Fast inclusion for the matrix inverse square root

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Inverse square root of nonsingular $A \in \mathbb{C}^{n \times n}$

is $X^* \in \mathbb{C}^{n \times n}$ s.t. ${X^*}^2 A = I_n$,

always exists for A being nonsingular,

is not unique.

If $\lambda_i(A) \notin \mathbb{R}_-$, $\forall i$, the principal inverse square root can be uniquely defined by requiring $\mathrm{Re}\lambda_i(X^*) > 0$, $\forall i$.

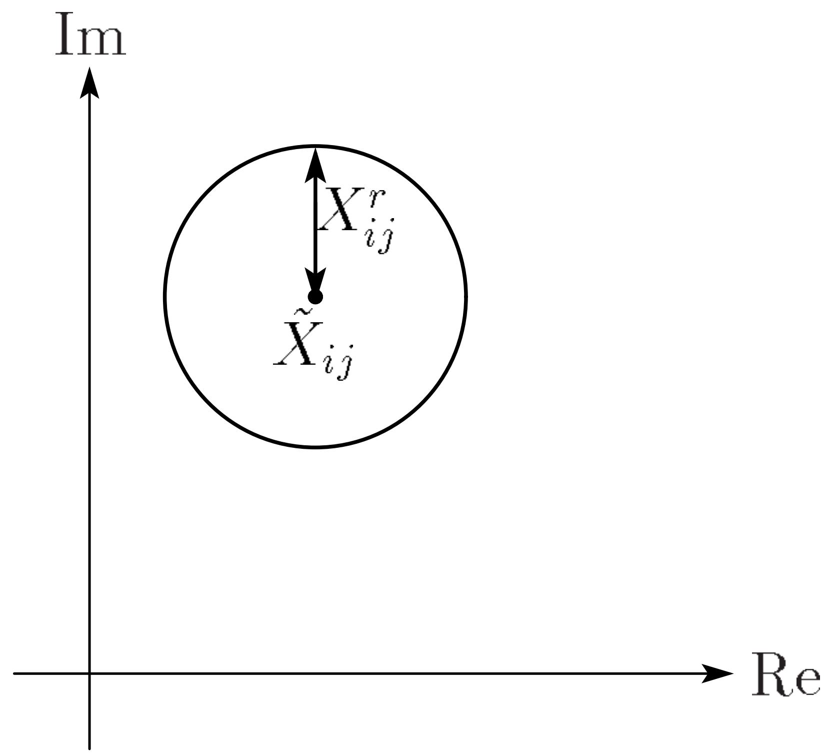
The principal inverse square root is of particular interest.

Purpose

Numerically computing $\tilde{X}$ and X^r s.t. $X^* \in \langle \tilde{X}, X^r \rangle$

Preferable

- Smaller X^r_{ij}
- Fast algorithm



Previous work

2 algorithms by Frommer-Hashemi-Sablik (2014)

- numerical spectral decomposition is utilized $\Rightarrow \mathcal{O}(n^3)$ operations
- Krawczyk operator is applied for nonlinear matrix equations

1st algorithm ($F(X) = 0$, where $F(X) := XAX - I_n$)

The uniqueness of the contained inverse square root is verified

2nd algorithm (an affine transformation of $F(X) = 0$)

Although the uniqueness is not verified, more effective than the 1st

Our contribution

Algorithm for computing $\tilde{X}$ and X^r s.t. $X^* \in \langle \tilde{X}, X^r \rangle$

- utilizes the spectral decomposition $\Rightarrow \mathcal{O}(n^3)$ operations
- adopts the affine transformation and Newton operator
- verifies the principal property and uniqueness

Affine transformation (1/2)

Assume we have diagonal $\tilde{D} \in \mathbb{C}^{n\times n}$ and $\tilde{V}, W \in \mathbb{C}^{n\times n}$ s.t. $A\tilde{V} \approx \tilde{V}\tilde{D}$, $W \approx \tilde{V}^{-1}$, and $\tilde{V}$ and W are nonsingular (verifiable).

$Q := \tilde{D} - WA\tilde{V}$, $S := I_n - W\tilde{V}$ ($Q \approx 0$, $S \approx 0$), $Y := \tilde{V}^{-1}XW^{-1}$

$$
\begin{aligned}
F(X) = 0 \;&\Leftrightarrow\; \tilde{V}^{-1}XW^{-1}WA\tilde{V}\tilde{V}^{-1}XW^{-1} - \tilde{V}^{-1}W^{-1} = 0 \\
&\Leftrightarrow\; Y(\tilde{D} - (\tilde{D} - WA\tilde{V}))Y - (W\tilde{V})^{-1} = 0 \\
&\Leftrightarrow\; Y(\tilde{D} - Q)Y - (I_n - S)^{-1} = 0 \\
&\Leftrightarrow\; Y(\tilde{D} - Q)Y - I_n - (I_n - S)^{-1}S = 0.
\end{aligned}
$$

Affine transformation (2/2)

$F(X) = 0 \Leftrightarrow \hat{F}(Y) = 0$, $\hat{F}(Y) := Y(\tilde{D} - Q)Y - I_n - (I_n - S)^{-1}S$.

We compute an interval matrix $\boldsymbol{Y}$ s.t. $Y^* \in \boldsymbol{Y}$ and $\hat{F}(Y^*) = 0$

and enclose X^* by computing the superset of $\{\tilde{V}YW : Y \in \boldsymbol{Y}\}$.

Since $X^* = \tilde{V}Y^*W$, the superset contains X^*.

The superset can be obtained by interval arithmetic.

How to obtain Y?

$\hat{F}'_Y(H) = Y(\tilde{D} - Q)H + H(\tilde{D} - Q)Y$. Let $\tilde{Y} \approx Y^*$ be diagonal.

If $\hat{F}'_{\tilde{Y}}(H)$ is invertible, $\hat{N}(Y) := Y - (\hat{F}'_{\tilde{Y}})^{-1}(\hat{F}(Y))$.

$\hat{N}(Y) = Y$ is a fixed point equation for Y.

We thus verify the invertibility and

$\{\hat{N}(Y) : Y \in \langle \tilde{Y}, Y^r \rangle\} \subseteq \mathrm{int}(\langle \tilde{Y}, Y^r \rangle)$ for given $Y^r \in \mathbb{R}^{n \times n}$.

The Brouwer theorem then implies $Y^* \in \{\hat{N}(Y) : Y \in \langle \tilde{Y}, Y^r \rangle\}$.

$\boldsymbol{Y}$ can be obtained s.t. $\{\hat{N}(Y) : Y \in \langle \tilde{Y}, Y^r \rangle\} \subseteq \boldsymbol{Y}$.

How to verify the invertibility?

$\hat{F}'_{\tilde{Y}}(H)$ can be represented in terms of matrix vector products as

$\mathrm{vec}(\hat{F}'_{\tilde{Y}}(H)) = \hat{\mathsf{P}}\mathrm{vec}(H)$, $\hat{\mathsf{P}} := I_n \otimes \tilde{Y}(\tilde{D} - Q) + \tilde{Y}^T(\tilde{D} - Q)^T \otimes I_n$

If $\hat{\mathsf{P}}$ is nonsingular, $\hat{F}'_{\tilde{Y}}(H)$ is invertible. We verify the nonsingularity.

$\hat{\mathsf{P}}$ is a $n^2 \times n^2$ matrix.

By exploiting the sparsity of $\tilde{D}$ and $\tilde{Y}$, however, this can be achieved with $\mathcal{O}(n^3)$ operations.

$\{\hat{N}(Y) : Y \in \langle \tilde{Y}, Y^r \rangle\} \subseteq \mathrm{int}(\langle \tilde{Y}, Y^r \rangle)$? (1/2)

We compute $Y^\varepsilon \in \mathbb{R}^{n\times n}$ s.t. $\{\hat{N}(Y) : Y \in \langle \tilde{Y}, Y^r \rangle\} \subseteq \langle \tilde{Y}, Y^\varepsilon \rangle$ and verify $Y^\varepsilon < Y^r$. Y^ε can be obtained by the following idea:

$\hat{N}(Y) = Y - (\hat{F}'_{\tilde{Y}})^{-1}(\hat{F}(Y)) \Leftrightarrow \hat{F}'_{\tilde{Y}}(\hat{N}(Y)) = \hat{F}'_{\tilde{Y}}(Y) - \hat{F}(Y)$

LHS $= \tilde{Y}(\tilde{D} - Q)\hat{N}(Y) + \hat{N}(Y)(\tilde{D} - Q)\tilde{Y}$

RHS $= \tilde{Y}(\tilde{D} - Q)Y + Y(\tilde{D} - Q)\tilde{Y} - Y(\tilde{D} - Q)Y + I_n + (I_n - S)^{-1}S$

$\{\hat{\boldsymbol{N}}(\boldsymbol{Y}) : \boldsymbol{Y} \in \langle \tilde{\boldsymbol{Y}}, \boldsymbol{Y}^r \rangle\} \subseteq \mathbf{int}(\langle \tilde{\boldsymbol{Y}}, \boldsymbol{Y}^r \rangle)$? (2/2)

$\{\hat{N}(Y) : Y \in \langle \tilde{Y}, Y^r \rangle\}$ is the set of all solutions of an equation

$$\tilde{Y}(\tilde{D} - Q)\hat{N}_Y + \hat{N}_Y(\tilde{D} - Q)\tilde{Y}$$

$$= \tilde{Y}(\tilde{D} - Q)Y + Y(\tilde{D} - Q)\tilde{Y} - Y(\tilde{D} - Q)Y + I_n + (I_n - S)^{-1}S,$$

where $\hat{N}_Y \in \mathbb{C}^{n\times n}$ is unknown and $Y \in \langle \tilde{Y}, Y^r \rangle$ is the parameter.

We hence enclose the solution set, which can be achieved with $\mathcal{O}(n^3)$ operations.

How to determine Y^r?

In the computation of Y^ε, Y^r is required.

Let Y_0^ε be Y^ε when $Y^r = 0$. For $\eta \in \mathbb{R}$, we put $Y^r = \eta Y_0^\varepsilon$ and determine η s.t. $Y^\varepsilon < \eta Y_0^\varepsilon = Y^r$.

Note The determination of η includes some assumptions. If one of the assumptions cannot be verified, this determination fails.

How to verify the principal property?

Let $X^* \in \langle \tilde{X}, X^r \rangle$ and $X \in \langle \tilde{X}, X^r \rangle$ be arbitrary.

We show $\mathrm{Re}\lambda_i(X) > 0$, $\forall i$. Then $\mathrm{Re}\lambda_i(X^*) > 0$, $\forall i$.

Since the principal square root is unique, the uniqueness can also be verified.

By reusing the previously computed matrices, this can be achieved with $\mathcal{O}(n^2)$ operations.

The uniqueness when $\lambda_i(A) \in \mathbb{R}_-$? (1/2)

Let X^* and X^{**}, and X_1 and X_2 be the inverse square roots and arbitrarily matrices contained in $\langle \tilde{X}, X^r \rangle$, respectively. We show the invertibility of $F'_{\tilde{V}\tilde{Y}W}(H)$, use $N(X) := X - (F'_{\tilde{V}\tilde{Y}W})^{-1}(F(X))$ (Note $N(X^*) = X^*$, $N(X^{**}) = X^{**}$), derive $\mathsf{S}(X_1, X_2)$ s.t.

$\mathrm{vec}(N(X_1) - N(X_2)) = \mathsf{S}(X_1, X_2)\mathrm{vec}(X_1 - X_2)$,

and prove $\|\mathsf{S}(X_1, X_2)\|_\infty < 1$, which gives $\|\mathsf{S}(X^*, X^{**})\|_\infty < 1$.

The uniqueness when $\lambda_i(A) \in \mathbb{R}_-$? (2/2)

We obtain

$$\begin{aligned} \|\mathrm{vec}(X^* - X^{**})\|_\infty &= \|\mathrm{vec}(N(X^*) - N(X^{**}))\|_\infty \\ &= \|\mathsf{S}(X^*, X^{**})\mathrm{vec}(X^* - X^{**})\|_\infty \\ &\leq \|\mathsf{S}(X^*, X^{**})\|_\infty \|\mathrm{vec}(X^* - X^{**})\|_\infty, \end{aligned}$$

so that $(1 - \|\mathsf{S}(X^*, X^{**})\|_\infty)\|\mathrm{vec}(X^* - X^{**})\|_\infty \leq 0$.

This and $\|\mathsf{S}(X^*, X^{**})\|_\infty < 1$ implies $X^* = X^{**}$.

These can be achieved with $\mathcal{O}(n^3)$ operations.

Numerical results (1/2)

Intel Xeon 2.66GHz Dual CPU, 4.00GB RAM, MATLAB 7.5 with Intel MKL, and IEEE 754 double precision

- `FHS1`: 1st algorithm by Frommer-Hashemi-Sablik (2014) (the uniqueness is verified)
- `FHS2`: 2nd algorithm by Frommer-Hashemi-Sablik (2014) (the uniqueness is not verified)
- `M`: the proposed algorithm (the principal property and uniqueness are verified)

–: `FHS1` or `FHS2` did not succeed after 30 iterations

Numerical results (2/2)

Let $X^* \in \langle \tilde{X}, X^r \rangle$, mrp $:= \max_{i,j} X^p_{ij}$ and arp $:= (\sum_{i,j=1}^n X^p_{ij})/n^2$,

where $X^p_{ij} := \begin{cases} \min\left(1, \dfrac{X^r_{ij}}{|\tilde{X}_{ij}|}\right) & (\tilde{X}_{ij} \neq 0) \\ 1 & (\tilde{X}_{ij} = 0) \end{cases}$.

mrp and arp by `M` with underline: both of the principal property and uniqueness could not be verified

Results for "frank" matrix

n	FHS1 mrp arp	FHS2 mrp arp	M mrp arp	FHS1 time	FHS2 time	M time
7	2.6e–10	2.6e–10	6.2e–11	4.3e–1	1.3e–2	3.4e–3
	4.4e–11	4.4e–11	1.6e–11			
8	–	5.5e–9	1.0e–9	1.7e–1	1.1e–2	3.4e–3
	–	1.0e–9	2.1e–10			
9	–	–	1.5e–8	1.4e–1	1.3e–1	3.3e–3
	–	–	2.9e–9			
12	–	–	1.4e–1	1.4e–1	1.3e–1	4.1e–3
	–	–	2.8e–3			
13	–	–	fail	1.4e–1	1.3e–1	3.5e–3
	–	–	fail			

Results for “poisson” matrix

n	FHS1 mrp arp	FHS2 mrp arp	M mrp arp	FHS1 time	FHS2 time	M time
400	5.7e–7	5.5e–7	4.3e–8	3.7e+0	3.6e+0	8.2e–1
	3.0e–9	2.8e–9	2.2e–10			
625	–	3.2e–6	1.9e–7	1.4e+2	1.3e+1	2.8e+0
	–	9.6e–9	5.6e–10			
900	–	1.4e–5	6.6e–7	3.8e+2	3.5e+1	7.9e+0
	–	2.7e–8	1.2e–9			
1225	–	5.0e–5	2.0e–6	9.2e+2	8.6e+1	1.9e+1
	–	6.0e–8	2.4e–9			
1600	–	1.5e–4	4.7e–6	1.9e+3	1.8e+2	4.2e+1
	–	1.3e–7	4.1e–9			

Results for "prolate" matrix

n	FHS1 mrp arp	FHS2 mrp arp	M mrp arp	FHS1 time	FHS2 time	M time
10	4.6e–9	4.6e–9	6.2e–10	6.7e–2	1.2e–2	3.6e–3
	3.5e–10	3.5e–10	1.8e–10			
12	–	2.2e–7	1.9e–8	1.4e–1	3.6e–2	3.4e–3
	–	1.5e–8	5.7e–9			
14	–	–	1.6e–6	1.4e–1	1.3e–1	3.5e–3
	–	–	4.0e–7			
20	–	–	2.3e–1	1.5e–1	1.4e–1	4.4e–3
	–	–	4.8e–2			
22	–	–	fail	1.6e–1	1.4e–1	3.6e–3
	–	–	fail			

Results for “toeppen” matrix

n	FHS1 mrp arp	FHS2 mrp arp	M mrp arp	FHS1 time	FHS2 time	M time
400	1.0e+0	1.0e+0	1.0e+0	1.4e+1	1.4e+1	2.8e+0
	2.0e–1	2.0e–1	1.7e–1			
600	–	1.0e+0	1.0e+0	4.1e+2	4.0e+1	7.8e+0
	–	4.1e–1	3.8e–1			
800	–	1.0e+0	1.0e+0	8.8e+2	8.8e+1	1.7e+1
	–	5.4e–1	5.1e–1			
1000	–	1.0e+0	1.0e+0	1.6e+3	1.6e+2	3.2e+1
	–	6.2e–1	6.0e–1			
1200	–	1.0e+0	1.0e+0	2.6e+3	2.7e+2	5.3e+1
	–	6.8e–1	6.6e–1			