# THE FACTORS IN THE SR DECOMPOSITION AND THEIR CONDITIONING

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# Orthogonalization with respect to an inner product

$B \in \mathcal{R}^{m,m}$ symmetric positive definite, inner product $\langle \cdot, \cdot \rangle_B$

$A = (a_1, \ldots, a_n) \in \mathcal{R}^{m,n}$, $m \geq n = rank(A)$

$B$-orthonormal basis of $span(A)$:

$Q = (q_1, \ldots, q_n) \in \mathcal{R}^{m,n}$, $Q^T BQ = I_n$

$A = QR$, $R \in \mathcal{R}^{n,n}$ upper triangular with positive diagonal entries

$B^{1/2}A = (B^{1/2}Q)R$, $\kappa(B^{1/2}Q) = 1$,
$\kappa(R) = \kappa(B^{1/2}A)$, but $\kappa(Q) \leq \kappa^{1/2}(B))$ !

$$C = A^T BA = R^T R$$

# Orthogonalization with respect to a symmetric bilinear form

$B \in \mathcal{R}^{m,m}$ symmetric indefinite and nonsingular

$$A = (a_1, \ldots, a_n) \in \mathcal{R}^{m,n},\ m \geq n = rank(A)$$

$B$-orthonormal basis of $span(A)$:

$$Q = (q_1, \ldots, q_n) \in \mathcal{R}^{m,n},\ Q^T B Q = \Omega \in \mathrm{diag}(\pm 1)$$

$A = QR$, $R \in \mathcal{R}^{n,n}$ upper triangular with positive diagonal

if no principal minor of $C$ vanishes (if $C$ is strongly nonsingular)

$$C = A^T B A = R^T \Omega R$$

Bunch 1971, Bunch-Parlett 1971

Della Dora 1975, Elsner 1979, Bunse-Gerstner 1981

Slapničar, Veselić, 1999, Slapničar 1999, Singer and Singer 2000, Singer 2006

Higham, $J$-orthogonal matrices, SIAM Review 2003

Fiedler, Hall, Markham, $G$-matrices, 2012-2013

# Cholesky-like factorization of a symmetric indefinite matrix

$$C_j = A_j^T B A_j = \begin{pmatrix} C_{j-1} & c_{1:j-1,j} \\ c_{1:j-1,j}^T & c_{j,j} \end{pmatrix} =$$

$$\begin{pmatrix} R_{j-1}^T & 0 \\ r_{1:j-1,j}^T & r_{j,j} \end{pmatrix} \begin{pmatrix} \Omega_{j-1} & 0 \\ 0 & \omega_j \end{pmatrix} \begin{pmatrix} R_{j-1} & r_{1:j-1,j} \\ 0 & r_{j,j} \end{pmatrix}$$

$$r_{j,j}^2 \omega_j = c_{j,j} - c_{1:j-1,j}^T C_{j-1}^{-1} c_{1:j-1,j} = s_j$$

$$C_j^{-1} = \begin{pmatrix} C_{j-1}^{-1} + C_{j-1}^{-1} c_{1:j-1,j} s_j^{-1} c_{1:j-1,j}^T C_{j-1}^{-1} & -C_{j-1}^{-1} c_{1:j-1,j} s_j^{-1} \\ -s_j^{-1} c_{1:j-1,j}^T C_{j-1}^{-1} & s_j^{-1} \end{pmatrix}$$

$$\sqrt{\frac{1}{\|C_j^{-1}\|}} \le r_{j,j} = \sqrt{|s_j|} \le \sqrt{(\|C_{j-1}^{-1}\| \|C_j\| + 1)\|C_j\|}$$

# The inverse of the triangular factor in Cholesky-like factorization

$$R_j^{-1} = \begin{pmatrix} R_{j-1}^{-1} & -C_{j-1}^{-1} c_{1:j-1,j} / \sqrt{|s_j|} \\ 0 & 1/\sqrt{|s_j|} \end{pmatrix}$$

$$(R_j^T R_j)^{-1} = \begin{pmatrix} (R_{j-1}^T R_{j-1})^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \omega_j \left[ C_j^{-1} - \begin{pmatrix} C_{j-1}^{-1} & 0 \\ 0 & 0 \end{pmatrix} \right]$$

$$\|R_j^{-1}\|^2 \leq \|C_j^{-1}\| + 2 \sum_{i=1,\dots,j-1;\ \omega_{i+1} \neq \omega_i} \|C_i^{-1}\|$$

$$C_j = R_j^T \Omega_j R_j, \quad \|R_j\| \leq \|C_j\| \|R_j^{-1}\|$$

# Example with $\kappa(R) \approx \kappa^{1/2}(B)$

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; B = \begin{pmatrix} 1 & \sqrt{\varepsilon} \\ \sqrt{\varepsilon} & -\varepsilon \end{pmatrix}$$

$$Q = R^{-1} = \begin{pmatrix} 1 & -1 \\ 0 & \frac{1}{\sqrt{\varepsilon}} \end{pmatrix}, \quad R = Q^{-1} = \begin{pmatrix} 1 & \sqrt{\varepsilon} \\ 0 & \sqrt{\varepsilon} \end{pmatrix}, \quad \Omega = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\|B\| \approx 1 + \varepsilon \text{ and } \sigma_{min}(B) = 2\varepsilon$$

$$\|R\| \approx \sqrt{1+\varepsilon}, \;\; \sigma_{min}(R) \approx \sqrt{\varepsilon}, \;\; \kappa(R) = \kappa(Q) \approx \frac{1}{\sqrt{\varepsilon}}$$

## Example with $\kappa(R) \gg \kappa^{1/2}(B)$

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ B = \begin{pmatrix} \varepsilon & 1 \\ 1 & -\varepsilon \end{pmatrix}$$

$$Q = R^{-1} = \begin{pmatrix} \frac{1}{\sqrt{\varepsilon}} & -\frac{1}{\sqrt{\varepsilon(1+\varepsilon^2)}} \\ 0 & \frac{\sqrt{\varepsilon}}{\sqrt{1+\varepsilon^2}} \end{pmatrix}, \quad R = Q^{-1} = \begin{pmatrix} \sqrt{\varepsilon} & \frac{1}{\sqrt{\varepsilon}} \\ 0 & \frac{\sqrt{1+\varepsilon^2}}{\sqrt{\varepsilon}} \end{pmatrix}, \quad \Omega = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\|B\| = \sigma_{min}(B) = \sqrt{1+\varepsilon^2}$$

$$\|R\| \approx \frac{\sqrt{2}}{\sqrt{\varepsilon}},\ \sigma_{min}(R) \approx \frac{\sqrt{\varepsilon}}{\sqrt{2}}, \quad \kappa(R) = \kappa(Q) \approx \frac{2}{\varepsilon}$$

# Orthogonalization with respect to a skew-symmetric bilinear form

$$A = (A_1, \ldots, A_n) \in \mathcal{R}^{2m,2n},\ m \geq n,\ rank(A) = 2n,$$
$$A_j \in \mathcal{R}^{2m,2},\ j = 1, \ldots, n$$

$J$-orthonormal basis of $span(A)$:

$$Q = (Q_1, \ldots, Q_n) \in \mathcal{R}^{2m,2n},\ Q_j \in \mathcal{R}^{2m,2},\ j = 1, \ldots, n$$

$J$ skew-symmetric, $J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix} \in \mathcal{R}^{2m,2m}$

$$Q^T J Q = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & & \\ & \ddots & \\ & & \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{pmatrix} \in \mathcal{R}^{2n,2n}$$

# SR decomposition

$$A = QR$$

$Q$ semi-symplectic and $R$ upper triangular with positive diagonal

$$Q = (Q_1, \ldots, Q_n) \in \mathcal{R}^{2m,2n},\ R = \begin{pmatrix} R_{1,1} & \ldots & R_{1,n} \\ & \ddots & \vdots \\ & & R_{n,n} \end{pmatrix} \in \mathcal{R}^{2n,2n}$$

if no minor of $C$ with even dimension vanishes

$$C = A^T JA = R^T \mathrm{diag}(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \ldots, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix})R$$

Della Dora 1975, Elsner 1979, Bunse-Gerstner 1981
Mehrmann 1979, Bunse-Gerstner and Mehrmann 1986
Benner, Byers, Fassbender, Mehrmann, Watkins 2000

# Uniqueness of the Cholesky-like factorization? 2 x 2 case

$$C = R^T J R = \begin{pmatrix} r_{11} & 0 \\ r_{12} & r_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & r_{11}r_{22} \\ -r_{11}r_{22} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \pm\|C\| \\ \mp\|C\| & 0 \end{pmatrix}$$

How to choose the factor $R = \begin{pmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{pmatrix}$?

Mehrmann 1979, Bunse-Gerstner and Mehrmann 1986
Fassbender 2000, Benner 2003
Salam 2005
Ferng, Lin, Wang 1997
Bhatia 1994, Chang, 1998

## Minimization of the condition number of $R$

$$\kappa^2(R) = \frac{\|R\|_F^2 + \sqrt{\|R\|_F^4 - 4r_{11}^2 r_{22}^2}}{\|R\|_F^2 - \sqrt{\|R\|_F^4 - 4r_{11}^2 r_{22}^2}}$$

As $r_{11}r_{22} = \pm\|C\|$ is fixed and $\kappa(R)$ is an increasing function of $\|R\|_F$, it is minimized if $r_{12} = 0$ and $r_{11} = \pm\sqrt{\|C\|}$, $r_{22} = \pm\sqrt{\|C\|}$. Then

$$R^T R = \|C\| \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \kappa(R) = 1$$

.

$$A = \begin{pmatrix} \sqrt{\varepsilon} & 1 \\ 1 & 0 \\ 0 & \sqrt{\varepsilon} \\ 0 & 0 \end{pmatrix}, A^T J A = \begin{pmatrix} 0 & \varepsilon \\ -\varepsilon & 0 \end{pmatrix}, R = \begin{pmatrix} \sqrt{\varepsilon} & 0 \\ 0 & \sqrt{\varepsilon} \end{pmatrix}$$

$$Q = AR^{-1} = \begin{pmatrix} 1 & 1/\sqrt{\varepsilon} \\ 1/\sqrt{\varepsilon} & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}$$

# Orthogonal factor $Q$?

$$r_{11} = \|a_1\| = \sqrt{1+\varepsilon},\ q_1 = \frac{1}{\sqrt{1+\varepsilon}} \begin{pmatrix} \sqrt{\varepsilon} \\ 1 \\ 0 \\ 0 \end{pmatrix},\ r_{12} = q_1^T a_2 = \frac{\sqrt{\varepsilon}}{\sqrt{1+\varepsilon}},$$

$$r_{22} = \frac{a_1^T J a_2}{r_{11}} = \frac{\varepsilon}{\sqrt{1+\varepsilon}},\ q_2 = \frac{1}{r_{22}}(a_2 - r_{12} q_1) = \frac{1}{\varepsilon} \begin{pmatrix} \frac{1}{\sqrt{1+\varepsilon}} \\ -\frac{\sqrt{\varepsilon}}{\sqrt{1+\varepsilon}} \\ \sqrt{\varepsilon}\sqrt{1+\varepsilon} \\ 0 \end{pmatrix}$$

$$Q^T Q = \begin{pmatrix} 1 & 0 \\ 0 & \approx \frac{1}{\varepsilon^2(1+\varepsilon)} \end{pmatrix},\ \kappa(Q) \approx \frac{1}{\varepsilon}$$

$$R = \begin{pmatrix} \sqrt{1+\varepsilon} & \frac{\sqrt{\varepsilon}}{\sqrt{1+\varepsilon}} \\ 0 & \frac{\varepsilon}{\sqrt{1+\varepsilon}} \end{pmatrix},\ \lambda(R^T R) \approx 1 + 2\varepsilon, \varepsilon^2/16,\ \kappa(R) \approx \frac{4}{\varepsilon}$$

## Minimization of the condition number of $Q$

$$Q = AR^{-1},\ \kappa^2(Q) = \frac{\|Q\|_F^2 + \sqrt{\|Q\|_F^4 - 4\frac{(\|A\|\sigma_{min}(A))^2}{\|C\|^2}}}{\|Q\|_F^2 - \sqrt{\|Q\|_F^4 - 4\frac{(\|A\|\sigma_{min}(A))^2}{\|C\|^2}}}$$

As $\kappa(A)/\|C\|$ is fixed and $\kappa(Q)$ is an increasing function of $\|Q\|_F$, it is minimized if $r_{12}$ is chosen so that $q_1 \perp q_2$ with $\|q_1\| = \|q_2\|$, $r_{11} = \|a_1\|\|C\|^{1/2}/(\|A\|\sigma_{min}(A))^{1/2}$ and $r_{22} = \|C\|/r_{1,1}$. Then

$$Q^TQ = \frac{\|A\|\sigma_{min}(A)}{\|C\|}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \kappa(Q) = 1$$

.

$$R = \begin{pmatrix} \frac{\sqrt{\varepsilon}\sqrt{1+\varepsilon}}{\sqrt[4]{1+\varepsilon+\varepsilon^2}} & \frac{\varepsilon}{\sqrt{1+\varepsilon}\sqrt[4]{1+\varepsilon+\varepsilon^2}} \\ 0 & \frac{\sqrt{\varepsilon}\sqrt[4]{1+\varepsilon+\varepsilon^2}}{\sqrt{1+\varepsilon}} \end{pmatrix}$$

$$Q = AR^{-1} = \begin{pmatrix} \frac{\sqrt[4]{1+\varepsilon+\varepsilon^2}}{\sqrt{1+\varepsilon}} & \frac{1}{\sqrt{\varepsilon}\sqrt{1+\varepsilon}\sqrt[4]{1+\varepsilon+\varepsilon^2}} \\ \frac{\sqrt[4]{1+\varepsilon+\varepsilon^2}}{\sqrt{\varepsilon}\sqrt{1+\varepsilon}} & -\frac{1}{\sqrt{1+\varepsilon}\sqrt[4]{1+\varepsilon+\varepsilon^2}} \\ 0 & \frac{\sqrt{1+\varepsilon}}{\sqrt[4]{1+\varepsilon+\varepsilon^2}} \\ 0 & 0 \end{pmatrix}$$

# Cholesky-like factorization of a skew-symmetric matrix

$$C_{2k} = A_{2k}^T J A_{2k} = \begin{pmatrix} & C_{2(k-1)} & & \begin{matrix} C_{1,k} \\ \vdots \\ C_{k-1,k} \end{matrix} \\ -C_{1,k}^T & \dots & -C_{k-1,k}^T & \hat{C}_{k,k} \end{pmatrix} =$$

$$R_{2k}^T \begin{pmatrix} \hat{J}_{2(k-1)} & 0 \\ 0 & \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{pmatrix} R_{2k}, R_{2k} = \begin{pmatrix} R_{2(k-1)} & \begin{matrix} R_{1,k} \\ \vdots \\ R_{k-1,k} \end{matrix} \\ 0 & R_{k,k} \end{pmatrix}$$

$$R_{i,k} = \hat{J}_{2(k-1)}^{-1} R_{2(k-1)}^{-T} C_{i,k}$$

$$R_{k,k}^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} R_{k,k} = C_{k,k} + \sum_{i=1}^{k-1} C_{i,k}^T C_{2(k-1)}^{-1} C_{i,k} = C_{2k} \backslash C_{2(k-1)}$$

# The inverse of the triangular factor in Cholesky-like factorization

$$R_{2k}^{-1} = \begin{pmatrix} R_{2(k-1)}^{-1} & -R_{2(k-1)}^{-1} \begin{pmatrix} R_{1,k} \\ \vdots \\ R_{k-1,k} \end{pmatrix} R_{k,k}^{-1} \\ 0 & R_{k,k}^{-1} \end{pmatrix}$$

$$= \begin{pmatrix} R_{2(k-1)}^{-1} & -C_{2(k-1)}^{-1} \begin{pmatrix} C_{1,k} \\ \vdots \\ C_{k-1,k} \end{pmatrix} R_{k,k}^{-1} \\ 0 & R_{k,k}^{-1} \end{pmatrix}$$

$$\|R_{2n}^{-1}\|^2 \leq \|C_{2n}^{-1}\| + \sqrt{2} \sum_{k=1}^{n-1} (\|C_{2(k-1)}^{-1} \begin{pmatrix} C_{1,k} \\ \vdots \\ C_{k-1,k} \end{pmatrix} \| + 1)^2 \|R_{k,k}^{-1}\|$$

$$\|R_{2n}\| \leq \|C_{2n}\| \|R_{2n}^{-1}\|$$

# Example with $\kappa(R) \approx \kappa(A)$

$$A = \begin{pmatrix} \sqrt{\varepsilon} & 0 & 0 & -\frac{1}{\sqrt{\varepsilon}} \\ 0 & 0 & 0 & \frac{\sqrt{1-\varepsilon^2}}{\sqrt{\varepsilon}} \\ 0 & \sqrt{\varepsilon} & \frac{1}{\sqrt{\varepsilon}} & 0 \\ 0 & 0 & \frac{\sqrt{1-\varepsilon^2}}{\sqrt{\varepsilon}} & 0 \end{pmatrix}, \; A^T J A = \begin{pmatrix} 0 & \varepsilon & 1 & 0 \\ -\varepsilon & 0 & 0 & 1 \\ -1 & 0 & 0 & \varepsilon \\ 0 & -1 & -\varepsilon & 0 \end{pmatrix}$$

$$Q = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad R = \begin{pmatrix} \sqrt{\varepsilon} & 0 & 0 & -\frac{1}{\sqrt{\varepsilon}} \\ 0 & \sqrt{\varepsilon} & \frac{1}{\sqrt{\varepsilon}} & 0 \\ 0 & 0 & \frac{\sqrt{1-\varepsilon^2}}{\sqrt{\varepsilon}} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{1-\varepsilon^2}}{\sqrt{\varepsilon}} \end{pmatrix}$$

$$\sigma(A) \approx \frac{\sqrt{2}}{\sqrt{\varepsilon}}, \frac{\sqrt{\varepsilon}}{\sqrt{2}}, \; \kappa(A) \approx \frac{2}{\varepsilon},$$
$$\sigma(R) \approx \frac{\sqrt{2}}{\sqrt{\varepsilon}}, \frac{\sqrt{\varepsilon}}{\sqrt{2}}, \; \kappa(R) \approx \frac{2}{\varepsilon}, \; \kappa(Q) = 1$$

## Example with $\kappa(R) \gg \kappa(A)$

$$A = \begin{pmatrix} \sqrt{\varepsilon} & 1 & 0 & 0 \\ 1 & 0 & 0 & -\varepsilon \\ 0 & \sqrt{\varepsilon} & 0 & 1 \\ 0 & 0 & 1 & -\sqrt{\varepsilon} \end{pmatrix}, \; A^T J A = \begin{pmatrix} 0 & \varepsilon & 1 & 0 \\ -\varepsilon & 0 & 0 & 1 \\ -1 & 0 & 0 & \varepsilon \\ 0 & -1 & -\varepsilon & 0 \end{pmatrix}$$

$$Q = \begin{pmatrix} 1 & 0 & \frac{\sqrt{\varepsilon}}{\sqrt{1-\varepsilon^2}} & -\frac{1}{\sqrt{1-\varepsilon^2}} \\ \frac{1}{\sqrt{\varepsilon}} & 0 & 0 & -\frac{\sqrt{1-\varepsilon^2}}{\sqrt{\varepsilon}} \\ 0 & 0 & \frac{\sqrt{\varepsilon}}{\sqrt{1-\varepsilon^2}} & -\frac{\sqrt{\varepsilon}}{\sqrt{1-\varepsilon^2}} \\ 0 & \frac{1}{\sqrt{\varepsilon}} & -\frac{\sqrt{\varepsilon}}{\sqrt{1-\varepsilon^2}} & \frac{\varepsilon}{\sqrt{1-\varepsilon^2}} \end{pmatrix},$$

$$R = \begin{pmatrix} \sqrt{\varepsilon} & 0 & 0 & -\frac{1}{\sqrt{\varepsilon}} \\ 0 & \sqrt{\varepsilon} & \frac{1}{\sqrt{\varepsilon}} & 0 \\ 0 & 0 & \frac{\sqrt{1-\varepsilon^2}}{\sqrt{\varepsilon}} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{1-\varepsilon^2}}{\sqrt{\varepsilon}} \end{pmatrix}$$

$$\sigma(A) \approx 1, \; \kappa(A) \approx 1,$$
$$\sigma(R) \approx \frac{\sqrt{2}}{\sqrt{\varepsilon}}, \frac{\sqrt{\varepsilon}}{\sqrt{2}}, \; \kappa(R) \approx \frac{2}{\varepsilon}, \; \sigma(Q) \approx \frac{\sqrt{2}}{\sqrt{\varepsilon}}, \frac{\sqrt{\varepsilon}}{\sqrt{2}}$$

Thank you for your attention!!!

References:

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