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Computing the Square Root of a Low-Rank Perturbation of the Scaled Identity Matrix

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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.

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \pm 1 & 0 \\ 0 & \pm 1 \end{bmatrix}^2 = \begin{bmatrix} a & b \\ c & -a \end{bmatrix}^2, \quad a^2 + bc = 1.$$

Definition

For A with no eigenvalues on $\mathbb{R}^- = \{x \in \mathbb{R} \colon x \le 0\}$ the principal square root $A^{1/2}$ is unique square root X with spectrum in the region

$$-\pi/2 < \arg(\lambda(X)) < \pi/2.$$

Matrix Square Roots in Machine Learning

Shampoo (Gupta, Koren, & Singer, 2018): preconditioned stochastic gradient method for second-order optimization. Needs

$$L_t^{-1/2p} G_t R_t^{-1/2q}, \quad t = 1, \dots, \ell,$$

where

$$L_t = \alpha I_n + \sum_{s=1}^{t} G_s G_s^*, \quad R_t = \alpha I_k + \sum_{s=1}^{t} G_s^* G_s, \quad \alpha > 0,$$

and $G_1, \dots, G_t \in \mathbb{R}^{n \times k}$ are of rank at most r.

Visual recognition (Lin, 2020): features aggregated via bilinear pooling, using the square root of

$$A = \alpha I_n + \frac{1}{k} \sum_{i=1}^{k} x_i x_i^*, \quad \alpha > 0.$$

Computing the (principal) square root

$$A = \alpha I_n + UV^*, \quad \alpha \in \mathbb{C},\ U, V \in \mathbb{C}^{n\times k},\ k \le n,\ \Lambda(A) \cap \mathbb{R}^- = \emptyset.$$

Theorem (Harris, 1993; Higham, 2008)

Let $U, V \in \mathbb{C}^{n\times k}$ with $k \le n$ and assume that V^*U is nonsingular. Then

$$f(A) = f(\alpha) I_n + U(V^*U)^{-1}\Big(f(\alpha I_k + V^*U) - f(\alpha) I_k\Big) V^*.$$

Explicit Formula for General Functions

Theorem (Harris, 1993; Higham, 2008)

Let $U, V \in \mathbb{C}^{n\times k}$ with $k \le n$ and assume that V^*U is nonsingular. Then

$$f(A) = f(\alpha)I_n + U(V^*U)^{-1}\Big(f(\alpha I_k + V^*U) - f(\alpha)I_k\Big)V^*.$$

- $f(A)$ is a perturbation of rank at most k of the scaled identity matrix.
- $f(A)$ can be computed by evaluating f and the inverse at two $k \times k$ matrices.

Problem: requires V^*U nonsingular, which is not required for f to exist!

Sherman–Morrison–Woodbury Formula

If $U, V \in \mathbb{C}^{n\times k}$ and $I_k + V^*A^{-1}U$ is nonsingular then

$$(A + UV^*)^{-1} = A^{-1} - A^{-1}U(I_k + V^*A^{-1}U)^{-1}V^*A^{-1}.$$

- Does not require V^*U nonsingular!

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Derivation

Obtained using $A + UV^* = A(I_n + A^{-1}U \cdot V^*)$ and

$$(I_n + BC)^{-1} = I_n - B(I_k + CB)^{-1}C, \quad B \in \mathbb{C}^{n\times k}, C \in \mathbb{C}^{k\times n}$$

$$\begin{aligned} I &= I + BC - (I + BC)B(I + CB)^{-1}C \\ &= I + BC - B(I + CB)(I + CB)^{-1}C \\ &= I + BC - BC \end{aligned}$$

Square Root Update Formula

Theorem

Let $U, V \in \mathbb{C}^{n\times k}$ with $k \leq n$ have full rank and let the matrix $A = \alpha I_n + UV^*$ have no eigenvalues on $\mathbb{R}^-$. Then

$$A^{1/2} = \alpha^{1/2} I_n + U\Big((\alpha I_k + V^* U)^{1/2} + \alpha^{1/2} I_k\Big)^{-1} V^*.$$

- Does not contain the factor $(V^*U)^{-1}$!

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- Does not contain the factor $(V^*U)^{-1}$!

Key idea: Taking for f the square root in the $f(A)$ formula:

$$A^{1/2} = \alpha^{1/2} I_n + U(V^*U)^{-1}\Big((\alpha I_k + V^*U)^{1/2} - \alpha^{1/2} I_k\Big) V^*$$

and use

$$(\alpha I_k + V^*U)^{1/2} - \alpha^{1/2} I_k = V^*U\Big((\alpha I_k + V^*U)^{1/2} + \alpha^{1/2} I_k\Big)^{-1},$$

which is essentially $(\sqrt{1+x} - 1)/x = 1/(\sqrt{1+x} + 1)$!

Schur Method for the Square Root

- Compute Schur decomp. $A = QTQ^*$.

- Expand $U^2 = T$, where U is upper triangular, for primary square root:

$$u_{ii}^2 = t_{ii},$$

$$(u_{ii} + u_{jj})u_{ij} = t_{ij} - \sum_{k=i+1}^{j-1} u_{ik}u_{kj}.$$

U is found either a column or a superdiagonal at a time.

- $\sqrt{A} = QUQ^*$.

- **Schur decomp. may not be available**
  - In low precisions or on custom hardware. No nonsymmetric dense eigensolver in NVIDIA cuSOLVER library.
  - In multiprecision environments. E.g., Julia (Version 1.7.1) and MATLAB Symbolic Math Toolbox in VPA arithmetic.
- **Matrix Iterations** are attractive. Newton–Schulz iteration is being used in deep learning.

Newton methods

The (scaled) DB iteration is (Denman & Beavers, 1976)

$$X_{i+1} = \frac{1}{2}\left(\mu_i X_i + \mu_i^{-1} Y_i^{-1}\right), \quad X_0 = A,$$
$$Y_{i+1} = \frac{1}{2}\left(\mu_i Y_i + \mu_i^{-1} X_i^{-1}\right), \quad Y_0 = I,$$

for some scaling parameter $\mu_i \in \mathbb{R}$.

Product form DB (Cheng, Higham, Kenney, & Laub, 2001)

$$M_{i+1} = \frac{1}{2}\left(I + \frac{\mu_i^2 M_i + \mu_i^{-2} M_i^{-1}}{2}\right), \quad M_0 = A,$$
$$X_{i+1} = \frac{1}{2}\mu_i X_i\left(I + \mu_i^{-2} M_i^{-1}\right), \quad X_0 = A.$$
$$Y_{i+1} = \frac{1}{2}\mu_i Y_i\left(I + \mu_i^{-2} M_i^{-1}\right), \quad Y_0 = I.$$

The Structured DB Iteration

Facts: $A^{1/2}$ is a rank-k prturbation to $\alpha^{1/2} I_n$, and

$$A^{1/2} = \alpha^{1/2} I_n + U\big((\alpha I_k + V^* U)^{1/2} + \alpha^{1/2} I_k\big)^{-1} V^*.$$

is in the form $A^{1/2} = \alpha^{1/2} I_n + UZV^*$ for some $Z \in \mathbb{C}^{k\times k}$.

Key idea: For $A = \alpha I_n + UV^*$, write the DB iterates in the form

$$\begin{aligned} X_i &= \beta_i I_n + UB_i V^*, \quad \beta_i \in \mathbb{C}, \quad B_i \in \mathbb{C}^{k\times k}, \\ Y_i &= \gamma_i I_n + UC_i V^*, \quad \gamma_i \in \mathbb{C}, \quad C_i \in \mathbb{C}^{k\times k}, \end{aligned}$$

and use SMW

$$(A + UV^*)^{-1} = A^{-1} - A^{-1} U (I_k + V^* A^{-1} U)^{-1} V^* A^{-1}.$$

for X_i^{-1} and Y_i^{-1}.

The Structured DB Iteration

For $A = \alpha I_n + UV^*$, the DB iterates are

$$X_i = \beta_i I_n + UB_i V^*, \quad \beta_i \in \mathbb{C}, \quad B_i \in \mathbb{C}^{k\times k},$$
$$Y_i = \gamma_i I_n + UC_i V^*, \quad \gamma_i \in \mathbb{C}, \quad C_i \in \mathbb{C}^{k\times k},$$

where $\beta_0 = \alpha$, $B_0 = I_k$, $\gamma_0 = 1$, $C_0 = 0$, and

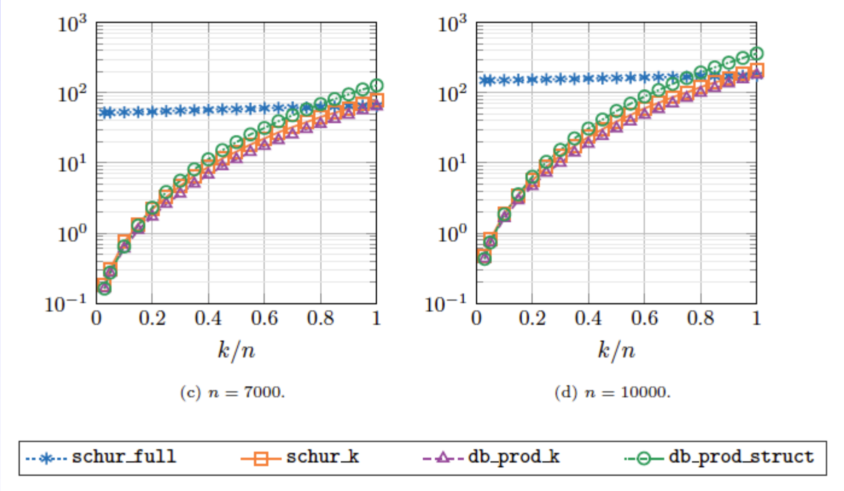
$$\beta_{i+1} = \frac{\mu_i\beta_i + (\mu_i\gamma_i)^{-1}}{2},$$
$$B_{i+1} = \frac{1}{2}\left(\mu_i B_i - (\mu_i\gamma_i)^{-1} C_i(\gamma_i I_k + V^* UC_i)^{-1}\right),$$
$$\gamma_{i+1} = \frac{\mu_i\gamma_i + (\mu_i\beta_i)^{-1}}{2},$$
$$C_{i+1} = \frac{1}{2}\left(\mu_i C_i - (\mu_i\beta_i)^{-1} B_i(\beta_i I_k + V^* UB_i)^{-1}\right).$$

Methods

$$A^{1/2} = \alpha^{1/2} I_n + U\Big((\alpha I_k + V^* U)^{1/2} + \alpha^{1/2} I_k\Big)^{-1} V^*$$

- Schur method on A.
- Schur method on $(\alpha I_k + V^* U)^{1/2}$.
- DB method on $(\alpha I_k + V^* U)^{1/2}$.
- Structured DB method on A.

Numerical Experiment



$A = \alpha I + UV^*$ with $\alpha = 0.1$ and U, V normal$(0, n^{-2})$.

Concluding Remarks

- $\sqrt{A}$ is enjoying new interest in machine learning applications. Exploiting the structure yields much faster algorithms than the standard Schur method!

- Schur decomposition is not always available, in which case matrix iterations are attractive!

M. Fasi, N. J. Higham and X. Liu. Computing the square root of a low-rank perturbation of the scaled identity matrix. MIMS EPrint 2022.1, Janurary 2022. Revised May 2022.

- Codes available at https://github.com/Xiaobo-Liu/sqrtm-lrpsi

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