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Strong rank revealing LU factorizations

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Abstract

For any $m \times n$ matrix A we introduce a definition of strong rank revealing LU (RRLU) factorization related to the definition presented by Pan, but with some extensions similar to the notion of strong rank revealing QR factorization developed in the joint work of Gu and Eisenstat. A pivoting strategy based on the idea of local maximum volumes is introduced and a proof of the existence of strong RRLU is given.
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1. Introduction

Gaussian elimination (GE), along with its modifications like GE with partial pivoting, complete pivoting and block GE, is a fundamental tool in numerical linear algebra, and hence, so is LU decomposition. In some applications, it is necessary to compute decompositions with linearly independent columns being separated from linearly dependent ones, i.e. compute the rank revealing decomposition, which is not usually achieved by standard algorithms. One application of rank revealing factorizations comes from constrained optimization problems discussed in Chan and Resasco [1–3]. Another application is the active-set method discussed by Fletcher [4]. Also, rank revealing factorization can be used to solve least-squares problems using the method proposed by Björck [5,6]. In particular, rank revealing LU (RRLU)

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factorization for a rank deficient square matrix with well known numerical nullity arises from the path-following problem [7].

Usually rank revealing factorizations produce a decomposition with two components: the full-rank portion, and the rank deficient, or redundant, part. In practice, the quality of rank revealing decomposition is governed by the following two distances: how far from singular the full-rank portion is, and how close the exact rank deficient part is to the numerical rank deficient portion, where rank deficiency is estimated with some tolerance. We develop theoretical bounds (presented in Theorem 2) for full-rank and rank deficient components of RRLU decomposition, which are very similar to those obtained for rank revealing QR (RRQR) factorizations.

In particular, consider block LU decomposition

$$\begin{aligned}\Pi_1 A \Pi_2 &= \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \\ &= \begin{pmatrix} I_{k,k} & \\ A_{21}A_{11}^{-1} & I_{m-k,n-k} \end{pmatrix} \begin{pmatrix} A_{11} & \\ & S(A_{11}) \end{pmatrix} \begin{pmatrix} I_{k,k} & A_{11}^{-1}A_{12} \\ & I_{m-k,n-k} \end{pmatrix},\end{aligned}$$

where Π_1, Π_2 are permutation matrices, $A \in \mathbf{R}^{m,n}$, $A_{11} \in \mathbf{R}^{k,k}$, $A_{12} \in \mathbf{R}^{m-k,k}$, $A_{21} \in \mathbf{R}^{k,n-k}$, $A_{22} \in \mathbf{R}^{m-k,n-k}$, $S(A_{11})$ is the Schur complement of A_{11} and $I_{p,q}$ is $p \times q$ identity matrix. The numerical approximations to the left and right null spaces of A are correspondingly

$$N_{\mathrm{l}} = \begin{pmatrix} I_{n-k,m-k} \\ -A_{11}^{-\mathrm{T}} A_{21}^{\mathrm{T}} \end{pmatrix} \quad \text{and} \quad N_{\mathrm{r}} = \begin{pmatrix} -A_{11}^{-1}A_{12} \\ I_{m-k,n-k} \end{pmatrix},$$

which are governed by matrices $V = A_{11}^{-1}A_{12}$ and $W = A_{21}A_{11}^{-1}$. Hence, we need a pivoting strategy that reveals the linear dependence among columns of a matrix and keeps elements of N_{r} and N_{l} bounded by some slow growing polynomial in k, m and n.

Pan in [9] uses a pivoting strategy based on the idea of local maximum volumes to prove the existence of LU factorization where the smallest singular value of A_{11} is significantly larger than the kth singular value of A, and the largest singular value of $S(A_{11})$ is significantly smaller than the $(k+1)$th singular value of A, where k is the numerical rank of A. In this paper we use the maximum local volumes strategy that was introduced by Gu and Eisenstat in [8], Pan in [9] and Chandrasekaran and Ipsen in [10] to prove the existence of LU factorization with the property described above and elements of W and V small, which is crucial for the stability of LU factorization.

The importance of matrix W in the context of backward stability of the Cholesky decomposition for a symmetric matrix A was first discovered by Higham in [11]. Following Higham's discussion, in Theorem 3 we consider a matrix with $\operatorname{rank}(A) = r$ and show that the error bound for $\|A - \hat{L}_{\mathrm{r}}\hat{U}_{\mathrm{r}}\|_2$, where $\hat{L}_{\mathrm{r}}$ and $\hat{U}_{\mathrm{r}}$ are the computed lower and upper triangular matrices, is governed by V and W which implies that the stability of the algorithm depends on how small $\|V\|_2$ and $\|W\|_2$ are.

The rest of the paper is organized as follows: in Section 2, we give an overview of the previous results on RRLU and RRQR factorizations. In Section 3, we introduce a definition of strong RRLU decomposition, and, in Section 4, we discuss the existence of the strong RRLU defined in Section 3. In Section 5, we perform backward stability analysis for partial LU decomposition. Concluding remarks are in the final Section 6.

2. Previous results on RRLU and RRQR decompositions

Assume $A \in \mathbf{R}^{n,m}$ has numerical rank k. Then the factorization

$$\Pi_1 A \Pi_2^{\mathrm{T}} = \begin{pmatrix} L_{11} & \\ L_{21} & I_{n-k} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ & U_{22} \end{pmatrix},$$

where $L_{11}, U_{11} \in \mathbf{R}^{k,k}$, $U_{12} \in \mathbf{R}^{k,m-k}$, $U_{22} \in \mathbf{R}^{m-k,m-k}$, $L_{21} \in \mathbf{R}^{n-k,k}$, $I_{n-k} \in \mathbf{R}^{n-k,m-k}$ and Π_1 and Π_2 are permutation matrices, is a RRLU factorization if

$$\sigma_k(A) \geqslant \sigma_{\min}(L_{11}U_{11}) \gg \sigma_{\max}(U_{22}) \geqslant \sigma_{k+1}(A) \approx 0.$$

Given any rank-deficient matrix $A \in \mathbf{R}^{n,m}$, exact arithmetic Gaussian elimination with complete pivoting, unlike partial pivoting, will reveal the rank of the matrix. However, for nearly singular matrices even complete pivoting may not reveal the rank correctly. This is shown in the following example by Peters and Wilkinson [12] (see also Kahan, [13]):

$$A = \begin{pmatrix} 1 & -1 & -1 & \dots & -1 \\ & 1 & -1 & \dots & -1 \\ & & \ddots & & \vdots \\ & & & & 1 \end{pmatrix}.$$

There are no small pivots, but this matrix has a very small singular value when size of A is sufficiently large.

Several papers [1,14,15], were dedicated to the question of whether there is a pivoting strategy that will force entries with magnitudes comparable to those of small singular values to concentrate in the lower-right corner of U, so that LU decomposition reveals the numerical rank. In [1] the existence of such pivoting is shown for the case of only one small singular value. Later, in [14] the generalized case of more than one small singular value is discussed. However, bounds obtained in [14] may increase very rapidly (faster than exponential, in the worst case) because of its combinatorial nature. In [15] improved bounds are obtained. Pan, in [9], using Schur complement factorizations and local maximum volumes, deduced the following bounds:

Theorem 1 [9]. *Let $A \in \mathbf{R}^{n,n}$ with $\sigma_1 \geqslant \cdots \geqslant \sigma_k \geqslant \sigma_{k+1} \cdots \geqslant \sigma_n \geqslant 0$. Then there exist permutations Π_1 and Π_2 such that*

$$\Pi_1 A \Pi_2^{\mathrm{T}} = \begin{pmatrix} L_{11} & \\ L_{21} & I_{n-k} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ & U_{22} \end{pmatrix},$$

where L_{11} is unit lower triangular and U_{11} is upper triangular,

$$\|U_{22}\|_2 \leqslant (k(n-k)+1)\sigma_{k+1}$$

and

$$\sigma_{\min}(L_{11}U_{11}) \geqslant \frac{\sigma_k}{k(n-k)+1}.$$

These bounds are very similar to those obtained in RRQR factorizations in [8,10,16]. One of the definitions of RRQR factorization presented in [10,16] is the following: assume $M \in \mathbf{R}^{m,n}$ has numerical rank k, Q is orthogonal, $A_k \in \mathbf{R}^{k,k}$ is upper triangular with nonnegative diagonal entries, $B_k \in \mathbf{R}^{k,n-k}$, $C_k \in \mathbf{R}^{m-k,n-k}$ and Π is a permutation matrix. Then we call factorization

$$M\Pi = QR = Q\begin{pmatrix} A_k & B_k \\ & C_k \end{pmatrix} \tag{1}$$

RRQR factorization if

$$\sigma_{\min}(A_k) \geqslant \frac{\sigma_k(M)}{p(k,n)} \quad \text{and} \quad \sigma_{\max}(C_k) \leqslant \sigma_{k+1}(M)p(k,n), \tag{2}$$

where $p(k,n)$ is a function bounded by low-degree polynomial in k and n. Other, less restrictive definitions are discussed in [10,17].

RRQR factorization was first introduced by Golub [18], who, with Businger [19], developed the first algorithm for computing the factorization. The algorithm was based on QR with column pivoting, and worked well in practice. However, there are examples (Kahan matrix [13]) where the factorization it produces fails to satisfy condition (2).

Pierce and Lewis in [20] developed an algorithm to compute sparse multi-frontal RRQR factorization. In [21] Meyer and Pierce present advances towards the development of an iterative rank revealing method. Hough and Vavasis in [22] developed an algorithm to solve an ill-conditioned full rank weighted least-squares problem using RRQR factorization as a part of their algorithm. Also, a URV rank revealing decomposition was proposed by Stewart in [23].

In [16] Hong and Pan showed that there exists RRQR factorization with $p(k,n) = \sqrt{k(n-k)+\min(k,n-k)}$ and Chandrasekaran and Ipsen in [10] developed an efficient algorithm that is guaranteed to find an RRQR given k.

In some applications, such as rank-deficient least-squares computations and subspace tracking, where elements of $A_k^{-1}B_k$ are expected to be small, RRQR does not lead to a stable algorithm. In these cases strong RRQR, first presented in [8], is being used: factorization (1) is called a *strong RRQR factorization* if

1. $\sigma_i(A_k) \geqslant \sigma_i(M)/q_1(k,n),\ \sigma_j(C_k) \leqslant \sigma_{k+j}(M)q_1(k,n)$
2. $|(A_k^{-1}B_k)_{i,j}| \leqslant q_2(k,n)$

for $1 \leqslant i \leqslant k$ and $1 \leqslant j \leqslant n-k$, where $q_1(k,n)$ and $q_2(k,n)$ are functions bounded by low-degree polynomials in k and n.

Pan and Tang in [17] developed an algorithm that, given $f > 1$ computes strong RRQR with $q_1(k,n) = \sqrt{1+f^2k(n-k)}$ and $q_2(k,n) = f$. Later, in [8], a different, but mathematically equivalent algorithm, was presented by Gu and Eisenstat. The new algorithm was based on the idea of local maximum volumes. The same idea will be used in this paper to prove the existence of strong RRLU.

3. Strong rank revealing LU decomposition

In this section, we explore the idea of using significant gaps between singular values to define the numerical rank of a matrix and introduce strong RRLU factorization.

Given any matrix $A \in \mathbf{R}^{m,n}$, we consider a Schur complement factorization

$$\Pi_1 A \Pi_2^{\mathrm{T}} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} I_{k,k} & \\ A_{21}A_{11}^{-1} & I_{m-k,n-k} \end{pmatrix} \begin{pmatrix} A_{11} & \\ & S(A_{11}) \end{pmatrix} \begin{pmatrix} I_{k,k} & A_{11}^{-1}A_{12} \\ & I_{m-k,n-k} \end{pmatrix}, \tag{3}$$

where $S(A_{11}) = A_{22} - A_{21}A_{11}^{-1}A_{12}$, $A_{11} \in \mathbf{R}^{k,k}$, $A_{12} \in \mathbf{R}^{m-k,k}$, $A_{21} \in \mathbf{R}^{k,n-k}$, $A_{22} \in \mathbf{R}^{m-k,n-k}$ and $I_{p,q}$ denotes the $p \times q$ identity matrix. According to the interlacing property of singular values, for any permutation matrices Π_1 and Π_2, we have

$$\sigma_i(A_{11}) \leqslant \sigma_i(A) \quad \text{and} \quad \sigma_j(S(A_{11})) \geqslant \sigma_{j+k}(A)$$

for $1 \leqslant i \leqslant k$ and $1 \leqslant j \leqslant n-k$. Hence,

$$\sigma_{\min}(A_{11}) \leqslant \sigma_k(A) \quad \text{and} \quad \sigma_{\max}(S(A_{11})) \geqslant \sigma_{k+1}(A).$$

Assume that $\sigma_k(A) \gg \sigma_{k+1}(A) \approx 0$, so that k would be the numerical rank of A. Then we would like to choose permutation matrices Π_1 and Π_2 in such a way that $\sigma_{\min}(A_{11})$ is sufficiently large and $\sigma_{\max}(S(A_{11}))$ is sufficiently small. In this paper we will call factorization (3) a *strong RRLU decomposition* if it satisfies the following conditions:

1. $\sigma_i(A_{11}) \geqslant \sigma_i(A)/q_1(k,n,m);\ \sigma_j(S(A_{11})) \leqslant \sigma_{k+j}(A)q_1(k,n,m)$
2. $|(A_{21}A_{11}^{-1})_{ij}| \leqslant q_2(k,n,m)$
3. $|(A_{11}^{-1}A_{12})_{ij}| \leqslant q_3(k,n,m)$,

where $1 \leqslant i \leqslant k$, $1 \leqslant j \leqslant n-k$, $q_1(k,n,m)$, $q_2(k,n,m)$ and $q_3(k,n,m)$ are functions bounded by some low degree polynomials in k, m and n.

4. The existence of strong rank revealing LU decomposition

In this section we prove the existence of permutation matrices Π_1 and Π_2 which make a strong RRLU decomposition possible. It is proven in Theorem 2 of this section that permutation matrices obtained using Proposition 1 are those necessary for RRLU factorization with elements of $W = A_{21}A_{11}^{-1}$ and $V = A_{11}^{-1}A_{12}$ bounded by some slow growing functions in n, m and k.

The bounds obtained by Pan in [9] are sharper than those proved in Theorem 2, but they do not provide connections with matrices W and V.

As first observed in [8],

$$\det(\Pi_1 A \Pi_2^{\mathrm{T}}) = \det(A_{11})\det(S(A_{11})),$$

hence

$$\det(A_{11}) = \prod_{i=1}^{k}\sigma_i(A_{11}) = \det(A) \Bigg/ \prod_{j=1}^{n-k}\sigma_j(S(A_{11})).$$

We are looking for permutations Π_1 and Π_2 which would extract from A a matrix A_{11} with the largest possible singular values and $S(A_{11})$ with the smallest. Observation above implies that a search for A_{11} with the largest determinant will result in A_{11} with the largest singular values, as well as $S(A_{11})$ having the smallest singular values.

Since we wish to maximize $\det(A_{11})$, we are going to use the local maximum volume idea to permute rows and columns of A. The following proposition tells us how the determinant of A_{11} may change if we perform a row and column swap.

Proposition 1. *Suppose we have matrix*

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where $A_{11} \in \mathbf{R}^{k,k}$, $A_{22} \in \mathbf{R}^{m-k,n-k}$, $A_{21} \in \mathbf{R}^{k,n-k}$, $A_{12} \in \mathbf{R}^{m-k,k}$. *If* $1 \leqslant i \leqslant k$, $k \leqslant j \leqslant n-k$ *and we interchange*:

1. *rows* i *and* $k+j$ *in matrix* A, *then*
$$\frac{\det(\tilde{A}_{11})}{\det(A_{11})} = \left(A_{21}A_{11}^{-1}\right)_{ji}$$
2. *columns* i *and* $k+j$ *in matrix* A, *then*
$$\frac{\det(\tilde{A}_{11})}{\det(A_{11})} = \left(A_{11}^{-1}A_{12}\right)_{ij}$$

3. *rows i and $k+j$; columns s and $k+t$ in matrix A, then*

$$\frac{\det(\tilde{A}_{11})}{\det(A_{11})} = \left(A_{11}^{-1}A_{12}\right)_{st}\left(A_{21}A_{11}^{-1}\right)_{ji} + \left(A_{11}^{-1}\right)_{si}\left(A_{22} - A_{21}A_{11}^{-1}A_{12}\right)_{jt},$$

where in each of these cases matrix $\tilde{A}$ is the result of corresponding interchanges, and $\tilde{A}_{11}$ is the upper left $k \times k$ portion of it.

Proof. For simplicity, we assume that $i = k$ and $j = 1$. Other cases can be obtained similarly. Consider the following partition of a matrix A:

$$A = \begin{pmatrix} U_{11} & a_1 & a_2 & U_{12} \\ b_1^{\mathrm{T}} & \gamma_{11} & \gamma_{12} & d_1^{\mathrm{T}} \\ b_2^{\mathrm{T}} & \gamma_{21} & \gamma_{22} & d_2^{\mathrm{T}} \\ U_{21} & c_1 & c_2 & U_{22} \end{pmatrix},$$

$$A_{11} = \begin{pmatrix} U_{11} & a_1 \\ b_1^{\mathrm{T}} & \gamma_{11} \end{pmatrix}, \quad A_{21} = \begin{pmatrix} b_2^{\mathrm{T}} & \gamma_{21} \\ U_{21} & c_1 \end{pmatrix}, \quad A_{12} = \begin{pmatrix} a_2 & U_{12} \\ \gamma_{12} & d_1^{\mathrm{T}} \end{pmatrix},$$

$$A_{22} = \begin{pmatrix} \gamma_{22} & d_2^{\mathrm{T}} \\ c_2 & U_{22} \end{pmatrix},$$

where $A_{11} \in \mathbf{R}^{k,k}$, $A_{22} \in \mathbf{R}^{m-k,n-k}$, $A_{21} \in \mathbf{R}^{k,n-k}$, $A_{12} \in \mathbf{R}^{m-k,k}$.

1. To prove part 1, we notice that

$$\frac{\det(\tilde{A}_{11})}{\det(A_{11})} = \det(\tilde{A}_{11}A_{11}^{-1})$$

and

$$\tilde{A}_{11} = \begin{pmatrix} U_{11} & a_1 \\ b_2^{\mathrm{T}} & \gamma_{21} \end{pmatrix} = \begin{pmatrix} U_{11} & a_1 \\ b_1^{\mathrm{T}} & \gamma_{22} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ b_2^{\mathrm{T}} - b_1^{\mathrm{T}} & \gamma_{21} - \gamma_{11} \end{pmatrix}$$

$$= \begin{pmatrix} U_{11} & a_1 \\ b_1^{\mathrm{T}} & \gamma_{11} \end{pmatrix} + e_k^{\mathrm{T}} v = A_{11} + e_k^{\mathrm{T}} v,$$

where $e_k = (0, \ldots, 1)$, $v = (b_2^{\mathrm{T}} - b_1^{\mathrm{T}}, \gamma_{21} - \gamma_{11})$.
Hence

$$\tilde{A}_{11}A_{11}^{-1} = \left(A_{11} + e_k^{\mathrm{T}} v\right) A_{11}^{-1} = I + e_k^{\mathrm{T}} v A_{11}^{-1},$$

which implies that

$$\frac{\det(\tilde{A}_{11})}{\det(A_{11})} = 1 + \left(vA_{11}^{-1}\right)_{kk} = 1 + v\ A_{11}^{-1}e_k^{\mathrm{T}} = \left(A_{21}A_{11}^{-1}\right)_{1k},$$

where the last equality follows from the calculation below.

Call $e_1 = (1, \dots, 0)$, then

$$\begin{aligned}\left(A_{21}A_{11}^{-1}\right)_{1k} - vA_{11}^{-1}e_k^{\mathrm{T}} &= e_1A_{21}A_{11}^{-1}e_k^{\mathrm{T}} - vA_{11}^{-1}e_k^{\mathrm{T}}\\ &= \left(e_1A_{21} - v\right)A_{11}^{-1}e_k^{\mathrm{T}}\\ &= \left(\left(b_2^{\mathrm{T}}, \gamma_{21}\right) - v\right)A_{11}^{-1}e_k^{\mathrm{T}}\\ &= \left(b_1^{\mathrm{T}}, \gamma_{11}\right)A_{11}^{-1}e_k^{\mathrm{T}}.\end{aligned}$$

Here $A_{11}^{-1}e_k^{\mathrm{T}}$ produces the last column of A_{11}^{-1}, which is equal to

$$\begin{pmatrix} U_{11}^{-1}a_1\left(b_1^{\mathrm{T}}U_{11}^{-1}a_1 - \gamma_{11}\right)^{-1} \\ -\left(b_1^{\mathrm{T}}U_{11}^{-1}a_1 - \gamma_{11}\right)^{-1} \end{pmatrix}.$$

Then,

$$(b_1^{\mathrm{T}}, \gamma_{11})A_{11}^{-1}e_k^{\mathrm{T}} = (b_1^{\mathrm{T}}, \gamma_{11})\begin{pmatrix} U_{11}^{-1}a_1\left(b_1^{\mathrm{T}}U_{11}^{-1}a_1 - \gamma_{11}\right)^{-1} \\ -\left(b_1^{\mathrm{T}}U_{11}^{-1}a_1 - \gamma_{11}\right)^{-1} \end{pmatrix} = 1,$$

which proves the statement.

2. Similar to part 1.
3. After the row swap which results in matrix $\tilde{A}$ we have

$$\frac{\det(\tilde{A}_{11})}{\det(A_{11})} = \left(A_{21}A_{11}^{-1}\right)_{1k}.$$

After the column swap which results in matrix $\tilde{\tilde{A}}$ we have

$$\frac{\det(\tilde{\tilde{A}}_{11})}{\det(\tilde{A}_{11})} = \left(\tilde{A}_{11}^{-1}\tilde{A}_{12}\right)_{k1},$$

where

$$\tilde{A}_{11} = \begin{pmatrix} a_2 & U_{12} \\ \gamma_{12} & d_1^{\mathrm{T}} \end{pmatrix}, \quad \tilde{A}_{12} = \begin{pmatrix} a_2 & U_{12} \\ \gamma_{22} & d_2^{\mathrm{T}} \end{pmatrix}.$$

Hence,

$$\frac{\det(\tilde{\tilde{A}}_{11})}{\det(A_{11})} = \left(A_{21}A_{11}^{-1}\right)_{1k}\left(\tilde{A}_{11}^{-1}\tilde{A}_{12}\right)_{k1}.$$

As in part 1, $\tilde{A}_{11} = A_{11} + e_k^{\mathrm{T}}v$, where $e_k = (0, \dots, 1)$ and

$$v = \left(b_2^{\mathrm{T}} - b_1^{\mathrm{T}}, \gamma_{21} - \gamma_{11}\right) = e_1A_{12} - \left(b_1^{\mathrm{T}}, \gamma_{11}\right) = e_1A_{12} - e_kA_{11}.$$

By the same reasoning, $\tilde{A}_{12} = A_{12} + e_k^{\mathrm{T}}w$, where

$$w = \left(\gamma_{22} - \gamma_{12}, d_2^{\mathrm{T}} - d_1^{\mathrm{T}}\right) = e_1 A_{22} - e_k A_{12}.$$

So, $\tilde{A}_{12} = A_{12} + e_k^{\mathrm{T}}(e_1 A_{22} - e_k A_{12})$.

Using the fact that $1 + vA_{11}^{-1}e_k^{\mathrm{T}} = e_1 A_{21} A_{11}^{-1} e_k^{\mathrm{T}}$ and the Sherman–Morrison formula, we obtain

$$\begin{aligned}\tilde{A}_{11}^{-1} &= A_{11}^{-1} - \left(A_{11}^{-1}e_k^{\mathrm{T}}vA_{11}^{-1}\right)/\left(1 + vA_{11}^{-1}e_k^{\mathrm{T}}\right)\\ &= \left(A_{11}^{-1}e_1A_{21}A_{11}^{-1}e_k^{\mathrm{T}} - A_{11}^{-1}e_k^{\mathrm{T}}e_1A_{21}A_{11}^{-1} + A_{11}^{-1}e_k^{\mathrm{T}}e_k\right)/\left(e_1A_{21}A_{11}^{-1}e_k^{\mathrm{T}}\right).\end{aligned}$$

Using the fact that $\left(\tilde{A}_{11}^{-1}\tilde{A}_{12}\right)_{k1} = e_k\tilde{A}_{11}^{-1}\tilde{A}_{12}e_1^{\mathrm{T}}$, we obtain

$$\begin{aligned}&\left(A_{21}A_{11}^{-1}\right)_{1k}\left(\tilde{A}_{11}^{-1}\tilde{A}_{12}\right)_{k1}\\ &\quad= \left(A_{21}A_{11}^{-1}\right)_{1k}e_k\tilde{A}_{11}^{-1}\tilde{A}_{12}e_1^{\mathrm{T}}\\ &\quad= \left(A_{21}A_{11}^{-1}\right)_{1k}e_k\left[A_{11}^{-1} - \left(A_{11}^{-1}e_k^{\mathrm{T}}vA_{11}^{-1}\right)/\left(1 + vA_{11}^{-1}e_k^{\mathrm{T}}\right)\right]\\ &\qquad\times\left[A_{12} + e_k^{\mathrm{T}}(e_1A_{22} - e_kA_{12})\right]e_1^{\mathrm{T}}.\end{aligned}$$

After plugging in $v = e_1A_{12} - e_kA_{11}$ and simplifying the expression we arrive to the formula

$$\begin{aligned}\frac{\det(\tilde{\tilde{A}}_{11})}{\det(A_{11})} &= \left(A_{11}^{-1}A_{12}\right)_{k1}\left(A_{21}A_{11}^{-1}\right)_{1k} + \left(A_{11}^{-1}\right)_{k,k}\left(A_{22} - A_{21}A_{11}^{-1}A_{12}\right)_{11}\\ &= \left(A_{11}^{-1}A_{12}\right)_{k1}\left(A_{21}A_{11}^{-1}\right)_{1k} + \left(A_{11}^{-1}\right)_{k,k}S(A_{11})_{11}. \qquad \square\end{aligned}$$

According to this proposition, we can permute rows and columns of matrix A, accumulating these permutations in matrices Π_1 and Π_2 so that

$$\Pi_1 A \Pi_2^{\mathrm{T}} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

until $\det(A_{11})$ is sufficiently large. The following theorem proves that by setting bounds for elements of $A_{11}^{-1}A_{12}$ and $A_{21}A_{11}^{-1}$ we in fact obtain strong RRLU factorization. Theorem 2 establishes bounds for $\sigma_i(A_{11})$ and $\sigma_j(S(A_{11}))$ in terms of some function $q_1(n, m, k)$ and the singular values of A.

Theorem 2. *Let*

$$\Pi_1 A \Pi_2^{\mathrm{T}} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

and $f \geqslant 1$, $g \geqslant 1$, $h \geqslant 1$. *Suppose*

$$|A_{21}\ A_{11}^{-1}|_{\max} \leqslant f, \quad |A_{11}^{-1}\ A_{12}|_{\max} \leqslant g \quad \textit{and} \quad \frac{\det(\tilde{A}_{11})}{\det(A_{11})} \geqslant h.$$

Then

$$\sigma_i(A_{11}) \geqslant \frac{\sigma_i(A)}{q_1(k,n)}, \quad 1 \leqslant i \leqslant k, \tag{4}$$

and

$$\sigma_j(S(A_{11})) \leqslant \sigma_{k+j}(A) q_1(k,n), \quad k \leqslant j \leqslant n, \tag{5}$$

where

$$q_1(n,m,k) = 3\max(h, f^2, g^2)\big(1 + k\{\max(m,n) - k\}\big).$$

Proof. Let us define

$$\alpha\beta = \frac{\sigma_{\max}(S(A_{11}))}{\sigma_{\min}(A_{11})}.$$

Suppose

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} I & \\ A_{21}A_{11}^{-1} & \alpha I \end{pmatrix} \begin{pmatrix} A_{11} & \\ & \frac{1}{\alpha\beta} S(A_{11}) \end{pmatrix} \begin{pmatrix} I & A_{11}^{-1}A_{12} \\ & \beta I \end{pmatrix} = \bar{W} D \bar{V},$$

where $\bar{W}$ is the leftmost matrix, D is the matrix in between, and $\bar{V}$ is the rightmost matrix. According to theorem 3.3.16 in [24],

$$\sigma(A) \leqslant \sigma(A_{11}) \|\bar{W}\|_2 \|\bar{V}\|_2, \quad 1 \leqslant i \leqslant n.$$

Since

$$\sigma_{\min}(A_{11}) = \sigma_{\max}\left(\frac{S(A_{11})}{\alpha\beta}\right),$$

we have that $\sigma_i(A_{11}) = \sigma_i(D)$, $1 \leqslant i \leqslant k$.
Moreover,

$$\begin{aligned} \|\bar{W}\|_2^2 &\leqslant 1 + \alpha^2 + \|A_{21}A_{11}^{-1}\|_2^2 \\ &\leqslant 1 + \alpha^2 + \|A_{21}A_{11}^{-1}\|_{\mathrm{F}}^2 \\ &\leqslant 1 + \alpha^2 + \sum_{i=1}^{k} \sum_{j=1}^{n-k} \left(A_{21}A_{11}^{-1}\right)_{ij}^2 \\ &\leqslant 1 + \alpha^2 + k(n-k) f^2. \end{aligned}$$

By the same reasoning we may conclude that $\|\bar{V}\|_2^2 \leqslant 1 + \beta^2 + k(m-k)g^2$.
Hence,

$$\sigma(A) \leqslant \sigma(A_{11}) \sqrt{[1 + \beta^2 + k(m-k)g^2][1 + \alpha^2 + k(n-k) f^2]}.$$

Now we need to find α and β such that

$$H(\alpha,\beta) = [1+\beta^2+k(m-k)g^2][1+\alpha^2+k(n-k)f^2]$$

is the smallest, given that

$$\alpha\beta = \frac{\sigma_{\max}(S(A_{11}))}{\sigma_{\min}(A_{11})}.$$

For the sake of clarity, define

$$a = 1+k(n-k)f^2 \quad \text{and} \quad b = 1+k(m-k)g^2.$$

After minimizing $H(\alpha,\beta)$ over the given set we arrive to

$$\alpha = \sqrt{\frac{\sigma_{\max}(S(A_{11}))}{\sigma_{\min}(A_{11})}}\sqrt[4]{\frac{a}{b}} \quad \text{and} \quad \beta = \sqrt{\frac{\sigma_{\max}(S(A_{11}))}{\sigma_{\min}(A_{11})}}\sqrt[4]{\frac{b}{a}}.$$

Notice that

$$\frac{\sigma_{\max}(S(A_{11}))}{\sigma_{\min}(A_{11})} = \|S(A_{11})\|_2\|A_{11}^{-1}\|_2 \leqslant k(fg+h)\sqrt{(n-k)(m-k)}.$$

For simplicity, define $c = k(fg+h)\sqrt{(n-k)(m-k)}$, then

$$1+\beta^2+g^2k(m-k) = \beta^2+b \leqslant b+c\sqrt{\frac{b}{a}} = \left(\sqrt{ab}+c\right)\sqrt{\frac{b}{a}}$$

and

$$1+\alpha^2+k(n-k)f^2 = \alpha^2+a \leqslant a+c\sqrt{\frac{a}{b}} = \left(\sqrt{ab}+c\right)\sqrt{\frac{a}{b}}.$$

Hence, $[1+\beta^2+k(m-k)g^2][1+\alpha^2+k(n-k)f^2] \leqslant (c+\sqrt{ab})^2$, which implies

$$\begin{aligned}\sigma(A) &\leqslant \sigma(A_{11})\left(c+\sqrt{ab}\right)\\ &\leqslant \sigma(A_{11})\,(2Mk\{\max(m,n)-k\}+1+Mk\{\max(m,n)-k\})\\ &\leqslant \sigma(A_{11})3M\,(1+k\{\max(m,n)-k\}) = \sigma(A_{11})q_1(n,m,k),\end{aligned}$$

where $M = \max(h, f^2, g^2)$. Similarly,

$$\begin{aligned}D = \begin{pmatrix}\alpha\beta A_{11} & \\ & S(A_{11})\end{pmatrix} &= \begin{pmatrix}A_{11}/\alpha & \\ -A_{21}A_{11}^{-1} & I\end{pmatrix}\begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}\begin{pmatrix}I/\beta & -A_{11}^{-1}A_{12}\\ & I\end{pmatrix}\\ &= \bar{W}A\bar{V}.\end{aligned}$$

Then $\sigma_j(S(A_{11})) = \sigma_{j+k}(D) \leqslant \sigma_{j+k}(A)\|\bar{W}\|_2\|\bar{V}\|_2 = \sigma_{j+k}(A)q_1(n,m,k)$. $\square$

So, if we put $q_2(k,n,m) = f$, $q_3(k,n,m) = g$ and q_1 as defined in Theorem 2, the resulting decomposition is strong RRLU according to our definition in Section

3. Observe that $q_1(n, m, k)$ is very similar to the bounds established in [8]. While the bound obtained by Pan in [9] is a factor of $3\max(f^2, g^2, h)$ better than the one proved in this section, our bound provides connections with important matrices W and V, the usefulness of which is discussed in the next section.

5. Backward error analysis for RRLU factorization

In this section, which is similar to Section 3 in [11] by Higham, we perform a backward error analysis of LU decomposition. The main purpose of this section is to show that for any given ordering of rows and columns of matrix A, Eq. (20) relates the difference $A - \hat{L}_{\mathrm{r}}\hat{U}_{\mathrm{r}}$ to the norms of matrices V and W. Hence if the given order is in strong rank-revealed form, the backward error can be expected to be small, and it could be large otherwise. While we do not discuss ways to compute the ordering, its importance can be seen from (20).

Consider a matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \tag{6}$$

where $A_{11} \in \mathbf{R}^{k,k}$, $A_{12} \in \mathbf{R}^{k,n-k}$, $A_{21} \in \mathbf{R}^{m-k,k}$, $A_{22} \in \mathbf{R}^{m-k,n-k}$. Following [11] for Cholesky decomposition, we find an error bound for $\|A - \hat{L}_{\mathrm{r}}\hat{U}_{\mathrm{r}}\|$, where $\hat{L}_{\mathrm{r}}$ and $\hat{U}_{\mathrm{r}}$ are the computed lower and upper-triangular LU factors, in the special case where $\mathrm{rank}(A) = r = k$.

Denote $S_k(A) = A_{22} - A_{21}A_{11}^{-1}A_{12}$ to be the Schur complement of A_{11} in A. First we will prove a lemma which shows how Schur complement changes when matrix A is perturbed.

Lemma 1. *Assume* $\|A_{11}^{-1}E_{11}\|_2 < 1$. *Then*

$$S_k(A + E) = S_k(A) + E_{22} - (E_{21}W + VE_{12}) + VE_{11}W + \mathrm{O}(\|E\|_2^2),$$

where $W = A_{21}A_{11}^{-1}$, $V = A_{11}^{-1}A_{12}$, *and* E *is partitioned the same way as* A.

The proof is similar to the one presented in [11, Lemma 2.1] .

Let A be a matrix of floating point numbers. We will write

$$A = \tilde{A} + \Delta A,$$

where $\tilde{A}$ is the rounded computer representation of A and ΔA is assumed to have small entries. Standard error analysis (see [25, Chapter 3]) reveals that

$$A - \hat{L}_{\mathrm{r}}\hat{U}_{\mathrm{r}} = E + \hat{A}^{(r+1)}, \tag{7}$$

where

$$\hat{L}_{\mathrm{r}} = \begin{pmatrix} \hat{L}_{11} & 0 \\ \hat{L}_{21} & I \end{pmatrix} \quad \text{and} \quad \hat{U}_{\mathrm{r}} = \begin{pmatrix} \hat{U}_{11} & \hat{U}_{12} \\ 0 & 0 \end{pmatrix},$$

$$|E| \leqslant \epsilon_{r+1}\big(|\hat{L}_{\rm r}||\hat{U}_{\rm r}| + |\hat{A}^{(r+1)}|\big),$$

$\epsilon_k = ku/(1-ku)$ and u is the machine precision. Observe that

$$\begin{aligned} |\hat{L}_{\rm r}||\hat{U}_{\rm r}| &\leqslant \begin{pmatrix} I & 0 \\ |\hat{L}_{21}\hat{L}_{11}^{-1}| & I \end{pmatrix} \begin{pmatrix} |\hat{L}_{11}||\hat{U}_{11}| & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} I & |\hat{U}_{11}^{-1}\hat{U}_{12}| \\ 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} I & 0 \\ |W| & I \end{pmatrix} \begin{pmatrix} |\hat{L}_{11}||\hat{U}_{11}| & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} I & |V| \\ 0 & 0 \end{pmatrix} = W_1 A_1 V_1, \end{aligned}$$

where W_1 is the leftmost matrix, A_1 is the matrix in between, and V_1 is the rightmost matrix. Using inequalities $\|B\|_2 \leqslant \||B|\|_2 \leqslant \sqrt{\operatorname{rank}(B)}\|B\|_2$ it is now easy to see that

$$\|W_1\|_2^2 \leqslant 1 + (m-r)\|W\|_2^2 \quad \text{and} \quad \|V_1\|_2^2 \leqslant 1 + (n-r)\ \|V\|_2^2.$$

Let us introduce a new quantity

$$\rho = \||\hat{L}_{11}||\hat{U}_{11}|\|_2 / \|A_{11}\|_2. \tag{8}$$

Then we obtain

$$\begin{aligned} \|E\|_2 &\leqslant \epsilon_{r+1}\rho\|A_{11}\|_2\sqrt{\big(1+(m-r)\|W\|_2^2\big)\big(1+(n-r)\|V\|_2^2\big)} \\ &\quad + \epsilon_{r+1}\sqrt{n-r}\|\hat{A}^{(r+1)}\|_2 \\ &= \epsilon_{r+1}\big(\rho\lambda_1\|A_{11}\|_2 + \sqrt{n-r}\|\hat{A}^{(r+1)}\|_2\big), \end{aligned} \tag{9}$$

where

$$\lambda_1 = \sqrt{\big(1+(m-r)\|W\|_2^2\big)\big(1+(n-r)\|V\|_2^2\big)}. \tag{10}$$

Since our goal is to obtain a bound for $\|A - \hat{L}_{\rm r}\hat{U}_{\rm r}\|_2$, we have to find a bound for $\|A^{(r+1)}\|_2$. Eq. (7) shows that $\hat{A}^{(r+1)}$ is the exact Schur complement for the matrix

$$A - E = \tilde{A} + (\Delta A - E) =: \tilde{A} + F.$$

Applying Lemma 1 to matrix $\tilde{A}$ and using the fact that the Schur complement of $\tilde{A}$ is zero, we obtain

$$\begin{aligned} \|S_{\rm r}(\tilde{A}+F)\|_2 = \|\hat{A}^{(r+1)}\|_2 = \|A_{r+1}\| &\leqslant \|F_{22}\|_2 + \|F_{21}\|_2\|W\|_2 + \|F_{12}\|_2\|V\|_2 \\ &\quad + \|V\|_2\|W\|_2\|F_{11}\|_2 + \mathrm{O}\big(\|F_{11}\|_2^2\big) \\ &\leqslant \|F\|_2\,(1 + \|W\|_2 + \|V\|_2 + \|V\|_2\|W\|_2) + \mathrm{O}\big(\|F\|_2^2\big) \\ &= \|F\|_2\lambda_2 + \mathrm{O}\big(\|F\|_2^2\big), \end{aligned} \tag{11}$$

where

$$\lambda_2 = 1 + \|W\|_2 + \|V\|_2 + \|V\|_2\|W\|_2. \tag{12}$$

We use (11) and the fact that $\|F\|_2 \leqslant \|\Delta A\|_2 + \|E\|_2$ to obtain

$$\|\hat{A}^{(r+1)}\|_2 \leqslant \Psi\,(\|\Delta A\|_2\lambda_2 + \epsilon_{r+1}\rho\lambda_1\lambda_2\|A_{11}\|_2) + \mathrm{O}\big(\|F\|_2^2\big), \tag{13}$$

where

$$\Psi = \big(1 - \epsilon_{r+1}\lambda_2\sqrt{n-r}\,\big)^{-1}. \tag{14}$$

Combining (7), (9) and (13) we get

$$\begin{aligned}\|A - \hat{L}_{\mathrm{r}}\hat{R}_{\mathrm{r}}\|_2 &\leqslant \|E\|_2 + \|\hat{A}^{(r+1)}\|_2 \\ &\leqslant \Psi\,(\|\Delta A\|_2\lambda_2 + \epsilon_{r+1}\rho\lambda_1\lambda_2\|A_{11}\|_2)\big(1 + \epsilon_{r+1}\sqrt{n-r}\,\big) \\ &\quad + \epsilon_{r+1}\rho\lambda_1\|A_{11}\|_2 + \mathrm{O}\big(\|F\|_2^2\big).\end{aligned} \tag{15}$$

Now we can formulate the following backward analysis result: Denote $W = \tilde{A}_{21}\tilde{A}_{11}^{-1}$, $V = \tilde{A}_{11}^{-1}\tilde{A}_{12}$, and define ρ, λ_1, λ_2, and Ψ as in (8), (10), (12) and (14).

Theorem 3. *Let $A = \tilde{A} + \Delta A$ be a $m \times n$, $m \geqslant n$ matrix of floating point numbers where $\tilde{A}$ has rank $r < n$ and partition it like in* (6) *with $r = k$.*
Assume that

$$\max\left\{\frac{\|\Delta A_{11}\|_2}{\|A_{11}\|_2};\ \frac{\|\Delta A\|_2}{\|A\|_2}\right\} = \theta u, \tag{16}$$

where θ is a small constant;

$$\max\left\{20r^{3/2}u;\ 2(\theta u + \epsilon_{r+1}\lambda_1)\right\}k_2(A_{11}) < 1, \tag{17}$$

$$\epsilon_{r+1}\lambda_2\sqrt{n-r} < 1/2, \tag{18}$$

$$u(r+1) < 1/2. \tag{19}$$

Then, in floating point arithmetic with round off u, the LU algorithm applied to A successfully completes r stages, and the computed LU factors satisfy the following inequality

$$\|A - \hat{L}_{\mathrm{r}}\hat{U}_{\mathrm{r}}\|_2 \leqslant (1 + 2\lambda_2)(\theta + 4\lambda_1(r+1))\|A\|_2 u + \mathrm{O}(u^2). \tag{20}$$

Proof. Condition (16) allows us to replace $\mathrm{O}\big(\|F\|_2^2\big)$ with $\mathrm{O}(u^2)$. Condition (17) provides two things: the first part makes sure that the first r stages of LU decomposition are completed without breakdowns (the $20r^{3/2}u$ part); the second part ensures that $\|\tilde{A}_{11}^{-1}F_{11}\|_2 < 1$ which is required for applicability of Lemma 1. Indeed, it can easily be shown that

$$\|E_{11}\|_2 \leqslant \epsilon_{r+1}\lambda_1\|A_{11}\|_2.$$

Also,

$$\|\tilde{A}_{11}^{-1}\|_2 = \|(A_{11} - \Delta A_{11})^{-1}\|_2 \leqslant \frac{\|A_{11}^{-1}\|_2}{1 - \|A_{11}^{-1}\Delta A_{11}\|_2} \leqslant 2\|A_{11}^{-1}\|_2.$$

Since $F = \Delta A - E$ we have

$$\|\tilde{A}_{11}^{-1}F_{11}\|_2 \leqslant 2\|A_{11}^{-1}\|_2\big(\epsilon_{r+1}\lambda_1\|A_{11}\|_2 + \theta u\|A_{11}\|_2\big) < 1.$$

Condition (18) provides that $\Psi < 2$ and $1 + \epsilon_{r+1}\lambda_2 < (1 + 2\lambda_2)/2\lambda_2$, and now by combining conditions (16)–(19) we get (20). □

Observe that $\rho = \||\hat{L}_{\mathrm{r}}||\hat{U}_{\mathrm{r}}|\|_2/\|A_{11}\|_2$ is the growth factor which relates only to the pivoting strategy applied to A_{11} and does not depend on W or V. For example, if we factor A_{11} using GEPP we would have $\rho = 2^{r-1}$, in case of GECP we would have $\rho = \sqrt{r}\big(2^1 \cdot 3^{1/2} \cdots r^{1/r-1}\big)^{1/2}$.

6. Conclusion

We have introduced a definition of strong RRLU factorization similar to the notion of strong RRQR. We proved the existence of a pivoting strategy that efficiently extracts full rank and rank deficient portions of matrix A and keeps elements of $V = A_{11}^{-1}A_{12}$ and $W = A_{21}A_{11}^{-1}$ small. Backward error analysis has revealed the key role played by matrices V and W in the bound (20) on the error term $A - \hat{L}_{\mathrm{r}}\hat{U}_{\mathrm{r}}$, where $\hat{L}_{\mathrm{r}}$ and $\hat{U}_{\mathrm{r}}$ are the computed lower and upper-triangular LU factors.

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