

# Structured Matrix Computations

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Joint work with **N. J. Higham**,  
**D. S. Mackey** and **N. Mackey**.



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# Outline

- What kind of structures? Those arising in the context of a bilinear or sesquilinear form.
- Basic actions and structured tools to perform these actions.
- Structured factorizations.
- Iterations in matrix groups for
  - polar decomposition,
  - matrix sign decomposition,
  - matrix square root.

# Background

A **scalar product**  $\langle \cdot, \cdot \rangle_M$  is a non degenerate ( $M$  nonsingular) **bilinear** or **sesquilinear** form on  $\mathbb{K}^n$  ( $\mathbb{K} = \mathbb{R}$  or  $\mathbb{C}$ ).

$$\langle x, y \rangle_M = \begin{cases} x^T M y, & \text{real or complex bilinear forms,} \\ x^* M y, & \text{sesquilinear forms.} \end{cases}$$

$\langle \cdot, \cdot \rangle_M$  does not have to be symmetric, skew-symmetric, Hermitian or positive definite.

Recall **adjoint**  $A^*$  of  $A \in \mathbb{K}^{n \times n}$  wrt  $\langle \cdot, \cdot \rangle_M$  defined by

$$\langle Ax, y \rangle_M = \langle x, A^* y \rangle_M \quad \forall x, y \in \mathbb{K}^{n \times n}.$$

Can show: 
$$A^* = \begin{cases} M^{-1} A^T M, & \text{for bilinear forms,} \\ M^{-1} A^* M, & \text{for sesquilinear forms.} \end{cases}$$

# Structured Classes Associated with a Scalar Product

- $\langle Ax, Ay \rangle = \langle x, y \rangle, \forall x, y \in \mathbb{K}^n$ .  
**Automorphisms or isometries** of  $\langle \cdot, \cdot \rangle$ .
- $\langle Kx, y \rangle = -\langle x, Ky \rangle, \forall x, y \in \mathbb{K}^n$ .  
**Skew-adjoint** with respect to  $\langle \cdot, \cdot \rangle$ .
- $\langle Sx, y \rangle = \langle x, Sy \rangle, \forall x, y \in \mathbb{K}^n$ .  
**Self-adjoint** with respect to  $\langle \cdot, \cdot \rangle$ .

In terms of adjoint:

$$\begin{array}{ll} \mathbb{G} & = \{A \in \mathbb{K}^{n \times n} : A^* = A^{-1}\} & \text{Automorphism group,} \\ \mathbb{L} & = \{K \in \mathbb{K}^{n \times n} : K^* = -K\} & \text{Lie algebra,} \\ \mathbb{J} & = \{S \in \mathbb{K}^{n \times n} : S^* = S\} & \text{Jordan algebra.} \end{array}$$

# Structure Preserving Transformations

Similarity by any matrix in  $\mathbb{G}$  preserves the structure of matrices in  $\mathbb{G}$ ,  $\mathbb{L}$  and  $\mathbb{J}$ .

That is, for any  $G \in \mathbb{G}$ ,

1.  $A \in \mathbb{G} \implies G^{-1}AG \in \mathbb{G}$ .
2.  $K \in \mathbb{L} \implies G^{-1}KG \in \mathbb{L}$ .
3.  $S \in \mathbb{J} \implies G^{-1}SG \in \mathbb{J}$ .

Matrices in  $\mathbb{G}$  are hence useful in the construction of structure-preserving algorithms.

# Familiar Classes

Space	$\langle x, y \rangle$	$\mathbb{G}$	$\mathbb{J}$	$\mathbb{L}$
<b>Bilinear forms</b>				
$\mathbb{R}^n$	$x^T y$	Real orthog	Symm	Skew-symm
$\mathbb{C}^n$	$x^T y$	Cplx orthog	Cplx symm	Cplx skew-symm
$\mathbb{R}^n$	$x^T R y$	Real perplectics	Persymmetrics	Perskew-symm
$\mathbb{R}^n$	$x^T \Sigma_{p,q} y$	Pseudo-orthog	Pseudo symm	Pseudo skew-symm
$\mathbb{R}^{2n}$	$x^T J y$	Real symplectics	Skew-Hamil	Hamiltonians

## Sesquilinear forms

$\mathbb{C}^n$	$x^* y$	Unitaries	Herm	Skew-Herm
$\mathbb{C}^n$	$x^* \Sigma_{p,q} x$	Pseudo unitaries	Pseudo Herm	Pseudo skew-Herm
$\mathbb{C}^{2n}$	$x^T J y$	Conj symplectics	$J$ -skew-Herm	$J$ -Herm

$$R = \begin{bmatrix} & & & & 1 \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ 1 & & & & \end{bmatrix}, \quad
 J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad
 \Sigma_{p,q} = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}$$

# Basic Actions

**Action:**  $x \mapsto Ax$ , where  $A \in \mathbb{G}$ .

## ▶ Making zeros

- ▶ Givens-like action: setting one component of  $x$  to zero (usually).
- ▶ Householder-like action:  $x \mapsto e_j$  by an elementary matrix in  $\mathbb{G}$ .
- ▶ Gauss-like action: introduce  $k$  zeros into the top or bottom part of  $x$  by an elementary matrix in  $\mathbb{G}$ .

## ▶ Scaling by diagonal matrices in $\mathbb{G}$ .

# Gauss-like Action with Symplectics

$A \in \mathbb{R}^{2n \times 2n}$  symplectic  $\Leftrightarrow A^T J A = J$ ,  $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$ .

Given  $x, y \in \mathbb{R}^n$  and  $k$  s.t.  $x_k \neq 0$ , the **symplectic shear**

$$S = \begin{bmatrix} I & 0 \\ Z & I \end{bmatrix} \quad \text{with} \quad Z = -\frac{y e_k^T - e_k y^T}{x_k} + \frac{(y^T x) e_k e_k^T}{x_k^2} = Z^T,$$

satisfies

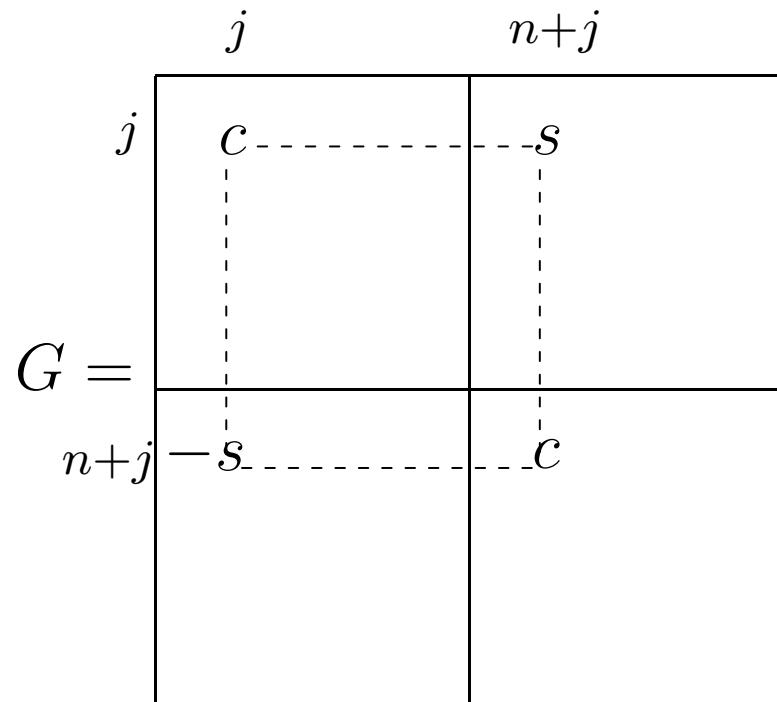
$$S \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x \\ 0 \end{bmatrix}.$$

- ▶ Can be modified to zero out any selected comp. of  $y$ .
- ▶ General form of  $S$  is new.
- ▶ **Symplectic Gauss** are special cases of symplectic shears used in reduction of Hamiltonians to  $J$ -Hessenberg forms.

# Givens-like Action with Symplectics (1)

Three possibilities with symplectic orthogonals :

- ▶ Embed symplectically  $2 \times 2$  Givens.



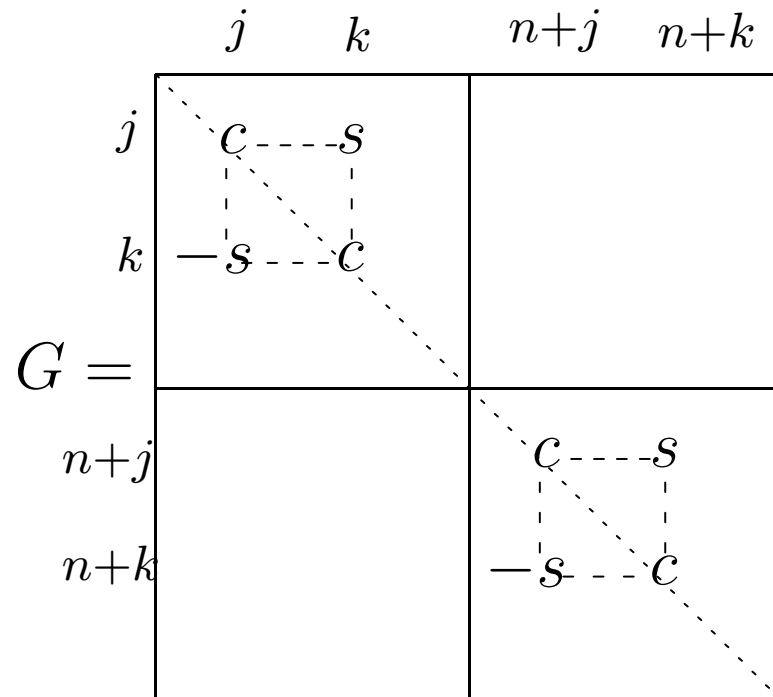
$$e_\ell^T Gx = 0 \text{ for } \ell \in \{j, n+j\}.$$

Used in symplectic and Hamiltonian eigenproblems.

# Givens-like Action with Symplectics (1)

Three possibilities with symplectic orthogonals :

- ▶ Embed symplectically  $2 \times 2$  Givens.
- ▶ Double Givens:
  - symplectic direct sum embedding.



$$e_\ell^T Gx = 0$$

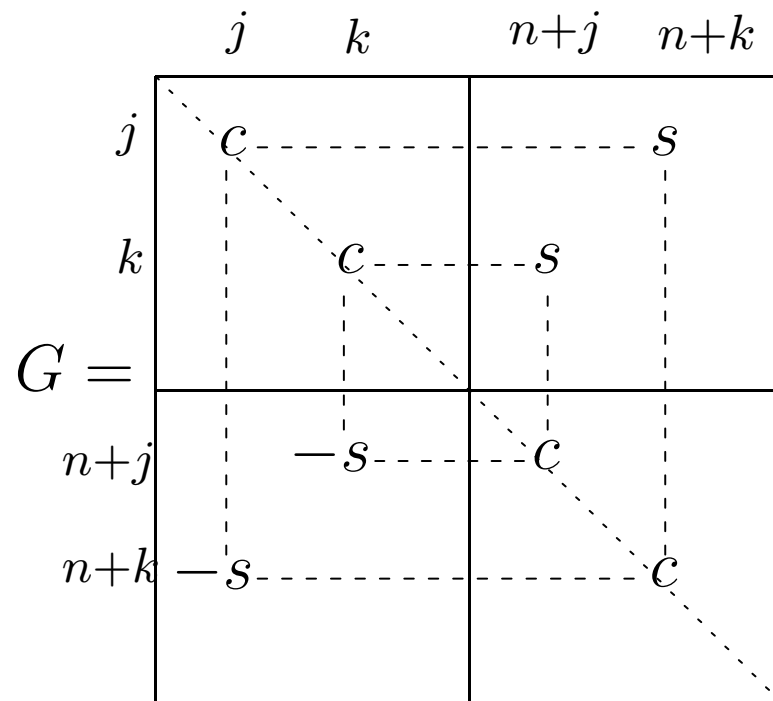
for  $\ell \in \{j, k, n + j, n + k\}$ .

Used in symplectic and Hamiltonian eigenproblems.

# Givens-like Action with Symplectics (1)

Three possibilities with symplectic orthogonals :

- ▶ Embed symplectically  $2 \times 2$  Givens.
- ▶ Double Givens:
  - symplectic **direct sum** embedding.
  - symplectic **concentric** embedding (new form).



$$e_\ell^T G x = 0$$

for  $\ell \in \{j, k, n + j, n + k\}$ .

# Givens-like Action with Symplectics (2)

Given  $x \in \mathbb{R}^4$ ,

$$G_4 = \frac{1}{\sqrt{x^T x}} \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \\ -x_2 & x_1 & x_4 & -x_3 \\ -x_3 & -x_4 & x_1 & x_2 \\ -x_4 & x_3 & -x_2 & x_1 \end{bmatrix}$$

is **symplectic orthogonal** and  $G_4 x = \sqrt{x^T x} e_1$ .

Symplectic embedding of  $G_4$  into  $I_{2n}$  simultaneously zeroes out three out of the four affected components of  $x \in \mathbb{R}^{2n}$ .

- ▶ Used in Jacobi-like algorithms for doubly structured Hamiltonians.

# Householder-like Actions with Symplectics

Two possibilities:

- ▶ **Symplectic Householder**:  $H \oplus H$  with  $H$   $n \times n$  Householder matrix. Can introduce up to  $n$  zeros. Used in Hamiltonian eigenproblems.
- ▶ **G-reflector** (new form):

$$G = I + \frac{(x - e_j)(x - e_j)^T J}{\alpha}, \quad \alpha = \begin{cases} x_{n+j}, & \text{if } 1 \leq j \leq n \\ -x_{j-n}, & \text{if } n+1 \leq j \leq 2n, \end{cases}$$

has the property  $Gx = e_j$ , as long as  $\alpha \neq 0$ .

Can introduce up to  $2n - 1$  zeros.

# G-Reflectors

A  $\mathbb{G}$ -reflector is a matrix in  $\mathbb{G}$  of the form

$$(1) \quad G = \begin{cases} I + \beta uu^T M & \text{(bilinear),} \\ I + \beta uu^* M & \text{(sesquilinear),} \end{cases}$$

where  $0 \neq \beta \in \mathbb{K}$  and  $0 \neq u \in \mathbb{K}^n$ .

**Theorem 1 (G-Reflector Mapping Theorem)** *For distinct nonzero  $x, b \in \mathbb{K}^n$ , there exists a  $\mathbb{G}$ -reflector  $G$  s.t.  $Gx = b$  iff  $\langle x, x \rangle_M = \langle b, b \rangle_M$  and  $\langle b - x, x \rangle_M \neq 0$ .*

*When  $G$  exists, it is unique and is specified by taking  $u = b - x$  and  $\beta = 1/\langle u, x \rangle_M$  in (1).*

Requires  $\langle \cdot, \cdot \rangle_M$  to be orthosymmetric.

# Structured Factorizations

Two basic types of questions:

- To what extent can a general unstructured matrix be factored into a product of structured matrices?  
E.g. LU, QR, polar, matrix sign, SVD, ...
- To what extent can a structured matrix in some class be factored within the class into even more structured factors?

We will investigate the second question.

# Structured Factorizations

- Polar Decomposition
- Matrix Sign Decomposition
- Square Roots

# Structure of Polar Factors

Recall **polar decomposition** of  $A \in \mathbb{C}^{n \times n}$ :

$$A = UH, \quad U^*U = I, \quad H = H^* \geq 0.$$

If  $A \in \mathbb{G}$ , are  $U$  and/or  $H$  also in  $\mathbb{G}$ ?

*For example, are the polar factors of a real symplectic matrix themselves real symplectic (in addition to being orthogonal and symmetric positive definite)?*

# Structure of Polar Factors

Recall **polar decomposition** of  $A \in \mathbb{C}^{n \times n}$ :

$$A = UH, \quad U^*U = I, \quad H = H^* \geq 0.$$

Denote by  $\mathfrak{U}$  the set of groups for which  $M$  defining the underlying form is unitary ( $M^{-1} = M^*$ ).

**Theorem 2** *If  $\mathbb{G} \in \mathfrak{U}$  then  $H, U$  always belong to  $\mathbb{G}$ .*

**Proof.**  $U$  unitary  $\Rightarrow U^*$  unitary,  $H$  hpd  $\Rightarrow H^*$  hpd. Hence,

$$\begin{aligned} A \in \mathbb{G} &\Rightarrow A = A^{-*} \\ &\Rightarrow A = UH = (UH)^{-*} = U^{-*}H^{-*} \end{aligned}$$

gives two polar decompositions of  $A$ . Uniqueness of polar factors implies  $U = U^{-*}$  and  $H = H^{-*}$ . So  $U, H \in \mathbb{G}$ .  $\square$

# Polar Factors for $\mathbb{L}$ , $\mathbb{J}$

One obstruction:  $\mathbb{L}(\mathbb{J})$  may contain no invertible elements, hence no unitaries.

**Theorem 3** *Let  $M$  be unitary and  $A \in \mathbb{L}$  (or  $\mathbb{J}$ ).*

- ▶  *$A$  nonsingular, then  $U \in \mathbb{L}(\mathbb{J})$ .*
- ▶  *$A$  singular and  $\mathbb{L}(\mathbb{J})$  has at least one nonsingular element, then  $\exists$  polar decomposition s.t.  $U \in \mathbb{L}(\mathbb{J})$ .*

What about the hpd factor  $H$ ?

In general  $H$  has no additional structure.

But  $A \in \mathbb{L}(\mathbb{J})$  is normal  $\Leftrightarrow H \in \mathbb{J}$ .

# Structure-Preserving Iterations

**Theorem 4** Consider

$$Z_{k+1} = Z_k P_{mm}(I - Z_k^* Z_k) Q_{mm}(I - Z_k^* Z_k)^{-1}, \quad Z_0 = A,$$

where  $P_{mm}(t)/Q_{mm}(t)$  is the  $[m/m]$  Padé approximant to  $(1 - t)^{-1/2}$  and  $m \geq 1$ . If  $\mathbb{G} \in \mathcal{U}$  and  $A \in \mathbb{G}$  then

- $Z_k \in \mathbb{G}$  for all  $k$ ,
- $Z_k \rightarrow U$  at order  $2m + 1$ .

# Structure-Preserving Iterations

**Theorem 4** Consider

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- $Z_k \in \mathbb{G}$  for all  $k$ ,
- $Z_k \rightarrow U$  at order  $2m + 1$ .

Iterations  $z_{k+1} = f(z_k)$ :

$m$	$f(x)$
1	$\frac{x(3 + x^2)}{1 + 3x^2}$ <b>Halley</b>
2	$\frac{x(5 + 10x^2 + x^4)}{1 + 10x^2 + 5x^4}$

# Iterations (all with $X_0 = A$ )

Cubic (structure-preserving):

$$X_{k+1} = \frac{1}{3} X_k [I + 8(I + 3X_k^* X_k)^{-1}].$$

Quintic (structure-preserving):

$$x_{k+1} = x_k \left[ \frac{1}{5} + \frac{8}{5x_k^2 + 7 - \frac{16}{5x_k^2 + 3}} \right].$$

Scaled Newton iteration (not structure-preserving):

$$X_{k+1} = \frac{1}{2} \left[ \gamma^{(k)} X_k + \frac{1}{\gamma^{(k)}} X_k^{-*} \right], \quad \gamma^{(k)} = \left( \frac{\|X_k^{-1}\|_F}{\|X_k\|_F} \right)^{1/2}.$$

$$X_0 \in \mathbb{G} \in \mathfrak{U} \quad \Rightarrow \quad \gamma^{(0)} = 1.$$

# Experiment

Random symplectic  $A \in \mathbb{R}^{12 \times 12}$ ,  $\|A\|_2 = 310 = \|A^{-1}\|_2$ .

$$\mu_{\mathbb{O}}(A) = \frac{\|A^*A - I\|_2}{\|A\|_2^2}, \quad \mu_{\mathbb{G}}(A) = \frac{\|A^*A - I\|_2}{\|A\|_2^2}.$$

$k$	Newton (scaled)		Cubic	
	$\mu_{\mathbb{O}}(X_k)$	$\mu_{\mathbb{G}}(X_k)$	$\mu_{\mathbb{O}}(X_k)$	$\mu_{\mathbb{G}}(X_k)$
0	1.0e+0	7.0e-18	1.0e+0	7.0e-18
1	1.0e+0	1.0e+0	1.0e+0	8.9e-17
2	8.6e-01	8.6e-01	1.0e+0	8.1e-16
3	2.0e-01	2.0e-01	9.9e-01	6.3e-15
4	3.2e-03	3.2e-03	9.4e-01	5.0e-14
5	9.0e-07	9.0e-07	5.7e-01	2.8e-13
6	6.0e-14	1.3e-13	3.6e-02	5.2e-13
7	4.3e-16	1.1e-13	3.2e-06	5.3e-13
8			3.8e-16	5.3e-13

# Newton Behaviour

**Theorem 5** Let  $\mathbb{G} \in \mathfrak{U}$ ,  $A \in \mathbb{G}$ , and  $X_k$  be the Newton iterates, either unscaled or with Frobenius scaling. Then

$$X_k^\star = X_k^*, \quad k \geq 1. \text{ Moreover,}$$

$$MX_k = X_kM, \quad \text{real bilinear, complex sesquilinear forms,}$$

$$MX_k = \overline{X_k}M, \quad \text{complex bilinear forms.}$$

Implications:

★ Tethering.

★ Structure in  $X_k$ :

A pseudo-orthogonal  $\Rightarrow X_k$  block-diagonal,

$$\text{A symplectic} \Rightarrow X_k = \begin{bmatrix} E_k & F_k \\ -F_k & E_k \end{bmatrix}.$$

# Structured Iterations Versus Scaled Newton

- ★ Newton has slightly better observed numerical stability.
- ★ Newton usually requires the fewest flops.
- ★ Convergence prediction possible with structured iterations.
- ★ Which is best depends on matrix  $A$ , group  $\mathbb{G}$ , and user's accuracy requirements.

# Structured Matrix Sign

**Theorem 6** *Suppose the sign decomposition  $A = SN$  exists, where  $S = \text{sign}(A)$  and  $N = (A^2)^{1/2}$ .*

•  $A \in \mathbb{G} \implies S \in \mathbb{G}$  and  $N \in \mathbb{G}$ ,

•  $A \in \mathbb{L} \implies S \in \mathbb{L}$  and  $N \in \mathbb{J}$ ,

•  $A \in \mathbb{J} \implies S \in \mathbb{J}$  and  $N \in \mathbb{J}$ .

► Holds in any scalar space.

► Have (structured) iterations for matrix sign function analogous to polar factors ones.

Rule of thumb: replace  $A^*A$  by  $A^2$ .

# Structured Square Roots

**Theorem 7** *Suppose  $A$  has no eigenvalues on  $\mathbb{R}^-$ . Then*

- $A \in \mathbb{G} \implies A^{1/2} \in \mathbb{G},$
- $A \in \mathbb{J} \implies A^{1/2} \in \mathbb{J}.$
- $A \in \mathbb{L} \implies A^{1/2}$  *is never in  $\mathbb{L}$ .*

**Proof.** Use  $(A^*)^{1/2} = (A^{1/2})^*.$   $\square$

Holds in any scalar product space.

# Matrix Sign Relations

For  $A \in \mathbb{C}^{n \times n}$  with no eigenvalues on  $\mathbb{R}^-$  (Higham, 1997):

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

$\Rightarrow$  enables results and iterations for the **sign function** to be translated into results for the **square root**.

# Coupled Square Root Iteration

**Theorem 8** *Let  $X_{k+1} = g(X_k) = X_k h(X_k^2)$ ,  $X_0 = A$  be such that  $X_k \mapsto \text{sign}(A)$  with order  $m$ . Consider coupled iteration*

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

*Then*

- ▶  $Y_k \rightarrow A^{1/2}$ ,  $Z_k \rightarrow A^{-1/2}$  with order  $m$ .
- ▶ If  $g$  is structure preserving for  $\mathbb{G}$  then  $A \in \mathbb{G} \Rightarrow X_k, Y_k \in \mathbb{G}$  for all  $k$ .
- ▶ The iteration is stable.

# Square Root Iterations for $A \in \mathbb{G}$

**Cubic (structure-preserving):**

$$Y_{k+1} = \frac{1}{3}Y_k [I + 8(I + 3Z_k Y_k)^{-1}], \quad Y_0 = A,$$
$$Z_{k+1} = \frac{1}{3} [I + 8(I + 3Z_k Y_k)^{-1}] Z_k, \quad Z_0 = I.$$

**Newton iteration (not structure-preserving):**

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

**Rewritten form for Newton (not structure-preserving):**

$$Y_{k+1} = \frac{1}{2}(Y_k + Y_k^{-\star}), \quad Y_1 = (1/2)(I + A).$$

# Experiment

Pseudo-orthogonal  $A \in \mathbb{R}^{10 \times 10}$  with  $\kappa_2(A) = 10^{10}$ .

$$\text{err}(X) = \frac{\|X - A^{1/2}\|_2}{\|A^{1/2}\|_2}, \quad \mu_G(A) = \frac{\|A^*A - I\|_2}{\|A\|_2^2}.$$

$k$	Newton	Rewritten Newton	
	$\text{err}(X_k)$	$\text{err}(Y_k)$	$\mu_G(Y_k)$
0	3.2e+2		
1	1.6e+2	1.6e+2	1.0e-5
3	3.9e+1	3.9e+1	1.0e-5
5	8.9e+0	8.9e+0	9.9e-6
7	3.2e+1	1.6e+0	8.5e-6
9	4.6e+9	8.2e-2	1.5e-6
10	2.3e+9	3.1e-3	6.1e-8
11	1.1e+9	4.7e-6	9.5e-11
12	5.6e+8	2.1e-11	2.4e-16

# Experiment

Pseudo-orthogonal  $A \in \mathbb{R}^{10 \times 10}$  with  $\kappa_2(A) = 10^{10}$ .

$$\text{err}(X) = \frac{\|X - A^{1/2}\|_2}{\|A^{1/2}\|_2}, \quad \mu_G(A) = \frac{\|A^*A - I\|_2}{\|A\|_2^2}.$$

$k$	Rewritten Newton (scaled)		Cubic	
	$\text{err}(Y_k)$	$\mu_G(Y_k)$	$\text{err}(Y_k)$	$\mu_G(Y_k)$
0			3.2e+2	1.4e-15
1	1.6e+2	1.0e-5	1.0e+2	7.2e-15
2	7.4e-1	2.1e-3	3.4e+1	6.0e-14
3	1.9e-1	1.8e-4	1.1e+1	5.1e-13
4	6.0e-2	1.7e-5	3.0e+0	2.9e-12
5	4.9e-3	1.6e-6	5.5e-1	4.4e-12
6	1.2e-4	3.1e-8	2.0e-2	4.1e-12
7	3.6e-8	1.4e-11	2.0e-6	4.1e-12
8	2.1e-11	1.3e-16	2.1e-11	4.1e-12

# Choice of Method for $A^{1/2}$ for $A \in \mathbb{G}$

Suggest to use rewritten form of Newton's iteration:

$$Y_{k+1} = \frac{1}{2}(Y_k + Y_k^{-\star}), \quad Y_1 = (1/2)(I + A).$$

- ▶ Overcomes instability in standard Newton.
- ▶ Less costly per iteration for classical  $\mathbb{G}$  than standard Newton.
- ▶ More efficient than cubic structure-preserving iteration.
- ▶ Produces  $A^{1/2}$  closer to the group than cubic iteration.
- ▶ Half the cost of Denman-Beavers iteration.

# Papers and Reports

- ▶ [M,M,T] **Structured Tools for Structured Matrices**, ELA (10)106-145, 2003.
- ▶ [M,M,T]  **$\mathbb{G}$ -Reflectors: Analogues of Householder Transformations in Scalar Product Spaces**, to appear in LAA.
- ▶ [H,M,M,T] **Computing the Polar Decomposition and the Matrix Sign Decomposition in Matrix Groups**, NA report 426. To appear in SIMAX.
- ▶ [H,M,M,T] **Functions Preserving Matrix Groups and Iterations for the Matrix Square Root**, NA Report in preparation.
- ▶ [M,M,T] **Structured Factorizations in Scalar Product Spaces**, NA Report in preparation.

# Thomas

