iff A has full rank and then

$$U = A(A^*A)^{-1/2}.$$

Newton's Method in 1984

For matrix sign (RB):

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

For unitary polar factor of nonsingular $A \in \mathbb{C}^{n\times n}$ (NJH):

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

Ralph's (1984) observation:

$$\operatorname{sign}\left(\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}\right) = \begin{bmatrix} 0 & U \\ U^* & 0 \end{bmatrix}.$$

First written down in H (1994).

Ralph's 1987 Paper (1)

Ralph Byers. Solving the algebraic Riccati equation with the matrix sign function. *Linear Algebra Appl.*, 85:267–279, 1987.

Hermitian stabilizing solution of

$$XFX - A^*X - XA - G = 0, \qquad F = F^*,\ G = G^*$$

obtained from sign of

$$W = \begin{bmatrix} A^* & G \\ F & -A \end{bmatrix}.$$

Ralph's 1987 Paper (2)

- Determinantal scaling:

$$X_{k+1} = \frac{1}{2}(\mu_k X_k + \mu_k^{-1} X_k^{-1}), \qquad \mu_k = |\det(X_k)|^{-1/n}.$$

  Minimizes $d(\mu X)$, where $d(X) = \sum_{i=1}^{n} (\log |\lambda_i(X)|)^2$.
- JW is Hermitian for $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$ so can use LINPACK Hermitian inversion code.
- Iterative refinement of the ARE.
- Implementation details.

Ralph's 1987 Paper (3)

- "The first twelve iterations of (1) differ insignificantly from $W^{(k+1)} := W^{(k)}/2$. At $O(n^3)$ floating-point operations per iteration, this is an expensive way to divide by 2."
- "Trivial cases are handled trivially by (2)."
- "The matrix sign function can be regarded simply as a way to obtain a good initial guess for Newton's method."

What do you get if you cross a matrix with a patrix?

Sign Function Developments

- Numerical stability of sign for invariant subspaces: Byers (1986), Byers, He & Mehrmann (1997), Bai & Demmel (1998) .
- Generalization.
- Parallelization.
- Analysis of scalings (Kenney & Laub).
- Padé family of iterations (Kenney & Laub).
- Conditioning of sign.
- Lattice quantum chromodynamics application.

Sign Function Stability and Termination

H (2008):

- (Roughly): all superlinearly convergent sign iterations $X_{k+1} = g(X_k)$ are stable and have idempotent Fréchet derivative at $S = \mathrm{sign}(X_0)$ given by $L_g(S, E) = \frac{1}{2}(E - SES) = L(S, E)$ (Fréchet derivative of sign function at S).
- Terminate Newton iteration when

$$\|X_{k+1} - X_k\| \le \left(2\eta \frac{\|X_{k+1}\|}{\|X_k^{-1}\|}\right)^{1/2}.$$

Based on quadratic convergence.

Polar Decomposition

$A \in \mathbb{C}^{m\times n}$, $A = UH$.

- Defined only for $m \geq n$.
- Unique U only if A has full rank.

Partial Isometry

$U \in \mathbb{C}^{m\times n}$ is a **partial isometry** if $\|Ux\|_2 = \|x\|_2$ for all $x \in \mathrm{range}(U^*)$; i.e., U norm-preserving on orthogonal complement of its null space.

Lemma

For $U \in \mathbb{C}^{m\times n}$ each of the following conditions is equivalent to U being a partial isometry:

(a) $U^+ = U^*$,

(b) $UU^*U = U$,

(c) *the singular values of U are all* 0 *or* 1.

Canonical Polar Decomposition

Theorem

*$A \in \mathbb{C}^{m\times n}$ has a **unique** decomp $A = UH$ with $U \in \mathbb{C}^{m\times n}$ a partial isometry, $H \in \mathbb{C}^{n\times n}$ Hermitian pos semidef, and*

$$\textbf{equivalent conditions} \begin{cases} \mathrm{range}(U^*) = \mathrm{range}(H) \\ U^*U = HH^+ \\ \mathrm{null}(U) = \mathrm{null}(H) \\ \mathrm{range}(U) = \mathrm{range}(A) \\ UU^+ = AA^+ \end{cases}$$

$H = (A^*A)^{1/2}$ and $U = AH^+$. Moreover, if $A = P\left[\begin{smallmatrix}\Sigma_r & 0 \\ 0 & 0_{m-r,n-r}\end{smallmatrix}\right]Q^*$ is an SVD then

$$U = P\begin{bmatrix} I_r & 0 \\ 0 & 0_{m-r,n-r}\end{bmatrix}Q^*, \qquad H = Q\begin{bmatrix}\Sigma_r & 0 \\ 0 & 0_{n-r}\end{bmatrix}Q^*.$$

Discussion

- **Polar decomp**:
  - $m \geq n$.
  - U has orthonormal cols.
  - U is nearest matrix with orthonormal columns.
- **Canonical polar decomp**:
  - Any m and n.
  - U and H both rank deficient if A is.
  - U is nearest partial isometry satisfying range condition.
- Some authors refer to canonical polar decomp as "*generalized polar decomp*".

Newton Iteration

Nonsingular $A \in \mathbb{C}^{n\times n}$:

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

Scaled iteration (H, 1986):

$$X_{k+1} = \tfrac{1}{2}\left(\mu_k X_k + \mu_k^{-1} X_k^{-*}\right), \quad \mu_k = \left(\frac{\|X_k^{-1}\|_1 \|X_k^{-1}\|_\infty}{\|X_k\|_1 \|X_k\|_\infty}\right)^{1/4}.$$

$\mu_k \approx \mu_k^{\mathrm{opt}} = \big(\sigma_1(X_k)\sigma_n(X_k)\big)^{-1/2}$, where latter gives convergence in d iterations, where A has d distinct singular values.

Stability of Scaled Newton

- Observed to be excellent, starting with H (1986).
- Computed factors proved backward stable, assuming matrix inverses are mixed backward–forward stable, by Byers & Xu (2008), following earlier analysis of Kielbasiński & Ziętak (2003) .

  See following talk for more. . .

Sign Connections

$$\mathrm{sign}\left(\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}\right) = \begin{bmatrix} 0 & U \\ U^* & 0 \end{bmatrix},$$

$$\mathrm{sign}\left(\begin{bmatrix} 0 & A \\ I & 0 \end{bmatrix}\right) = \begin{bmatrix} 0 & A^{1/2} \\ A^{-1/2} & 0 \end{bmatrix}.$$

Very useful for deriving new polar & square root iterations/results from existing sign iterations: H (1997), H, Mackey, Mackey & Tisseur (2004, 2005).

E.g.,

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

implies

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

Our “Gatlinburg” Papers

- Ralph Byers. Solving the algebraic Riccati equation with the matrix sign function. *Linear Algebra Appl.*, 85: 267–279, 1987.
- Nicholas J. Higham. Computing the polar decomposition—with applications. *SIAM J. Sci. Statist. Comput.*, 7(4):1160–1174, 1986.

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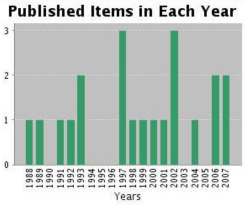

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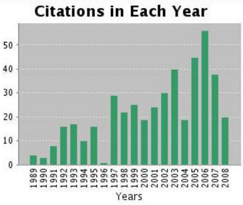

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Linear model reduction and solution of the algebraic Riccati equation by use of the **sign function**† - all 2 versions »
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This definition also leads immediately to a **matrix sign function** of any **matrix** Z

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