Rank Revealing *LU* Factorizations

Tsung-Min Hwang, Wen-Wei Lin,* and Eugene K. Yang
Institute of Applied Mathematics
National Tsing Hua University
Hsinchu
Taiwan 30043, R.O.C.

Submitted by Richard A. Brualdi

ABSTRACT

We consider permutations of any given squared matrix and the generalized $LU(r)$ factorization of the permuted matrix that reveals the rank deficiency of the matrix. Chan has considered the case with nearly rank deficiency equal to one. This paper extends his results to the case with nearly rank deficiency greater than one. Two applications in constrained optimization are given. We are primarily interested in the existence of such factorizations. In addition to the theories, we also present an efficient two-pass rank revealing $LU(r)$ algorithm.

---

1. INTRODUCTION

Let A be an n-by-n matrix. We shall consider the generalized $LU(r)$ factorization $P_1AQ_1 = LU$ which will reveal the nearly rank deficiency of A (herein P_1 and Q_1 always denote permutation matrices, L unit lower triangular and U upper triangular except for a small $r \times r$ block at its last $r \times r$ position; see the definition of $LU(r)$ factorization in Section 2 below). Our main interest is on the nearly singular case. Chan [4] considers the case when the nearly rank deficiency of A is one. In this paper, we extend his results to the case with higher-dimensional rank deficiency. Such a rank

*E-mail: wwlin@AM.nthu.edu.tw.

655 Avenue of the Americas, New York, NY 10010 0024-3795/92/$5.00

revealing (henceforth, RR) $LU(r)$ factorization is faster than either SVD (singular-value decomposition) or RR$QR(r)$ factorization (see Chan [3] and Foster [10]) and is important in matrix theory and linear algebra for its wide applications.

One kind of applications of such RR factorization arises from constrained optimization (see Chan [4, 5], Chan and Resasco [7]). When an equality constrained problem is solved by the Lagrange-multiplier approach, we have a symmetric but not positive definite system with the Hessian in the (1, 1) block and the constraints constituting the borders. If the Hessian is singular at the solution, then our RR factorization together with deflated block elimination [7] can be used to solve the problem (Chan [6]). The following is another application. If the active-set method is used to solve an inequality constrained optimization problem and the problem is (nearly) degenerate at an intermediate iteration, then the RR factorization is essential to make the method successful (Fletcher [9]). Besides, it can also be used to solve least-squares problems following the method proposed by Björk [1, 2].

Let $r \geqslant 1$ be the nearly rank deficiency of A. That is, the rth smallest singular value σ_{n-r+1} of A is of small magnitude, and the $(r+1)$th smallest singular value σ_{n-r} is of order one. We will show that, for this matrix A, there always exists a generalized $LU(r)$ factorization with an $r \times r$ position of U. Here "small" means $O(\sigma_{n-r+1})$. Chan [4] notes that the usual partial pivoting cannot guarantee to produce small pivots, i.e., to reveal the rank deficiency. In this paper, we shall concern ourselves with the theoretical questions of the existence of such RR$LU(r)$ factorizations but shall also give a practical (i.e. efficient) algorithm for computing such factorizations.

The following notation will be used throughout. $n(A)$ and $\det A$ denote the nullity and the determinant of A, respectively. $A[i_1, \dots, i_p | j_1, \dots, j_p]$ denotes the $p \times p$ submatrix of A obtained from the intersection of rows $i_1, \dots, i_p$ with columns $j_1, \dots, j_p$. When the two sets of indices are the same, we write $A[i_1, \dots, i_p]$ for short. $A(i_1, \dots, i_p | j_1, \dots, j_p)$ and $A(i_1, \dots, i_p)$ denote the determinants of $A[i_1, \dots, i_p | j_1, \dots, j_p]$ and $A[i_1, \dots, i_p]$, respectively.

In this paper some lemmas are simple extensions of those in [4], but others are not simple. In Section 2, we outline the ways to find permutations P and Q such that there exists a generalized $LU(r)$ factorization for PAQ. In Section 3, we discuss the exactly singular case; in Section 4, we discuss the nonsingular case. In Section 5, we present an efficient two-pass algorithm, RR$LU(r)$, that utilizes the theories in the previous sections. We give some numerical results to illustrate that the first pass of Algorithm RR$LU(r)$ fails but the second pass succeeds in revealing the nearly rank deficiency of a given nearly singular matrix.

2. EXISTENCE OF GENERALIZED $LU(r)$ FACTORIZATIONS

In this section, we first define the generalized $LU(r)$ factorization of a given matrix $A \in \mathbf{R}^{n \times n}$, and then we give an equivalence condition for the existence of the $LU(r)$ factorization.

DEFINITION. Let A be an $n \times n$ matrix and $0 \leqslant r \leqslant n$. If there exist permutations P_1 and Q_1 which, respectively, permute only the first $n - r$ rows and columns of A such that

$$P_1 A Q_1 = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I_r \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}, \tag{2.1}$$

where $U_{22} \in \mathbf{R}^{r \times r}$ (not necessary upper triangular), $U_{11} \in \mathbf{R}^{(n-r)\times(n-r)}$ is upper triangular, and $L_{11} \in \mathbf{R}^{(n-r)\times(n-r)}$ is unit lower triangular, then we say that A has a *generalized* $LU(r)$ *factorization.*

Note that the generalized $LU(0)$ factorization of A is the usual LU factorization of A (which always exists).

We first prove two lemmas for the fundamental existence theorem.

LEMMA 2.1.

(a) *If A is nonsingular and has a generalized $LU(r)$ factorization as in* (2.1), *then we can perturb the submatrix*

$$P_1 A Q_1[n - r + 1, \dots, n]$$

by U_{22} to make A singular with nullity equal to r.

(b) *If A is singular with nullity r and has a generalized $LU(r)$ factorization* (2.1) *with $U_{22} = 0$, then we can perturb the submatrix $P_1 A Q_1[n - r + 1, \dots, n]$ by a nonsingular $r \times r$ matrix to make A nonsingular.*

Proof. (a): Write

$$P_1 A Q_1 = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I_r \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} = \begin{bmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{21}U_{11} & L_{21}U_{12} + U_{22} \end{bmatrix}.$$

Let

$$\tilde{A} = P_1 A Q_1 - \operatorname{diag}\{0_{n-r}, U_{22}\} = \begin{bmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{21}U_{11} & L_{21}U_{12} \end{bmatrix}$$

$$= \begin{bmatrix} L_{11} & 0 \\ L_{21} & I_r \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & 0 \end{bmatrix}.$$

Thus $n(\tilde{A}) = r$. The proof for part (b) is similar. ■

LEMMA 2.2. *Let A, with nullity equal to 0 or r, be represented in the partitioned form*

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

where $A_{11} \in \mathbf{R}^{(n-r)\times(n-r)}$ and $A_{22} \in \mathbf{R}^{r\times r}$. Then we can change the nullity of A (from 0 to r or vice versa) by perturbing the submatrix A_{22} if and only if A_{11} is nonsingular.

Proof. The "only if" part: Suppose that A_{11} is singular and rank $A_{11} = k$. Let

$$A_{11} = U \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} V^T$$

be the SVD of A_{11}, where $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_k) > 0$. Define

$$S(A_{22}) \equiv \begin{bmatrix} U & 0 \\ 0 & I_r \end{bmatrix} A \begin{bmatrix} V & 0 \\ 0 & I_r \end{bmatrix}^T = \begin{bmatrix} \Sigma & 0 & S_{13} \\ 0 & 0 & S_{23} \\ S_{31} & S_{32} & A_{22} \end{bmatrix},$$

where S_{32} and S_{23}^T are in $\mathbf{R}^{r\times(n-k-r)}$.

For the case rank $A = n - r$:

(i) If S_{32} has deficient column rank, then rank $S(A_{22}) \leqslant n - 1$ for all A_{22}.

(ii) If S_{32} has full column rank, then

$$\operatorname{rank} \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \\ S_{31} & S_{32} \end{bmatrix} = n - r;$$

and since rank $A = n - r$, we have $S_{23} = 0$. Thus

$$\operatorname{rank} S(A_{22}) \leqslant n - 1 \qquad \text{for all } A_{22}.$$

From (i) and (ii), we know that there does not exist A_{22} such that rank $S(A_{22}) = n$, which is contradictory. Thus A_{11} is nonsingular.

For the case rank $A = n$: Since rank $A = n$, we have rank $S_{32} = n - k - r$ (full column rank), rank $S_{23} = n - k - r$ (full row rank), and $n - 2r \leqslant k \leqslant n - r - 1$. Thus

$$\operatorname{rank} S(A_{22}) \geqslant k + (n - k - r) + (n - k - r) = 2n - k - 2r.$$

From $n - 2r \leqslant k \leqslant n - r - 1$, we have $n - r + 1 \leqslant 2n - k - 2r \leqslant n$. Therefore, rank $S(A_{22}) \geqslant n - r + 1$ for all A_{22}; i.e. there does not exist a perturbation of A_{22}, say $\tilde{A}_{22}$, such that rank $S(\tilde{A}_{22}) = n - r$, which is contradictory. Thus A_{11} is nonsingular.

The "if" part: Suppose that A_{11} is nonsingular. Then

$$\begin{bmatrix} I & 0 \\ -A_{21}A_{11}^{-1} & I \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} I & -A_{11}^{-1}A_{12} \\ 0 & I \end{bmatrix} = \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{bmatrix}. \tag{2.2}$$

From (2.2), we have that

$$\operatorname{rank} A = \operatorname{rank} \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{bmatrix}.$$

Therefore, we can change the nullity of A (from 0 to r or vice versa) by perturbing the submatrix A_{22}. This complete the proof. ■

On the basis of Lemma 2.1 and 2.2, we want to find a submatrix H of A such that if we perturb H, then $n(A)$ is changed either from 0 to r or vice versa.

DEFINITION. Let $C_1(r)$ denote the set of all $r \times r$ submatrices

$$A[i_1, \ldots, i_r | j_1, \ldots, j_r] \equiv H$$

of A, where $n(A)$ can be changed (from 0 to r or vice versa) by perturbing the submatrix H of A alone.

When an element H in $C_1(r)$ is found, we use permutations, called P and Q, to permute H to the last $r \times r$ position of PAQ. In the following we will prove the fundamental theorem on the existence of a generalized $LU(r)$ factorization for PAQ.

THEOREM 2.3. *Let P and Q be two permutations. Then PAQ has a generalized $LU(r)$ factorization as in* (2.1) *if and only if P and Q permute a submatrix H in $C_1(r)$ to the last r-by-r position of PAQ.*

Proof. The "only if" part is Lemma 2.1. We prove the "if" part as follows. Let

$$PAQ = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \qquad \text{where} \quad A_{22} \in \mathbf{R}^{r \times r}.$$

By Lemma 2.2, A_{11} is nonsingular. So A_{11} has an $LU(0)$ factorization, say $\pi_1 A_{11} \theta_1 = L_{11} U_{11}$, where π_1, θ_1 are permutations and U_{11} has nonzero diagonal elements. Let

$$P_1 = \begin{bmatrix} \pi_1 & 0 \\ 0 & I_r \end{bmatrix} \quad \text{and} \quad Q_1 = \begin{bmatrix} \theta_1 & 0 \\ 0 & I_r \end{bmatrix}.$$

Thus

$$P_1 PAQQ_1 = \begin{bmatrix} L_{11} & 0 \\ A_{21}\theta_1 U_{11}^{-1} & I_r \end{bmatrix} \begin{bmatrix} U_{11} & L_{11}^{-1}\pi_1 A_{12} \\ 0 & U_{22} \end{bmatrix},$$

where $U_{22} = A_{22} - A_{21}\theta_1 U_{11}^{-1} L_{11}^{-1} \pi_1 A_{12} = A_{22} - A_{21} A_{11}^{-1} A_{12}$. Therefore, PAQ has a generalized $LU(r)$-factorization. ■

In the following two sections, we shall establish some subsets of $C_1(r)$ which will give further equivalent and sufficient conditions for the existence of the $LU(r)$ factorization of a singular or a nonsingular matrix. This information will lead to a practical algorithm in Section 5.

3. THE SINGULAR CASE

In this section, let A be a singular matrix with $n(A) = r$. We shall show how to find P and Q such that PAQ has a generalized $LU(r)$ factorization (2.1) with $U_{22} = 0$. First, we need the following two preliminary lemmas.

LEMMA 3.1. *Let* $D = \operatorname{diag}(d_1, \ldots, d_{n-r}, 0, \ldots, 0)$, $U_r \equiv [u_1, \ldots, u_r]$, *and* $V_r \equiv [v_1, \ldots, v_r] \in \mathbf{R}^{n \times r}$. *Then*

$$\det\left(D + \sum_{i=1}^{r} u_i v_i^T\right)$$
$$= \prod_{i=1}^{n-r} d_i U_r(n-r+1, \ldots, n|1, \ldots, r) V_r(n-r+1, \ldots, n|1, \ldots, r).$$

Proof. See appendix. ■

Now, let $A = X\Sigma Y^T$ be the SVD of A, where $\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_{n-r}, 0, \ldots, 0)$, $X \equiv [x_1, \ldots, x_n]$, and $Y \equiv [y_1, \ldots, y_n]$ are orthogonal. From now on, let H denote an $r \times r$ matrix $[\delta_{lk}]$. Then

LEMMA 3.2.

$$\det\left(A + \sum_{l=1}^{r} \sum_{k=1}^{r} \delta_{lk} e_{i_l} e_{j_k}^T\right)$$
$$= (\det X \det Y \det H) X(i_1, \ldots, i_r | n-r+1, \ldots, n)$$
$$\times Y(j_1, \ldots, j_r | n-r+1, \ldots, n) \prod_{i=1}^{n-r} \sigma_i.$$

Proof. See appendix. ■

The next lemma shows that $C_1(r)$ is related to the left and right singular vectors corresponding to $\sigma_{n-r+1} = \cdots = \sigma_n = 0$, respectively.

DEFINITION. Define the set

$$C_2(r) \equiv \{H : H \quad \text{is in } C_1(r)$$
$$\text{satisfying} \quad X(i_1, \ldots, i_r | n-r+1, \ldots, n) \neq 0$$
$$\text{and } Y(j_1, \ldots, j_r | n-r+1, \ldots, n) \neq 0\}.$$

Note that we use nonzero determinants instead of nonzero components to generalize the definition of $C_2(r)$ in Chan [4].

LEMMA 3.3. *If A is singular with $n(A) = r$, then $C_2(r) \equiv C_1(r)$ and is nonempty.*

Proof. By Lemma 3.2, we know that for a nonsingular matrix $H \equiv [\delta_{lk}] \in \mathbf{R}^{r \times r}$

$$\det\left(A + \sum_{l=1}^{r} \sum_{k=1}^{r} \delta_{lk} e_{i_l} e_{j_k}^T \right) \neq 0 \quad \text{if and only if}$$

$$X(i_1, \ldots, i_r | n - r + 1, \ldots, n) \neq 0 \text{ and } Y(j_1, \ldots, j_r | n - r + 1, \ldots, n) \neq 0.$$

Thus $C_2(r) = C_1(r)$.

It remains to show that $C_2(r)$ is nonempty. If $X(i_1, \ldots, i_r | n - r + 1, \ldots, n) = 0$ for any possible set of $i_l : l = 1, \ldots, r$, then $\{x_{n-r+1}, \ldots, x_n\}$ is linearly dependent, which is contradictory. This can be similarly shown for the determinant involving Y. Therefore, C_2 is nonempty. ■

Combining Theorem 2.3 and Lemma 3.3, we have the following primary result of this section.

THEOREM 3.4. *Suppose that $n(A) = r$. Then PAQ has a generalized $LU(r)$ factorization* (2.1) *with $U_{22} = 0$ if and only if P and Q permute an element in $C_2(r)$ to the last $r \times r$ position of PAQ. Moreover, there always exists at least one such factorization for any singular A.*

4. THE NONSINGULAR CASE

In this section, we assume that A is nonsingular but with r small singular values. We shall show how to find permutations P and Q such that PAQ has a generalized $LU(r)$ factorization (2.1) with such a small $U_{22} \in \mathbf{R}^{r \times r}$ that the factorization reveals the nearly rank r deficiency of A. First, we show that $C_1(r)$ is related to r-by-r submatrices of A^{-1} with nonzero determinants.

DEFINITION. Let $M = A^{-1}$. Define

$$C_3(r) \equiv \{H \equiv A[i_1, \ldots, i_r | j_1, \ldots, j_r] : \beta \equiv M(j_1, \ldots, j_r | i_1, \ldots, i_r) \neq 0\}.$$

LEMMA 4.1. *Let A be nonsingular. If $H \in C_3(r)$ and $H = [\delta_{lk}]$, for $l, k = 1, \ldots, r$, is the inverse of $M[j_1, \ldots, j_r | i_1, \ldots, i_r]$, i.e.,*

$$\delta_{lk} = \frac{(-1)^{l+k}}{\beta} M\left(j_1, \ldots, \hat{j}_k, \ldots, j_r | i_1, \ldots, \hat{\imath}_l, \ldots, i_r\right), \tag{4.1}$$

where $\hat{\imath}$ means "omit i," then

$$n\left(A - \sum_{l=1}^{r}\sum_{k=1}^{r}\delta_{lk}e_{i_l}e_{j_k}^T\right) = r.$$

In other words, we have $C_3(r) \subseteq C_1(r)$.

Proof. See appendix. ∎

THEOREM 4.2. *If P and Q permute a submatrix $A[i_1, \dots, i_r | j_1, \dots, j_r] \in C_1(r)$ to the last $r \times r$ position of PAQ, and*

$$n\left(A - \sum_{l=1}^{r}\sum_{k=1}^{r}\delta_{lk}e_{i_l}e_{j_k}^T\right) = r,$$

then PAQ has a generalized LU(r) factorization (2.1) *with $U_{22} = [\delta_{lk}]$.*

Proof. Let

$$PAQ = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \qquad \text{where} \quad A_{22} \in \mathbf{R}^{r\times r}.$$

By Lemma 2.2 and the definition of $C_1(r)$, we have that A_{11} is nonsingular. By Theorem 2.3, PAQ has a generalized $LU(r)$ factorization. Let it be

$$P_1 PAQQ_1 = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I_r \end{bmatrix}\begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}.$$

If $P_1 = \operatorname{diag}(\pi_1, I_r)$ and $Q_1 = \operatorname{diag}(\theta_1, I_r)$, then

$$\pi_1 A_{11}\theta_1 = L_{11}U_{11} \quad \text{and} \quad U_{22} = A_{22} - L_{21}U_{12}. \tag{4.2}$$

Let $\tilde{A} = A - \sum_{l=1}^{r}\sum_{k=1}^{r}\delta_{lk}e_{i_l}e_{j_k}^T$. Then

$$P\tilde{A}Q = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & \tilde{A}_{22} \end{bmatrix},$$

where

$$\tilde{A}_{22} = A_{22} - [\delta_{lk}]. \tag{4.3}$$

On the other hand,

$$P_1 P\tilde{A}QQ_1 = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I_r \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & \tilde{U}_{22} \end{bmatrix},$$

where

$$\tilde{U}_{22} = \tilde{A}_{22} - L_{21}U_{12}. \tag{4.4}$$

$n(\tilde{A}) = r$ implies $\tilde{U}_{22} = 0$. From (4.2), (4.3), and (4.4), we then have $U_{22} = [\delta_{lk}]$. ∎

Combining Lemma 4.1 and Theorem 4.2, we have the following theorem immediately.

THEOREM 4.3. *If A is nonsingular and P and Q permute an element of $C_3(r)$ to the last $r \times r$ position of PAQ, then PAQ has a generalized $LU(r)$ factorization* (2.1). *Moreover, the (l, k)th entry of U_{22}, say δ_{lk}, is equal to*

$$\frac{(-1)^{l+k}}{\beta} M\left(j_1, \dots, \hat{j}_k, \dots, j_r | i_1, \dots, \hat{i}_l, \dots, i_r\right) \tag{4.5}$$

for $l, k = 1, \dots, r$, where $\beta \equiv M(j_1, \dots, j_r | i_1, \dots, i_r)$.

Now, let $X^T AY = \Sigma \equiv \operatorname{diag}(\sigma_1, \dots, \sigma_n)$ be the SVD of A with $\sigma_1 \geqslant \cdots \geqslant \sigma_n > 0$, and denote the columns of X and Y by x_i and y_i, respectively. In the following, we will characterize the generalized $LU(r)$ factorization (2.1) of PAQ with small $U_{22} \in \mathbf{R}^{r\times r}$ by the singular vectors $x_{n-r+1}, \dots, x_n$ and $y_{n-r+1}, \dots, y_n$ corresponding to $\sigma_{n-r+1}, \dots, \sigma_n$, where $\sigma_{n-r} \gg \sigma_{n-r+1} = O(\epsilon)$ (small in magnitude).

DEFINITION. Define

$$C_4(r) = \Bigg\{ H \equiv A[i_1, \dots, i_r | j_1, \dots, j_r] :$$

$$\operatorname{abs} Y(j_1, \dots, j_r | n - r + 1, \dots, n) \geqslant \left(\frac{r!(n-r)!}{n!}\right)^{1/2}$$

$$\text{and abs } X(i_1, \dots, i_r | n - r + 1, \dots, n) \geqslant \left(\frac{r!(n-r)!}{n!}\right)^{1/2} \Bigg\},$$

where abs denotes the absolute value.

THEOREM 4.4. *$C_4(r)$ is nonempty.*

Proof. Let $Y_r \equiv Y[1,\dots,n|n-r+1,\dots,n]$. Since Y_r is orthogonal, by the Binet-Cauchy formula we have

$$1 = \det Y_r^T Y_r = \sum_{1 \leqslant k_1 < \cdots < k_r \leqslant n} Y_r(k_1,\dots,k_r|n-r+1,\dots,n)^2.$$

Hence, there exist indices $j_1,\dots,j_r$ such that

$$\operatorname{abs} Y(j_1,\dots,j_r|n-r+1,\dots,n) \geqslant \left(\frac{r!(n-r)!}{n!}\right)^{1/2}.$$

Similarly, there exist $i_1,\dots,i_r$ such that

$$\operatorname{abs} X(i_1,\dots,i_r|n-r+1,\dots,n) \geqslant \left(\frac{r!(n-r)!}{n!}\right)^{1/2}. \qquad \blacksquare$$

Next, we show our main result in this section. The next theorem, using the Binet-Cauchy formula, is also the main contribution of this paper.

THEOREM 4.5. *Let A be nonsingular. If P and Q permute an element in $C_4(r)$ to the last $r \times r$ position of PAQ, then PAQ has a generalized $LU(r)$ factorization* (2.1) *with $U_{22} \equiv [\delta_{lk}]$ satisfying the following upper bound:*

$$|\delta_{lk}| \leqslant \frac{n!}{r!(n-r)!}\sigma_{n-r+1}\left[1 - \frac{n!}{r!(n-r)!}\frac{\sigma_{n-r+1}}{\sigma_{n-r}}\right]^{-1}$$

for $l, k = 1,\dots,r$, provided that the quantity inside the bracket is positive.

Proof. For ease of exposition, we shall first use the case of $r = 2$ to illustrate the derivation. Let $A = X\Sigma Y^T$ and $M = A^{-1} = \sum_{k=1}^n \sigma_k^{-1} y_k x_k^T$. Then

$$M[j,k|i,l] = Y[j,k|1,\dots,n]\operatorname{diag}(\sigma_1^{-1},\dots,\sigma_n^{-1})X[i,l|1,\dots,n]^T.$$

By the Binet-Cauchy formula, we have

$$\beta \equiv M(j,k|i,l) = \sum_{1 \leqslant p < q \leqslant n} Y(j,k|p,q)X(i,l|p,q)\sigma_p^{-1}\sigma_q^{-1}$$

$$= Y(j,k|n-1,n)X(i,l|n-1,n)\sigma_{n-1}^{-1}\sigma_n^{-1}$$

$$+ \sum_{\substack{1 \leqslant p < q \leqslant n \\ (p,q) \neq (n-1,n)}} Y(j,k|p,q)X(i,l|p,q)\sigma_p^{-1}\sigma_q^{-1}. \tag{4.6}$$

In the following we will show the upper bound for the second term in (4.6) is $\sigma_n^{-1}\sigma_{n-2}^{-1}$:

$$\operatorname{abs}\left(\sum_{\substack{1 \leqslant p < q \leqslant n \\ (p,q) \neq (n-1,n)}} Y(j,k|p,q)X(i,l|p,q)\sigma_p^{-1}\sigma_q^{-1} \right)$$

$$\leqslant \sigma_n^{-1}\sigma_{n-2}^{-1} \sum_{\substack{1 \leqslant p < q \leqslant n \\ (p,q) \neq (n-1,n)}} \operatorname{abs}[Y(j,k|p,q)X(i,l|p,q)]$$

$$\leqslant \sigma_n^{-1}\sigma_{n-2}^{-1} \left\{ \sum_{\substack{1 \leqslant p < q \leqslant n \\ (p,q) \neq (n-1,n)}} Y(j,k|p,q)^2 \right\}^{1/2}$$

$$\left\{ \sum_{\substack{1 \leqslant p < q \leqslant n \\ (p,q) \neq (n-1,n)}} X(i,l|p,q)^2 \right\}^{1/2}$$

(by the Cauchy-Schwarz inequality)

$$\leqslant \sigma_n^{-1}\sigma_{n-2}^{-1}.$$

The last inequality follows from applying the Binet-Cauchy formula to the matrices

$$I_2 = Y[j,k|1,\ldots,n]Y[j,k|1,\ldots,n]^T \tag{4.7a}$$

and

$$I_2 = X[i,l|1,\ldots,n]X[i,l|1,\ldots,n]^T. \tag{4.7b}$$

By the definition of $C_4(r)$ and the assumption that the quantity inside the bracket is positive, we have

$$|\beta| \geqslant \frac{2}{n(n-1)} \sigma_n^{-1} \sigma_{n-1}^{-1} - \sigma_n^{-1} \sigma_{n-2}^{-1} > 0.$$

Hence $C_4(r) \subseteq C_3(r)$ and

$$|\beta|^{-1} \leqslant \frac{n(n-1)}{2} \sigma_n \sigma_{n-1} \left[1 - \frac{n(n-1)\sigma_{n-1}}{2\sigma_{n-2}} \right]^{-1}.$$

We show this similarly for the general case, i.e., when the nearly rank deficiency is r. By the Binet-Cauchy formula,

$$\begin{aligned} \beta &\equiv M(j_1, \dots, j_r | i_1, \dots, i_r) \\ &= Y(j_1, \dots, j_r | n - r + 1, \dots, n) \\ &\quad \times X(i_1, \dots, i_r | n - r + 1, \dots, n) \sigma_{n-r+1}^{-1} \cdots \sigma_n^{-1} \\ &\quad + \sum_{\substack{1 \leqslant p_1 < \cdots < p_r \leqslant n \\ (p_1, \dots, p_r) \neq (n-r+1, \dots, n)}} Y(j_1, \dots, j_r | p_1, \dots, p_r) \\ &\quad X(i_1, \dots, i_r | p_1, \dots, p_r) \sigma_{p_1}^{-1} \cdots \sigma_{p_r}^{-1}. \end{aligned} \tag{4.8}$$

The second term of (4.8) can be estimated as follows by using the Cauchy-Schwarz inequality and the Binet-Cauchy formula:

$$\begin{aligned} &\operatorname{abs}\left(\sum_{\substack{1 \leqslant p_1 < \cdots < p_r \leqslant n \\ (p_1, \dots, p_r) \neq (n-r+1, \dots, n)}} Y(j_1, \dots, j_r | p_1, \dots, p_r) \right. \\ &\qquad \left. \times X(i_1, \dots, i_r | p_1, \dots, p_r) \sigma_{p_1}^{-1} \cdots \sigma_{p_r}^{-1} \right) \\ &\leqslant \sigma_n^{-1} \cdots \sigma_{n-r+2}^{-1} \sigma_{n-r}^{-1} \left\{ \sum_{\substack{1 \leqslant p_1 < \cdots < p_r \leqslant n \\ (p_1, \dots, p_r) \neq (n-r+1, \dots, n)}} \right. \\ &\qquad \left. Y(j_1, \dots, j_r | p_1, \dots, p_r)^2 \right\}^{1/2} \end{aligned}$$

$$\times \left\{ \sum_{\substack{1 \leqslant p_1 < \cdots < p_r \leqslant n \\ (p_1, \ldots, p_r) \neq (n-r+1, \ldots, n)}} X(i_1, \ldots, i_r | p_1, \ldots, p_r)^2 \right\}^{1/2}$$

$$\leqslant \sigma_n^{-1} \cdots \sigma_{n-r+2}^{-1} \sigma_{n-r}^{-1}. \tag{4.9}$$

Hence, by the definition of $C_4(r)$, (4.8), (4.9), and the assumption of the theorem, a lower bound on $|\beta|$ is given by

$$|\beta| \geqslant \frac{r!(n-r)!}{n!} \prod_{p=n-r+1}^{n} \sigma_p^{-1} \left[1 - \frac{n!}{r!(n-r)!} \frac{\sigma_{n-r+1}}{\sigma_{n-r}} \right] > 0.$$

Thus, we have $C_4(r) \subseteq C_3(r)$ and

$$|\beta|^{-1} \leqslant \frac{n!}{r!(n-r)!} \prod_{p=n-r+1}^{n} \sigma_p \left[1 - \frac{n!}{r!(n-r)!} \frac{\sigma_{n-r+1}}{\sigma_{n-r}} \right]^{-1}. \tag{4.10}$$

By Theorem 4.3, PAQ has a generalized $LU(r)$ factorization (2.1). We have estimated an upper bound (4.10) for $|\beta|^{-1}$. To estimate an upper bound for $|\delta_{lk}|$ (see Theorem 4.3 for δ_{lk}), we only need to estimate an upper bound for the numerator of $|\delta_{lk}|$. By using the Cauchy-Schwarz inequality and the Binet-Cauchy formula in a similar way, we have

$$\operatorname{abs}\left(M\left(j_1, \ldots, \hat{j}_k, \ldots, j_r | i_1, \ldots, \hat{i}_l, \ldots, i_r\right)\right)$$

$$= \operatorname{abs}\left(\sum_{1 \leqslant p_1 < \cdots < p_{r-1} \leqslant n} Y\left(j_1, \ldots, \hat{j}_k, \ldots, j_r | p_1, \ldots, p_{r-1}\right) \right.$$

$$\left. \times X(i_1, \ldots, \hat{i}_l, \ldots, i_r | p_1, \ldots, p_{r-1}) \sigma_{p_1}^{-1} \cdots \sigma_{p_{r-1}}^{-1} \right)$$

$$\leqslant \sigma_n^{-1} \cdots \sigma_{n-r+2}^{-1}. \tag{4.11}$$

By (4.10) and (4.11) we complete the proof. ■

Theorem 4.4 and Theorem 4.5 together establish the *existence* of a generalized $LU(r)$ factorization with small U_{22} for any rank r deficient square matrix A. In addition to being nonempty, $C_4(r)$ is applicable in practical algorithms. In the next section, we propose such an algorithm for finding an element in $C_4(r)$, which leads to a generalized $LU(r)$ factorization with small U_{22} as bounded by the bound of Theorem 4.5.

5. ALGORITHM AND EXAMPLES

Suppose the matrix $A \in \mathbf{R}^{n\times n}$ has nearly rank deficiency r $(r \geqslant 1)$ and the quantity $[n!/r!(n-r)!]\sigma_{n-r+1}$ is sufficiently small, where σ_{n-r+1} is the rth smallest singular value of A. By using Theorem 4.4 and Theorem 4.5, we give an efficient algorithm for finding a rank revealing $LU(r)$ factorization for the matrix A.

ALGORITHM RR$LU(r)$. Given $A \in \mathbf{R}^{n\times n}$ with nearly rank deficiency r, where $r \geqslant 1$ (but r is unknown *a priori*). Let $X^TAY = \operatorname{diag}(\sigma_1, \dots, \sigma_n)$ be the SVD of A with $\sigma_1 \geqslant \cdots \geqslant \sigma_{n-r} \gg \sigma_{n-r+1} \geqslant \cdots \geqslant \sigma_n > 0$. This algorithm computes permutations P, Q and a generalized $LU(r)$ factorization of PAQ

$$P_1(PAQ)Q_1 = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I_r \end{bmatrix}\begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}$$

with a small $U_{22} \equiv [\delta_{lk}] \in \mathbf{R}^{r\times r}$, which reveals the rank r deficiency of A.

Step 1: Compute the $LU(0)$ factorization of A by some conventional pivoting strategy (e.g., partial pivoting):

$$\hat{\pi}A\hat{\theta} = \hat{L}\hat{U}. \tag{5.1}$$

Step 2: Determine a temporary rank deficiency $\hat{r}$. Determine the index $\hat{r}$ $(0 \leqslant \hat{r} < n)$ such that $|\hat{u}_{i,j}| <$ tolerance for all $i, j = n - \hat{r} + 1, \dots, n$ and there exists an index $k \in \{n - \hat{r}, \dots, n\}$ with $|\hat{u}_{n-r,k}|$ $>$ tolerance.

Step 3: Use inverse iteration to determine the true rank deficiency r and compute the approximate singular values $\sigma_{n-r+1}(A), \dots, \sigma_n(A)$, the corresponding approximate right singular vectors $Y_r \equiv [y_{n-r+1}, \dots, y_n]$, and the approximate left singular vectors $X_r \equiv [x_{n-r+1}, \dots, x_n]$.

If $\hat{r} = 0$, then set $m = 1$; else set $m := \hat{r}$.
For $k = 1, 2, \dots$
  $m := 2m$.
  Given an orthonormal matrix $Z \in \mathbf{R}^{n\times m}$

Set $Q = I$, $\lambda_1 = 1$.
While $\lambda_1 >$ tolerance, do
Set $U = ZQ$.
Solve $AW = U$ by using the factorization (5.1).
Solve $A^T V = W$ by using the factorization (5.1).
Let $Z = V(V^T V)^{-1/2}$ (e.g., Gram-Schmidt).
Compute the eigenvalues of $Z^T AA^T Z$. Since $Z^T AA^T Z = Z^T U(V^T V)^{-1/2}$, we compute an orthogonal $Q \in \mathbf{R}^{m \times m}$ so that

$$Q^T Z^T U(V^T V)^{-1/2} Q = \operatorname{diag}(\lambda_1, \dots, \lambda_m), \tag{5.2}$$

where $0 \leqslant \lambda_1 \leqslant \cdots \leqslant \lambda_m$.
Endwhile
If there exists index r $(1 \leqslant r < m)$ such that $\lambda_r \leqslant$ tolerance and $\lambda_{r+1} >$ tolerance then stop; else continue;
Endfor k.
Let $X_r = ZQ_r$, where Q_r is the first r columns of Q.

Remark: The convergence rate for the above inverse iteration process without adding (5.2) is $(\sigma_{n-r+1}/\sigma_{n-r})^2$. The convergence rate is now accelerated by the correction step (5.2) (see [8] for details).

Solve $A\hat{Y} = X_r$.
Let $Y_r = \hat{Y}(\hat{Y}^T\hat{Y})^{-1/2}$.
Compute the singular values of $X_r^T A Y_r$, which are approximations to the smallest singular values $\sigma_{n-r+1}(A), \dots, \sigma_n(A)$.
If $r = \hat{r}$, then done (first pass).

Step 4: Determine an element in the set $C_4(r)$.

Comment: Indeed, the maximal elements of the sets

$$\{\text{abs } Y_r(j_1, \dots, j_r | 1, \dots, r) : 1 \leqslant j_1 < \cdots < j_r \leqslant n\} \equiv \mathscr{Y}$$

and

$$\{\text{abs } X_r(i_1, \dots, i_r | 1, \dots, r) : 1 \leqslant i_1 < \cdots < i_r \leqslant n\} \equiv \mathscr{X}$$

satisfy the conditions in $C_4(r)$. That is, the corresponding indices $(j_1, \dots, j_r)$ and $(i_1, \dots, i_r)$ yield a submatrix $H \equiv A[i_1, \dots, i_r | j_1, \dots, j_r]$ in $C_4(r)$. Unfortunately, for an $r > 2$ it is not economical to find the maximums of $\mathscr{Y}$ and $\mathscr{X}$, because that needs $n!/[r!(n-r)!]$ flop counts. In the following we give an efficient algorithm to find an element in $C_4(r)$.

Compute the $LU(0)$ factorizations with complete pivoting of Y_r and X_r, respectively:

$$Q^T Y_r \theta_Y = L_Y \begin{bmatrix} R_Y \\ 0 \end{bmatrix}, \tag{5.3a}$$

$$P^T X_r \theta_X = L_X \begin{bmatrix} R_X \\ 0 \end{bmatrix}, \tag{5.3b}$$

where $P^T, Q^T \in \mathbf{R}^{n\times n}$, $\theta_Y, \theta_X \in \mathbf{R}^{r\times r}$ are permutations, $L_Y, L_X \in \mathbf{R}^{n\times n}$ are unit lower triangular, and R_Y, R_X are upper triangular.

Comment: Let $(1,\dots,n)Q = (j_1,\dots,j_n)$ and $(1,\dots,n)P = (i_1,\dots,i_n)$. It is easily seen that $Y_r(j_1,\dots,j_r|1,\dots,r) = \det R_Y$ and $X_r(i_1,\dots,i_r|1,\dots,r) = \det R_X$. Although we cannot prove that both $|\det R_Y|$ and $|\det R_X|$ are larger than $(r!(n-r)!/n!)^{1/2}$, a statistical result shows that there is no counterexample in up to a total of about 60,000 randomly generated tested orthonormal matrices Y_r and $X_r \in \mathbf{R}^{n\times r}$ for $n = 10, 12, \dots, 100$ and $r = 2, \dots, n/2$. That is, the corresponding submatrix $H \equiv A[i_1,\dots,i_r|j_1,\dots,j_r]$ produced by (5.3) is always in $C_4(r)$.

Step 5: Compute the generalized $LU(r)$ factorization (2.1) of PAQ: Perform the Gaussian eliminations by using the partial pivoting only on the 1st row to the $(n-r)$th row of the current matrix.

Comment: By Theorem 4.5, we have that the entries δ_{lk} of U_{22} satisfy

$$|\delta_{lk}| \leqslant \frac{n!}{r!(n-r)!}\sigma_{n-r+1}\left[1 - \frac{n!}{r!(n-r)!}\frac{\sigma_{n-r+1}}{\sigma_{n-r}}\right]^{-1}$$

for $l, k = 1, \dots, r$.

The main work of this algorithm consists of two parts. The first part (steps 1, 2, and 3), referred to as the first pass of the algorithm, computes an initial $LU(0)$ factorization of A. It requires $n^3/3 + O(n^2)$ flops. If and only if $r \neq \hat{r}$ in step 3, then we perform the second part of the algorithm (steps 4 and 5), which is referred as the second pass of Algorithm RR$LU(r)$. Step 3 computes the left and right singular vectors corresponding to $\sigma_{n-r+1}(A), \dots, \sigma_n(A)$ by using the inverse iteration method. It needs about $2Jn^2r$ flops, where J is the number of inverse iterations used for the computation of X_r and Y_r. Usually $J \leqslant 5$ is sufficient in practice. Step 4 computes the complete $LU(0)$-factorizations of X_r and Y_r as in (5.3). It requires about $2nr^2$ flops. Step 5 refactors the matrix PAQ. Here, we compute the Gaussian eliminations from the 1st column to the $(n-r)$th column by forcing the partial pivoting only on the submatrix $A^{(k)}[k, \dots, n-r|k, \dots, n-r]$, where $A^{(k)}$ denotes the current matrix in the elimination process with initial matrix $A^{(1)} = PAQ$. It requires about $n^3/3$ flops. Therefore, the total flop count $C(r)$ for Algorithm RR$LU(r)$ is given by

$$\begin{aligned} C(r) &= \tfrac{2}{3}n^3 + 2Jn^2r + 2nr^2 \\ &= \tfrac{2}{3}n^3 + 4n^2r + 2nr^2, \qquad \text{assuming that} \quad J = 2. \end{aligned}$$

Therefore, if $r \ll n$, the total work for Algorithm RR$LU(r)$ is the same as that for RR$QR(r)$ [3, 10]. However, Algorithm RR$LU(r)$ has the following practical advantage over RR$QR(r)$. Chan [4] notes that the rank deficiencies of almost all nearly singular matrices can be successfully detected by the first pass of RR$LU(r)$ algorithm, unless A is nearly singular and A^{-1} has a very skew distribution of the sizes of its elements. The first pass requires $\frac{1}{3}n^3 + O(n^2)$, which is only half the cost of computing the QR factorization in Algorithm RR$QR(r)$ [3, 10].

Chan [4] presented numerical results for two well-known matrices:

$$T_n = \begin{bmatrix} 1 & -1 & \cdot & \cdot & \cdot & -1 \\ & \ddots & \ddots & & & \vdots \\ & & \ddots & \ddots & & \vdots \\ & & & \ddots & \ddots & \vdots \\ & 0 & & & \ddots & -1 \\ & & & & & 1 \end{bmatrix} \in \mathbf{R}^{n \times n} \tag{5.4a}$$

and

$$W = \begin{bmatrix} 10 & 1 \\ 1 & 9 & 1 \\ & \ddots & \ddots & \ddots \\ & & 1 & 1 & 1 \\ & & & 1 & 0 & 1 \\ & & & & 1 & -1 & 1 \\ & & & & & \ddots & \ddots & \ddots \\ & & & & & & 1 & -9 & 1 \\ & & & & & & & 1 & -10 \end{bmatrix} \in \mathbf{R}^{21 \times 21}, \tag{5.4b}$$

which are nearly singular with nearly rank 1 deficiency. In the following, we construct some nearly singular matrices with higher-dimensional rank deficiency based on a direct sum of matrices T_n or W. All computations were performed on a PC MATLAB.

EXAMPLE 4.1. Let $A = \operatorname{diag}(T_{40}, T_{40})$. Compute elementary row and column operations of A by the following steps:

for $i = 1:40$
  $A(1:40, 81 - i) = A(1:40, 81 - i) + A(1:40, i)$
  $A(i, 41:80) = A(i, 41:80) + A(81 - i, 41:80)$
end

Then the resulting matrix is

$$A = \left[\begin{array}{cccccccccccc}
1 & -1 & \cdot & \cdot & \cdot & -1 & -1 & \cdot & \cdot & \cdot & -1 & 2 \\
 & \cdot & \cdot & & & \cdot & \cdot & & & \cdot & 2 & -1 \\
 & & \cdot & \cdot & & \cdot & \cdot & & \cdot & \cdot & \cdot & \cdot \\
 & & & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot \\
 & & & & \cdot & -1 & -1 & \cdot & \cdot & & & \cdot \\
 & & & & & 1 & 2 & -1 & \cdot & \cdot & \cdot & -1 \\
 & & & & & & 1 & -1 & \cdot & \cdot & \cdot & -1 \\
 & & & & & & & \cdot & \cdot & & & \cdot \\
 & & & & & & & & \cdot & \cdot & & \cdot \\
 & & & & & & & & & \cdot & \cdot & \cdot \\
 & 0 & & & & & & & & & \cdot & -1 \\
 & & & & & & & & & & & 1
\end{array}\right],$$

which has nearly rank 2 deficiency.

The three smallest singular values of A are 6.214×10^{-1}, 1.93×10^{-12}, and 1.93×10^{-12}. Algorithm RR$LU(r)$ produces the generalized $LU(2)$ factorization (2.1) with

$$U_{22} = \begin{bmatrix} 1.05 \times 10^{-15} & 3.638 \times 10^{-12} \\ -3.638 \times 10^{-12} & 1.323 \times 10^{-23} \end{bmatrix}.$$

The upper bound of elements of U_{22} in Theorem 4.5 is 6.098×10^{-9}.

EXAMPLE 4.2. Let $A = \operatorname{diag}(T_{30}, T_{30}, T_{30})$. Compute elementary row and column operations of A by the following steps:

for $i = 1:30$
  $A(1:90, 61 - i) = A(1:90, 61 - i) + A(1:90, i)$
  $A(i, 1:90) = A(i, 1:90) + A(61 - i, 1:90)$
end
for $i = 1:30$
  $A(1:90, 91 - i) = A(1:90, 91 - i) + A(1:90, 30 + i)$
  $A(30 + i, 1:90) = A(30 + i, 1:90) + A(91 - i, 1:90)$
end

Then the resulting matrix is

$$A = \begin{bmatrix}
1 & -1 & -1 & \cdots & -1 & -1 & & \cdots & -1 & 2 & 2 & -1 & -1 & \cdots & -1 \\
 & 1 & -1 & \cdots & -1 & -1 & & \cdots & 2 & -1 & -1 & 2 & -1 & \cdots & -1 \\
 & & 1 & \ddots & \vdots & \vdots & & & & \vdots & & \ddots & \ddots & \ddots & \vdots \\
 & & & \ddots & -1 & -1 & 2 & & & -1 & & & -1 & 2 & -1 \\
 & & & & 1 & 2 & -1 & \cdots & \cdot & -1 & \cdot & \cdot & \cdot & -1 & 2 \\
 & & & & & 1 & -1 & \cdots & \cdot & -1 & \cdot & \cdot & \cdot & -1 & 2 \\
 & & & & & & & \cdots & & \cdot & & & & 2 & -1 \\
 & & & & & & & \cdots & \cdot & \cdot & & & & \cdot & \cdot \\
 & & & & & & & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & \cdot & -1 & -1 & 2 & \cdot & \cdot & \cdot \\
 & & & & & 0 & & & & 1 & 2 & -1 & \cdots & -1 & -1 \\
 & & & & & & & & & & 1 & -1 & \cdots & -1 & -1 \\
 & & & & & & & & & & & 1 & \ddots & & \vdots \\
 & & & & & & & & & & & & \ddots & -1 & -1 \\
 & & & & & & & & & & & & & 1 & -1 \\
 & & & & & & & & & & & & & & 1
\end{bmatrix},$$

which has nearly rank 3 deficiency.

The smallest four singular values of A are 4.0204×10^{-1}, 2.794×10^{-9}, 1.397×10^{-9}, and 1.397×10^{-9}. Algorithm RR$LU(r)$ produces the generalized $LU(3)$ factorization (2.1) with

$$U_{22} = \begin{bmatrix} -3.725 \times 10^{-9} & -3.868 \times 10^{-17} & 1.388 \times 10^{-17} \\ 5.454 \times 10^{-17} & -3.726 \times 10^{-9} & 3.725 \times 10^{-9} \\ -1.585 \times 10^{-17} & 3.725 \times 10^{-9} & 5.906 \times 10^{-26} \end{bmatrix}.$$

The upper bound of elements of U_{22} in Theorem 4.5 is 3.285×10^{-4}.

EXAMPLE 4.3. Let $A = \operatorname{diag}(W, W)$. Compute elementary row and column operations of A by the following steps:

for $i = 1:21$
  $A(1:21, 43 - i) = A(1:21, 43 - i) + A(1:21, i)$
  $A(i, 22:42) = A(i, 22:42) + A(43 - i, 22:42)$
end

Then the resulting matrix is

$$A = \left[\begin{array}{cccccccccccccccccc}
10 & 1 & & & & & & & & & & & & & & & 2 & 0 \\
1 & 9 & 1 & & & & & & & & & & & & & 2 & 0 & 2 \\
 & \ddots & \ddots & \ddots & & & & & & & & & & & 2 & 0 & 2 & \\
 & & 1 & 1 & 1 & & & & & & & & & \cdot & \cdot & \cdot & & \\
 & & & 1 & 0 & 1 & & & & & & & \cdot & \cdot & \cdot & & & \\
 & & & & 1 & -1 & 1 & & & & & \cdot & \cdot & \cdot & & & & \\
 & & & & & \ddots & \ddots & \ddots & & & \cdot & \cdot & \cdot & & & & & \\
 & & & & & & 1 & -9 & 1 & 2 & 0 & 2 & & & & & & \\
 & & & & & & & 1 & -10 & 0 & 2 & & & & & & & \\
 & & & & & & & & & 10 & 1 & & & & & & & \\
 & & & & & & & & & 1 & 9 & 1 & & & & & & \\
 & & & & & & & & & & \ddots & \ddots & \ddots & & & & & \\
 & & & & & & & & & & & 1 & 1 & 1 & & & & \\
 & & & & & & & & & & & & 1 & 0 & 1 & & & \\
 & & & & & & & & & & & & & 1 & -1 & 1 & & \\
 & & & & & & & & & & & & & & \ddots & \ddots & \ddots & \\
 & & & & & & & & & & & & & & & 1 & -9 & 1 \\
 & & & & & & & & & & & & & & & & 1 & -10
\end{array}\right],$$

which has nearly rank deficiency $r = 2$.

The three smallest singular values of A are 5.523×10^{-1}, 8.675×10^{-16}, and 2.669×10^{-16}. Step 1 of Algorithm RR$LU(r)$ produces the last 3×3 submatrix of $\hat{U}$ as follows:

$$\hat{U}[n-2, n] = \begin{bmatrix} 1.0 \times 10^{0} & -9.0 \times 10^{0} & 1.0 \times 10^{0} \\ 0 & 1.0 \times 10^{0} & -1.0 \times 10^{1} \\ 0 & 0 & 8.1552 \times 10^{-11} \end{bmatrix},$$

which gives the temporary rank deficiency $\hat{r} = 1$. To illustrate in a general case, suppose that the true rank deficiency r is unknown *a priori*. Step 3 of the algorithm always determines correctly r. The second pass of Algorithm

RR $LU(2)$ produces the generalized $LU(2)$ factorization (2.1) with

$$U_{22} = \begin{bmatrix} -0.2097 \times 10^{-16} & -0.6775 \times 10^{-16} \\ 0.1106 \times 10^{-16} & -0.2944 \times 10^{-16} \end{bmatrix}.$$

The theoretical upper bound in Theorem 4.5 is 7.4692×10^{-13}. Note that only if the first pass produces a nearly rank deficiency r which is larger than $\hat{r}$ is the second pass required in order to obtain the correct RR $LU(r)$ factorization.

Although the theoretical bound in Theorem 4.5 is not always tight, it works well if $[n!/r!(n-r)!]\sigma_{n-r+1}$ is small [i.e., smaller than the tolerance we desire in Algorithm RR $LU(r)$]. Under this condition, Algorithm RR $LU(r)$ can produce small U_{22} even though the conventional partial-pivoting LU factorization fails to do so.

6. CONCLUSION

The main contribution of this paper is to extend the theory of Chan [4] for rank revealing LU factorizations to the general case when the nearly rank deficiency is greater than one. We have also proposed an efficient two-pass algorithm for finding an RR $LU(r)$ factorization which usually succeeds in the first pass, thus taking $\frac{1}{3}n^3 + O(n^2)$ flops. If the first pass fails (i.e., $r \neq \hat{r}$), then the current efficient implementation of the second pass, taking another $\frac{1}{3}n^3$ flops, finds RR $LU(r)$ factorizations for all of our 60,000 test problems. In comparison, Algorithm RR $QR(r)$ needs $\frac{2}{3}n^3$ flops in the first pass and $O(n^2)$ flops in the second pass. The rank deficiency of most randomly generated nearly singular matrices can be detected by the first pass of both algorithms. Therefore, for the square matrix A, Algorithm RR $LU(r)$ is in most cases twice as efficient as RR $QR(r)$. In the extreme case that the first pass fails and step 4 also fails to find an element in $C_4(r)$ (which never happened in our tests), we can switch to Algorithm RR $QR(r)$ of [4, 7] as a last resort. This hybrid strategy can take advantage of both the efficiency of our Algorithm RR $LU(r)$ and the hundred-percent guarantee of finding an RR(r) factorization given by Algorithm RR $QR(r)$.

APPENDIX

In this appendix, we shall prove Lemma 3.1, Lemma 3.2, and Lemma 4.1.

Proof of Lemma 3.1. Let

$$D_1 = \operatorname{diag}(d_1, \dots, d_{n-r}, 1, \dots, 1),$$

$$I_0 = \operatorname{diag}(1, \dots, 1, 0, \dots, 0).$$

Then

$$\begin{aligned}
D + \sum_{i=1}^{r} u_i v_i^T &= D_1 \left[I_0 + \sum_{i=1}^{r} (D_1^{-1} u_i) v_i^T \right] \\
&= D_1 \left[I + \sum_{i=1}^{r} (D_1^{-1} u_i) v_i^T - \sum_{i=1}^{r} e_{n-i+1} e_{n-i+1}^T \right] \\
&= D_1 \Big\{ I + \left[D_1^{-1} u_1, \dots, D_1^{-1} u_r, e_{n-r+1}, \dots, e_n \right] \\
&\qquad \times [v_1, \dots, v_r, -e_{n-r+1}, \dots, -e_n]^T \Big\} \\
&\equiv D_1 B. \qquad \text{(A.1)}
\end{aligned}$$

Let

$$\begin{aligned}
C = I &+ [v_1, \dots, v_r, -e_{n-r+1}, \dots, -e_n]^T \\
&\times \left[D_1^{-1} u_1, \dots, D_1^{-1} u_r, e_{n-r+1}, \dots, e_n \right].
\end{aligned}$$

Then

$$C = \begin{bmatrix} I_r + V_r^T D_1^{-1} U_r & V_r[n-r+1, \dots, n|1, \dots, r] \\ -U_r[n-r+1, \dots, n|1, \dots, r] & 0_r \end{bmatrix}.$$

Thus

$$\det C = U_r(n-r+1, \dots, n|1, \dots, r) V_r(n-r+1, \dots, n|1, \dots, r). \qquad \text{(A.2)}$$

From (A.1), (A.2), and the well-known result $\det B = \det C$, the conclusion follows. ∎

Proof of Lemma 3.2. From

$$\det\left(A + \sum_{l=1}^{r}\sum_{k=1}^{r} \delta_{lk} e_{i_l} e_{j_k}^T\right)$$

$$= \det\left\{X\left[\Sigma + \sum_{l=1}^{r}\left(X^T e_{i_l}\right)\left(\sum_{k=1}^{r} \delta_{lk}\left(Y^T e_{j_k}\right)^T\right)\right]Y^T\right\} \tag{A.3}$$

and Lemma 3.1, we have

(A.3)

$$= \det X \det Y \det\left(\Sigma + X^T[1,\dots,n|i_1,\dots,i_r] HY[j_1,\dots,j_r|1,\dots,n]\right)$$

$$= (\det X \det Y \det H) X^T(n-r+1,\dots,n|i_1,\dots,i_r)$$

$$\times Y(j_1,\dots,j_r|n-r+1,\dots,n)\prod_{i=1}^{n-r}\sigma_i.$$ ∎

Proof of Lemma 4.1. By defining U and V as

$$U \equiv \left[\delta_{11}(Me_{i_1}),\dots,\delta_{1r}(Me_{i_1}),\dots,\delta_{r1}(Me_{i_r}),\dots,\delta_{rr}(Me_{i_r})\right]$$

and

$$V \equiv [-e_{j_1},\dots,-e_{j_r},\dots,-e_{j_1},\dots,-e_{j_r}],$$

we have

$$A - \sum_{l=1}^{r}\sum_{k=1}^{r} \delta_{lk} e_{i_l} e_{j_k}^T = A\left[I - \sum_{l=1}^{r}\sum_{k=1}^{r} \delta_{lk}(Me_{i_l})e_{j_k}^T\right]$$

$$\equiv A[I - UV^T].$$

Let $W = I - V^T U$. We have $n(W) = n(A[I - UV^T])$. Since H is nonsingular, for each $i = 1, \dots, r$ there exists j such that $\delta_{ij} \neq 0$. By a careful computation, δ_{lk} $(l, k = 1, \dots, r)$ given by (4.1) in Lemma 4.1 solve the equations

$$\det \begin{bmatrix} m_{j_1 i_1} & \cdots & m_{j_1 i_{l-1}} & -\delta_{lk} m_{j_1 i_l} & m_{j_1 i_{l+1}} & \cdots & m_{j_1 i_r} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ m_{j_{k-1} i_1} & \cdots & m_{j_{k-1} i_{l-1}} & -\delta_{lk} m_{j_{k-1} i_l} & m_{j_{k-1} i_{l+1}} & \cdots & m_{j_{k-1} i_r} \\ m_{j_k i_1} & \cdots & m_{j_k i_{l-1}} & 1 - \delta_{lk} m_{j_k i_l} & m_{j_k i_{l+1}} & \cdots & m_{j_k i_r} \\ m_{j_{k+1} i_1} & \cdots & m_{j_{k+1} i_{l-1}} & -\delta_{lk} m_{j_{k+1} i_l} & m_{j_{k+1} i_{l+1}} & \cdots & m_{j_{k+1} i_r} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ m_{j_r i_1} & \cdots & m_{j_r i_{l-1}} & -\delta_{lk} m_{j_r i_l} & m_{j_r i_{l+1}} & \cdots & m_{j_r i_r} \end{bmatrix} = 0$$

and

$$\det \begin{bmatrix} 1 - \delta_{l1} m_{j_1 i_l} & \cdots & -\delta_{lr} m_{j_1 i_l} \\ \vdots & & \vdots \\ -\delta_{l1} m_{j_r i_l} & \cdots & 1 - \delta_{lr} m_{j_r i_l} \end{bmatrix} = 0 \qquad \text{for all} \quad l = 1, \dots, r.$$

Therefore, we have $n(W) \geqslant r$.

Next we need to show that $n(W) \leqslant r$. After row subtractions on the matrix

$$W = \begin{bmatrix} 1 - \delta_{11} m_{j_1 i_1} & \cdots & -\delta_{1r} m_{j_1 i_1} & \cdots & -\delta_{r1} m_{j_1 i_r} & \cdots & -\delta_{rr} m_{j_1 i_r} \\ \vdots & & \vdots & & \vdots & & \vdots \\ -\delta_{11} m_{j_r i_1} & \cdots & 1 - \delta_{1r} m_{j_r i_1} & \cdots & -\delta_{r1} m_{j_r i_r} & \cdots & -\delta_{rr} m_{j_r i_r} \\ \vdots & & \vdots & & \vdots & & \vdots \\ -\delta_{11} m_{j_1 i_1} & \cdots & -\delta_{1r} m_{j_1 i_1} & \cdots & -\delta_{r1} m_{j_1 i_r} & \cdots & -\delta_{rr} m_{j_1 i_r} \\ \vdots & & \vdots & & \vdots & & \vdots \\ -\delta_{11} m_{j_r i_1} & \cdots & -\delta_{1r} m_{j_r i_1} & \cdots & -\delta_{r1} m_{j_r i_r} & \cdots & -\delta_{rr} m_{j_r i_r} \\ -\delta_{11} m_{j_1 i_1} & \cdots & -\delta_{1r} m_{j_1 i_1} & \cdots & 1 - \delta_{r1} m_{j_1 i_r} & \cdots & -\delta_{rr} m_{j_1 i_r} \\ \vdots & & \vdots & & \vdots & & \vdots \\ -\delta_{11} m_{j_r i_1} & \cdots & -\delta_{1r} m_{j_r i_1} & \cdots & -\delta_{r1} m_{j_r i_r} & \cdots & 1 - \delta_{rr} m_{j_r i_r} \end{bmatrix},$$

we have the new transformed matrix

$$\tilde{W} = \begin{bmatrix} 1 & & & & & & -1 & \cdots & 0 \\ & \ddots & & 0 & & & \vdots & & \vdots \\ & & 1 & & & & 0 & \cdots & -1 \\ & & & \ddots & & & \vdots & & \vdots \\ & 0 & & & 1 & & -1 & \cdots & 0 \\ & & & & & \ddots & \vdots & & \vdots \\ & & & & & 1 & 0 & \cdots & -1 \\ -\delta_{11} m_{j_1 i_1} & \cdots & -\delta_{1r} m_{j_1 i_1} & \cdot & \cdot & -\delta_{r-1,r} m_{j_1 i_{r-1}} & 1 - \delta_{r1} m_{j_1 i_r} & \cdots & -\delta_{rr} m_{j_1 i_r} \\ \vdots & & \vdots & & & \vdots & \vdots & & \vdots \\ -\delta_{11} m_{j_r i_1} & \cdots & -\delta_{1r} m_{j_r i_1} & \cdot & \cdot & -\delta_{r-1,r} m_{j_r i_{r-1}} & -\delta_{r1} m_{j_r i_r} & \cdots & 1 - \delta_{rr} m_{j_r i_r} \end{bmatrix}.$$

Thus $\operatorname{rank} W = \operatorname{rank} \tilde{W} \geqslant r(r-1)$, which implies $n(W) \leqslant r$ and

$$n\left(A - \sum_{l=1}^{r} \sum_{k=1}^{r} \delta_{lk} e_{i_l} e_{j_k}^T\right) = n(W) = r.$$

Therefore, $C_3(r) \subseteq C_1(r)$. ■

We are grateful to Professor Tony Chan and an anonymous referee for their many helpful and detailed suggestions.

REFERENCES

1 A. Björck, Least squares methods, in *Handbook of Numerical Analysis* (P. G. Ciarlet and J. L. Lions, Eds.), Vol. 1, North-Holland, 1990, pp. 465–652.

2 A. Björck, A direct method for the solution of sparse linear least squares problems, in *Large Scale Matrix Problems* (A. Björck, R. J. Plemmons, and H. Schneider, Eds.), North-Holland, 1981.

3 T. F. Chan, Rank revealing *QR* factorizations, *Linear Algebra Appl.* 88/89:67–82 (1987).

4 T. F. Chan, On the existence and computation of *LU*-factorizations with small pivots, *Math. Comp.* 42:535–547 (1984).

5 T. C. Chan, An Efficient Modular Algorithm for Coupled Nonlinear Systems, Research Report YALEU/DCS/RR-328, Sept. 1984.

6 T. F. Chan, Private communication, 1990.

7 T. F. Chan and D. C. Resasco, Generalized deflated block-elimination, *SIAM J. Numer. Anal.* 23:913–924 (1986).

8 M. Clint and A. Jennings, The evaluation of eigenvalues and eigenvectors of real symmetric matrices by simultaneous iteration, *Comput. J.* 13:76–80 (1970).
9 R. Fletcher, *Practical Methods of Optimization*, Vol. 2, Wiley, 1981, pp. 38–39, 86–87, 103.
10 L. V. Foster, The probability of large diagonal elements in the *QR* factorization, *SIAM J. Sci. Statist. Comput.* 11:531–544 (1990).

Received 8 October 1990; final manuscript accepted 9 July 1991