

Rice condition numbers of QR and Cholesky factorizations

Li Xinxiu¹ Nie Xiaobing²

(¹ Department of Mathematics and Physics, Nanjing University of Posts and Telecommunications, Nanjing 210003, China)

(² Department of Mathematics, Southeast University, Nanjing 210096, China)

Abstract: A condition number is an amplification coefficient due to errors in computing. Thus the theory of condition numbers plays an important role in error analysis. In this paper, following the approach of Rice, condition numbers are defined for factors of some matrix factorizations such as the Cholesky factorization of a symmetric positive definite matrix and QR factorization of a general matrix. The condition numbers are derived by a technique of analytic expansion of the factor dependent on one parameter and matrix-vector equation. Condition numbers of the Cholesky and QR factors are different from the ones previously introduced by other authors, but similar to Chang's results. In Cholesky factorization, corresponding with the condition number of the factor matrix L , \mathcal{K}_L is a low bound of Stewart's condition number \mathcal{K} .

Key words: Rice condition number; Cholesky factorization; QR decomposition

Conditioning of problems has been studied by numerical analysts since the 1940's, but the first general theory was developed by Rice^[1]. Although condition numbers for certain numerical linear algebra problems have been derived by numerous authors^[1-8], relatively little attention has been paid to the approach of Rice. Wilkinson^[5] introduced the condition numbers of simple eigenvalue of a matrix. Sun^[2] defined the condition numbers of certain characteristic subspaces. Chang^[6, 7, 9] provided the condition number of QR and Cholesky factorizations in "matrix-vector equation" analysis and "matrix equation" analysis. Condition numbers of Cholesky factor and QR factors have been derived by several authors in other ways.

This paper derives condition numbers following Rice's approach. The new results are different from the previous ones, but they are similar to Chang's results.

Throughout this paper, we use the following notations. Let $\mathbf{SR}^{n \times n}$ stand for the set of all $n \times n$ symmetric real matrices. We will use $\| \cdot \|_2$ and $\| \cdot \|_F$ to denote the spectral norm and Frobenius norm, respectively. Let $\mathcal{L}_s^{n \times n}$ denote the set of $n \times n$ strictly lower triangular matrices. Obviously, any $X \in \mathbf{R}^{n \times n}$ can be split uniquely as

$$X = X_L + X_D + X_U$$

where X_L and X_U are strictly lower and upper triangular matrices, respectively. We denote $X_L = \text{Low}(X)$.

Similarly, we can define $\mathcal{L}_s^{n \times (n+1)}$ and the operator $\text{Low}()$ on $\mathcal{L}_s^{n \times (n+1)}$. Moreover, for $A = [a_1 \ a_2 \ \cdots \ a_n] \in$

$\mathbf{R}^{m \times n}$, define $A(1:k) = [a_1 \ a_2 \ \cdots \ a_k]$. For a matrix-valued function $M(t)$, we denote $\left. \frac{dM(t)}{dt} \right|_{t=0}$ by $\dot{M}(0)$.

1 Cholesky Factorization

Let A be a positive definite symmetric matrix. Then there exists a unique lower triangular matrix L with positive diagonal elements such that $A = LL^T$. The factorization $A = LL^T$ is known as the Cholesky factorization of A , and L is called the Cholesky factor.

Let $E \in \mathbf{SR}^{n \times n}$. Consider $A(t) = A + tE$, where t is a real parameter. We suppose $|t|$ is small enough so that $A(t)$ is positive definite and therefore has Cholesky factorization

$$A(t) = L(t)L^T(t) \quad (1)$$

Comparing both sides of elements of (1), we know that $L(t)$ is a differentiable function of t . Differentiating (1) at $t=0$, we get

$$E = \dot{L}(0)L^T + L\dot{L}^T(0) \quad (2)$$

Let

$$\begin{aligned} \mathbf{L} &= [\mathbf{l}_1 \quad \mathbf{l}_2 \quad \cdots \quad \mathbf{l}_n] = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 4l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix}, \dot{\mathbf{L}}(\mathbf{0}) = \begin{bmatrix} \delta_{11} & 0 & \cdots & 0 \\ \delta_{21} & \delta_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \delta_{n1} & \delta_{n2} & \cdots & \delta_{nn} \end{bmatrix} \\ \mathbf{E} &= \begin{bmatrix} e_{11} & e_{21} & \cdots & e_{n1} \\ e_{21} & e_{22} & \cdots & e_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ e_{n1} & e_{n2} & \cdots & e_{nn} \end{bmatrix}, \mathbf{I}_j^{(i)} = \begin{bmatrix} l_{ij} \\ l_{i+1,j} \\ \vdots \\ l_{nj} \end{bmatrix} \quad i, j = 1, 2, \dots, n \\ \Phi_L &= \begin{bmatrix} \mathbf{I}_1^{(1)} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_1^{(2)} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{I}_2^{(2)} & \mathbf{0} & \cdots & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_1^{(3)} & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{I}_2^{(3)} & \cdots & \mathbf{0} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{I}_1^{(n)} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{I}_2^{(n)} & \cdots & \mathbf{I}_n^{(n)} \end{bmatrix} \\ \Psi_L &= \begin{bmatrix} l_{11}\mathbf{I}_n & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ 0l_{21}\mathbf{I}_{n-1} & l_{22}\mathbf{I}_{n-1} & \mathbf{0} & \cdots & \mathbf{0} \\ 00l_{31}\mathbf{I}_{n-2} & 0l_{32}\mathbf{I}_{n-2} & l_{33}\mathbf{I}_{n-2} & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \ddots & \vdots \\ 0 \cdots 0l_{n1} & 0 \cdots 0l_{n2} & 0 \cdots 0l_{n3} & \cdots & l_{nn} \end{bmatrix}, \Phi_{\dot{\mathbf{L}}} = \begin{bmatrix} e_{11} \\ e_{21} \\ \vdots \\ e_{n1} \\ e_{22} \\ \vdots \\ e_{n2} \\ \vdots \\ e_{nn} \end{bmatrix}, \mathbf{l} = \begin{bmatrix} \delta_{11} \\ \delta_{21} \\ \vdots \\ \delta_{n1} \\ \delta_{22} \\ \vdots \\ \delta_{n2} \\ \vdots \\ \delta_{nn} \end{bmatrix} \end{aligned}$$

Then from (2), we get

$$(\Phi_L + \Psi_L) \dot{\mathbf{l}} = \Phi_{\dot{\mathbf{L}}} \quad (3)$$

Obviously the matrix of $\Phi_L + \Psi_L$ is nonsingular. The Rice condition number of \mathbf{L} is derived as

$$\begin{aligned} \mathcal{K}_L &= \limsup_{t \rightarrow 0} \left\{ \frac{\|\mathbf{L}(t) - \mathbf{L}\|_F}{|t| \|\mathbf{E} - \mathbf{E}_U\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} = \sup \left\{ \frac{\|\dot{\mathbf{L}}(0)\|_F}{\|\mathbf{E}_L + \mathbf{E}_D\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} = \\ &\quad \|\Phi_L + \Psi_L\|_2^{-1} \quad (4) \end{aligned}$$

Remark 1 Previously, the condition number of \mathbf{L} defined as^[6]

$$\mathcal{K} = (\|\mathbf{L}\|_2 \|\mathbf{L}^{-1}\|_2)^2 \quad (5)$$

From (2), we have

$$\|\dot{\mathbf{L}}(0)\|_F \leq \frac{\mathcal{K}}{\sqrt{2\|\mathbf{A}\|_2}} \|\mathbf{E}\|_F \quad (6)$$

Consequently

$$\mathcal{K}_L \leq \frac{\mathcal{K}}{\sqrt{2\|\mathbf{A}\|_2}} \quad (7)$$

2 QR Decomposition

Now we consider the Rice condition number of the factors of QR decomposition. Let $\mathbf{A} \in \mathbf{R}^{m \times n}$ with $\text{rank}(\mathbf{A}) = n$. The QR decomposition of \mathbf{A} is a decomposition of the form $\mathbf{A} = \mathbf{Q}\mathbf{R}$, in which $\mathbf{Q} \in \mathbf{R}^{m \times n}$ satisfies $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}_n$ and $\mathbf{R} \in \mathbf{R}^{n \times n}$ is an upper triangular matrix with positive diagonal elements.

Let $\mathbf{E} \in \mathbf{R}^{m \times n}$. Consider the matrix $\mathbf{A}(t) = \mathbf{A} + t\mathbf{E}$, where t is a real parameter. Suppose $|t|$ is small enough so that $\text{rank}(\mathbf{A}(t)) = n$, and therefore we have the QR decomposition of $\mathbf{A}(t)$:

$$\mathbf{A}(t) = \mathbf{Q}(t)\mathbf{R}(t) \quad (8)$$

Obviously

$$\mathbf{A}^T \mathbf{A} = \mathbf{R}^T \mathbf{R}, \quad \mathbf{A}^T(t) \mathbf{A}(t) = \mathbf{R}^T(t) \mathbf{R}(t) \quad (9)$$

Hence, \mathbf{R} and $\mathbf{R}(t)$ are Cholesky factors of $\mathbf{A}^T \mathbf{A}$ and $\mathbf{A}^T(t) \mathbf{A}(t)$, respectively. So $\mathbf{R}(t)$ is a differentiable function of t , and so is $\mathbf{Q}(t)$. Differentiating (8) at $t=0$, we get

$$\mathbf{E} = \dot{\mathbf{Q}}(0) \mathbf{R} + \dot{\mathbf{Q}} \mathbf{R}(0) \quad (10)$$

$$\mathbf{Q}^T \mathbf{E} = \mathbf{W} \mathbf{R} + \dot{\mathbf{R}}(0) \quad (11)$$

where $\mathbf{W} = \mathbf{Q}^T \dot{\mathbf{Q}}(0)$ is a skew-symmetric matrix, and we can split it as

$$\mathbf{W} = \mathbf{W}_L - \mathbf{W}_L^T, \quad \mathbf{W}_L \in \mathcal{L}_s^{n \times n} \quad (12)$$

Let

$$\mathbf{Q}^T \mathbf{E} = \begin{bmatrix} * & * & \cdots & * \\ m_{21} & * & \cdots & * \\ \vdots & \ddots & \ddots & \vdots \\ m_{n1} & \cdots & m_{nn-1} & * \end{bmatrix}, \quad \mathbf{W}_L = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ \omega_{21} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ \omega_{n1} & \cdots & \omega_{nn-1} & 0 \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}, \quad \mathbf{a} = \begin{bmatrix} m_{21} \\ \vdots \\ m_{n1} \\ m_{32} \\ \vdots \\ m_{nn-1} \end{bmatrix}, \quad \boldsymbol{\omega} = \begin{bmatrix} \omega_{21} \\ \vdots \\ \omega_{n1} \\ \omega_{32} \\ \vdots \\ \omega_{nn-1} \end{bmatrix}$$

$$\mathbf{R}_0 = \begin{bmatrix} r_{11} \mathbf{I}_{n-1} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ 0 & r_{12} \mathbf{I}_{n-2} & r_{22} \mathbf{I}_{n-2} & \mathbf{0} & \cdots & \mathbf{0} \\ 0 & 0 & r_{13} \mathbf{I}_{n-3} & 0 & r_{23} \mathbf{I}_{n-3} & r_{33} \mathbf{I}_{n-3} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & r_{1, n-1} & 0 & \cdots & 0 & r_{2, n-1} & 0 & \cdots & 0 & r_{3, n-1} & \cdots & r_{n-1, n-1} \end{bmatrix}$$

From (11), we get

$$\mathbf{R}_0 \boldsymbol{\omega} = \mathbf{a} \quad (13)$$

The Rice condition number of \mathbf{Q} is defined as

$$\mathcal{K}_Q = \limsup_{t \rightarrow 0} \left\{ \frac{\|\mathbf{Q}(t) - (\mathbf{Q})\|_F}{|t| \|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} \quad (14)$$

Obviously, we can construct an $m \times (m-n)$ matrix $\hat{\mathbf{Q}}_2$, such that $\hat{\mathbf{Q}} = [\mathbf{Q} \quad \hat{\mathbf{Q}}_2]$ is an $m \times m$ orthogonal matrix and

$$\mathbf{Q}_2^T \mathbf{E} = \mathbf{Q}_2^T \dot{\mathbf{Q}}(0) \mathbf{R} \quad (15)$$

Consequently

$$\mathcal{K}_Q = \sup \left\{ \frac{\|\dot{\mathbf{Q}}(0)\|_F}{\|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} = \sup \left\{ \frac{\|\hat{\mathbf{Q}}^T \dot{\mathbf{Q}}(0)\|_F}{\|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} =$$

$$\sup \left\{ \frac{\sqrt{2 \|\mathbf{R}_0^{-1} \mathbf{a}\|_2^2 + \|\mathbf{Q}_2^T \mathbf{E} \mathbf{R}^{-1}\|_F^2}}{\|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} \leq \max \{ \sqrt{2} \|\mathbf{R}_0^{-1}\|_2, \|\mathbf{R}^{-1}\|_2 \}$$

On the other hand, if $\sqrt{2} \|\mathbf{R}_0^{-1}\|_2 \geq \|\mathbf{R}^{-1}\|_2$, then we construct \mathbf{E} such that

$$\hat{\mathbf{Q}}^T \mathbf{E} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ m_{21} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ m_{n1} & \cdots & m_{nn-1} & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}, \quad \|\mathbf{R}_0^{-1} \mathbf{a}\|_2 = \|\mathbf{R}_0^{-1}\|_2 \|\mathbf{a}\|_2$$

If $\sqrt{2} \|\mathbf{R}_0^{-1}\|_2 \leq \|\mathbf{R}^{-1}\|_2$, we construct \mathbf{E} such that

$$\mathbf{Q}^T \mathbf{E} = \begin{bmatrix} \mathbf{0} \\ \mathbf{E}_2 \end{bmatrix}, \quad \|\mathbf{E}_2 \mathbf{R}^{-1}\|_2 = \|\mathbf{E}_2\|_F \|\mathbf{R}^{-1}\|_2$$

In fact, we can construct such a matrix as

$$\mathbf{E}_2 = \mathbf{u}\mathbf{v}^T, \quad \mathbf{u} \in \mathbf{R}^{m-n}, \quad \mathbf{v} \in \mathbf{R}^n, \quad \|\mathbf{u}\|_2 = \|\mathbf{v}\|_2 = 1, \quad \mathbf{v}^T \mathbf{R}^{-1} = \|\mathbf{R}\|_2^{-1} \mathbf{v}_0^T, \quad \|\mathbf{v}_0\|_2 = 1$$

For both cases, we always have

$$\mathcal{K}_Q \geq \max\{\sqrt{2}\|\mathbf{R}_0^{-1}\|_2, \|\mathbf{R}^{-1}\|_2\}$$

Consequently, we have

$$\mathcal{K}_Q = \max\{\sqrt{2}\|\mathbf{R}_0^{-1}\|_2, \|\mathbf{R}^{-1}\|_2\} \quad (16)$$

Next we consider the Rice condition number of \mathbf{R} . Differentiating (9), we get

$$\mathbf{E}^T \mathbf{A} + \mathbf{A}^T \mathbf{E} = \dot{\mathbf{R}}^T(0) \mathbf{R} + \mathbf{R}^T \dot{\mathbf{R}}(0) \quad (17)$$

Let

$$\begin{aligned} \mathbf{R} &= \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}, \quad \mathbf{r}_i^{(j)} = \begin{bmatrix} r_{ij} \\ r_{i,j+1} \\ \vdots \\ r_{in} \end{bmatrix} \quad i, j = 1, 2, \dots, n \\ \dot{\mathbf{R}}(0) &= \begin{bmatrix} \delta_{11} & \delta_{12} & \cdots & \delta_{1n} \\ 0 & \delta_{22} & \cdots & \delta_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \delta_{nn} \end{bmatrix}, \quad \mathbf{E}^T \mathbf{A} + \mathbf{A}^T \mathbf{E} = \begin{bmatrix} e_{11} & e_{12} & \cdots & e_{1n} \\ e_{21} & e_{22} & \cdots & e_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ e_{n1} & e_{n2} & \cdots & e_{nn} \end{bmatrix} \\ \boldsymbol{\Phi}_R &= \begin{bmatrix} \mathbf{r}_1^{(1)} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{r}_1^{(2)} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{r}_2^{(2)} & \mathbf{0} & \cdots & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{r}_1^{(3)} & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{r}_2^{(3)} & \cdots & \mathbf{0} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{r}_1^{(n)} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{r}_2^{(n)} & \cdots & \mathbf{r}_n^{(n)} \end{bmatrix} \\ \boldsymbol{\Psi}_R &= \begin{bmatrix} r_{11} \mathbf{I}_n & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ 0 & r_{12} \mathbf{I}_{n-1} & r_{22} \mathbf{I}_{n-1} & \mathbf{0} & \cdots & \mathbf{0} \\ 0 & 0 & r_{13} \mathbf{I}_{n-2} & 0 & r_{23} \mathbf{I}_{n-2} & r_{33} \mathbf{I}_{n-2} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & r_{1n} & 0 & \cdots & 0 & r_{2n} & 0 & \cdots & 0 & r_{3n} & \cdots & r_{nn} \end{bmatrix}, \quad \boldsymbol{\phi}_A = \begin{bmatrix} e_{11} \\ e_{12} \\ \vdots \\ e_{1n} \\ e_{22} \\ \vdots \\ e_{2n} \\ \vdots \\ e_{nn} \end{bmatrix}, \quad \boldsymbol{\gamma} = \begin{bmatrix} \delta_{11} \\ \delta_{12} \\ \vdots \\ \delta_{1n} \\ \delta_{22} \\ \vdots \\ \delta_{2n} \\ \vdots \\ \delta_{nn} \end{bmatrix} \end{aligned}$$

Similar to (3), we have

$$(\boldsymbol{\Phi}_R + \boldsymbol{\Psi}_R) \dot{\boldsymbol{\gamma}} = \boldsymbol{\phi}_A \quad (18)$$

Obviously, the matrix of $\boldsymbol{\Phi}_R + \boldsymbol{\Psi}_R$ is nonsingular. Consequently, the Rice condition number of \mathbf{R} is

$$\begin{aligned} \mathcal{K}_R &= \limsup_{t \rightarrow 0} \left\{ \frac{\|\mathbf{R}(t) - \mathbf{R}\|_F}{|t| \|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} = \sup \left\{ \frac{\|\dot{\mathbf{R}}(0)\|_F}{\|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} = \\ &= \sup \left\{ \frac{\|(\boldsymbol{\Phi}_R + \boldsymbol{\Psi}_R)^{-1} \boldsymbol{\phi}_A\|_2}{\|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} \leq \\ &= \|(\boldsymbol{\Phi}_R + \boldsymbol{\Psi}_R)^{-1}\|_2 \sup \left\{ \frac{\|\mathbf{E}^T \mathbf{A} + \mathbf{A}^T \mathbf{E}\|_F}{\|\mathbf{E}\|_F} \mid \|\mathbf{E}\|_F \leq \|\mathbf{A}\|_F \right\} \leq 2 \|\mathbf{A}\|_2 \|(\boldsymbol{\Phi}_R + \boldsymbol{\Psi}_R)^{-1}\|_2 \end{aligned}$$

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QR 分解和 Cholesky 分解的 Rice 条件数

李新秀¹ 聂小兵²

(¹ 南京邮电学院应用数理系, 南京 210003)

(² 东南大学数学系, 南京 210096)

摘要: 条件数是在计算过程中由于误差引起的放大系数, 所以条件数理论在误差分析中占有非常重要的地位. 本文运用 Rice 关于条件数的一般理论, 采取一种统一的方式, 在单参数扰动的前提下, 定义了与正定对称矩阵的 Cholesky 分解和一般矩阵的 QR 分解有关的一些矩阵因子的条件数. 利用解析展开和矩阵向量方程的方法, 求出了用 Frobenius 范数所定义的 Rice 条件数的具体表达式. 所得结果与常小文的结果类似. 在 Cholesky 分解情况下, 与因子矩阵 L 相对应的条件数 \mathcal{R}_L 是 Stewart 条件数 \mathcal{R} 的一个下界.

关键词: Rice 条件数; Cholesky 分解; QR 分解

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