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COMMUNICATION AVOIDING RANK REVEALING QR FACTORIZATION WITH COLUMN PIVOTING*

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Abstract. In this paper we introduce CARRQR, a communication avoiding rank revealing QR factorization with tournament pivoting. We show that CARRQR reveals the numerical rank of a matrix in an analogous way to QR factorization with column pivoting (QRCP). Although the upper bound of a quantity involved in the characterization of a rank revealing factorization is worse for CARRQR than for QRCP, our numerical experiments on a set of challenging matrices show that this upper bound is very pessimistic, and CARRQR is an effective tool in revealing the rank in practical problems. Our main motivation for introducing CARRQR is that it minimizes data transfer, modulo polylogarithmic factors, on both sequential and parallel machines, while previous factorizations as QRCP are communication suboptimal and require asymptotically more communication than CARRQR. Hence CARRQR is expected to have a better performance on current and future computers, where communication is a major bottleneck that highly impacts the performance of an algorithm.

Key words. QR factorization, rank revealing, column pivoting, minimize communication

AMS subject classifications. 65F25, 65F20

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1. Introduction.

Revealing the rank of a matrix is an operation that appears in many important problems as least squares problems, low rank approximations, regularization, and nonsymmetric eigenproblems (see, for example, [8] and the references therein). In this paper we focus on the rank revealing QR (RRQR) factorization [8, 7, 18], which computes a decomposition of a matrix $A \in \mathbb{R}^{m\times n}$ of the form

$$A\Pi = QR = Q \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix}, \tag{1.1}$$

where $Q \in \mathbb{R}^{m\times m}$ is orthogonal, $R_{11} \in \mathbb{R}^{k\times k}$ is upper triangular, $R_{12} \in \mathbb{R}^{k\times(n-k)}$, and $R_{22} \in \mathbb{R}^{(m-k)\times(n-k)}$. The column permutation matrix Π and the integer k are chosen such that $||R_{22}||_2$ is small and R_{11} is well-conditioned. This factorization was introduced in [18], and the first algorithm to compute it was proposed in [6] and is based on the QR factorization with column pivoting (QRCP). A BLAS-3 version

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of this algorithm [28] is implemented in LAPACK [1], and its parallel version in ScaLAPACK [5].

The performance of an algorithm is highly impacted by the amount of communication performed during its execution, where communication refers to both data transferred between different levels of the memory hierarchy of a processor and data transferred between different processors of a parallel computer. Research performed in recent years has shown that most of the classic algorithms in direct dense linear algebra transfer more data than lower bounds on communication indicate is necessary, and new, communication optimal algorithms can and should be developed. In this context, the goal of this paper is to design a pivoted QR factorization that is effective in revealing the rank of a matrix but also minimizes communication on both sequential and parallel machines.

There are several different definitions for determining when the factorization from (1.1) reveals the rank (see, for example, [17]); one of them [25, 9] says that the factorization from (1.1) is an RRQR factorization if

$$\sigma_{min}(R_{11}) \geq \frac{\sigma_k(A)}{p(k,n)} \quad \text{and} \quad \sigma_{max}(R_{22}) \leq \sigma_{k+1}(A)p(k,n), \tag{1.2}$$

where $\sigma_k(A)$ is the kth singular value of A, $\sigma_{max}(A) = \sigma_1(A)$ and $\sigma_{min}(A) = \sigma_n(A)$ are the largest and the smallest singular values of A, respectively, and $p(k,n)$ is a low degree polynomial in n and k. Since the $(k+1)$st largest singular value $\sigma_{k+1} \leq \sigma_{\max}(R_{22}) = ||R_{22}||_2$ and $||R_{22}||_2$ is small, A can be considered to have numerical rank k. The first k columns $Q(:,1:k)$ form an approximate orthogonal basis for the range of A, and $\Pi[\begin{smallmatrix} R_{11}^{-1}R_{12} \\ -I \end{smallmatrix}]$ are approximate null vectors.

Given a rank k and a parameter $f > 1$, it is shown in [22] that there exists a permutation Π such that the factorization displayed in (1.1) satisfies the inequality

$$\left(R_{11}^{-1}R_{12}\right)_{i,j}^2 + \omega_i^2\left(R_{11}\right)\gamma_j^2\left(R_{22}\right) \leq f^2, \tag{1.3}$$

where $R_{i,j}$ is the element in position (i,j) of R, $\omega_i(R_{11})$ denotes the 2-norm of the ith row of R_{11}^{-1}, and $\gamma_j(R_{22})$ denotes the 2-norm of the jth column of R_{22}. This factorization is called a *strong RRQR factorization* and is more powerful than the classic QR factorization with column pivoting which only guarantees that $f = O(2^n)$. A strong RRQR factorization is computed by performing first a QR factorization with column pivoting followed by additional swaps of columns. In section 2, we discuss in more detail the characterization of a strong RRQR factorization, as well as more relaxed versions of the bounds from (1.3).

In practice the QR factorization with column pivoting often works well, and it is widely used even if it is known to fail, for example, on the so-called Kahan matrix that we describe in more detail in section 4. However, in terms of communication, the QR factorization with column pivoting is suboptimal with respect to lower bounds on communication identified in [3] (under certain assumptions in the case of the QR factorization). If the algorithm is performed in parallel, then typically the matrix is distributed over P processors by using a two-dimensional block cyclic partitioning. This is indeed the approach used in the `psgeqpf` routine from ScaLAPACK. At each step of the decomposition, the QR factorization with column pivoting finds the column of maximum norm and permutes it to the leading position, and this requires exchanging $O(n)$ messages, where n is the number of columns of the input matrix. For square matrices, when the memory per processor used is on the order of $O(n^2/P)$, the lower bound on the number of messages to be exchanged is $\Omega(\sqrt{P})$. The number of messages exchanged during the QR factorization with column pivoting is larger by at least a factor of $n/\sqrt{P}$ than the lower bound. When QRCP is executed on a sequential machine with a fast memory of size M and a slow memory, then the volume of data transferred between fast and slow memory is on the order of $\Theta(n^3)$, and the number of messages is at least $\Theta(n^3/M)$. The lower bounds on the volume of communication and the number of messages are $\Omega(n^3/M^{1/2})$ and $\Omega(n^3/M^{3/2})$, respectively. We note that the classic QR factorization with no pivoting in which each column is annihilated by using one Householder transformation is also suboptimal in terms of communication. A communication optimal algorithm (modulo polylogarithmic factors), referred to as communication avoiding QR (CAQR), has been introduced in [11, 12].

In this paper we introduce communication avoiding rank revealing QR (CARRQR), a communication optimal (modulo polylogarithmic factors) RRQR factorization based on tournament pivoting. The factorization is based on an algorithm that computes the decomposition by blocks of b columns (panels). For each panel, tournament pivoting proceeds in two steps. The first step aims at identifying a set of b candidate pivot columns that are as well-conditioned as possible. These columns are permuted to the leading positions, and they are used as pivots for the next b steps of the QR factorization. To identify the set of b candidate pivot columns, a tournament is performed based on a reduction operation, where at each node of the reduction tree b candidate columns are selected by using the strong RRQR factorization. The idea of tournament pivoting was first used to reduce communication in Gaussian elimination [20, 21], and then in the context of a newly introduced LU factorization with panel rank revealing pivoting [27]. CARRQR is optimal in terms of communication, modulo polylogarithmic factors, on both sequential machines with two levels of slow and fast memory and parallel machines with one level of parallelism, while performing three times more floating point operations than QRCP. We expect that on computers where communication is the bottleneck, CARRQR will be faster than other algorithms such as QRCP which do not minimize communication. We believe that large speedups can be obtained on future computers (if not the present for sufficiently large matrices) where communication plays an increasingly important role for the performance and parallel scalability of an algorithm.

We show that CARRQR computes a permutation that satisfies

$$\left(R_{11}^{-1}R_{12}\right)_{i,j}^{2} + \left(\gamma_j\left(R_{22}\right)/\sigma_{\min}\left(R_{11}\right)\right)^2 \leq F^2, \tag{1.4}$$

where F is a constant dependent on k, f, and n. Equation (1.4) looks very similar to (1.3) and reveals the matrix numerical rank in a completely analogous way (see Theorems 2.2 and 2.4). While our upper bound on F is superexponential in n (see Theorem 2.10), our extensive experiments, including those on challenging matrices, show that this upper bound is very pessimistic in general (see section 4). These experiments demonstrate that CARRQR is as effective as QR with column pivoting in revealing the rank of a matrix. For the cases where QR with column pivoting does not fail, CARRQR also works well, and the values on the diagonal of the R factor are very close to the singular values of the input matrix computed with the highly accurate routine `dgesvj` [14, 15] (usually within a factor of 10, except when the values are close to the round-off threshold). The matrices in our set were also used in previous papers discussing rank revealing factorizations [4, 22, 29, 26].

The rest of this paper is organized as follows. Section 2 presents the algebra of CARRQR and shows that it is a rank revealing factorization that satisfies (1.4).

Section 3 analyzes the parallel and sequential performance of CARRQR and discusses its communication optimality. Section 4 discusses the numerical accuracy of CARRQR and compares it with QRCP and the singular value decomposition. Section 5 outlines how tournament pivoting can be extended to other factorizations such as Cholesky with diagonal pivoting, LU with complete pivoting, or LDL^T factorization with pivoting. Finally, section 6 concludes our paper.

2. Rank revealing QR factorization with tournament pivoting. This section presents the algebra of the QR factorization algorithm based on a novel pivoting scheme referred to as tournament pivoting and analyzes its numerical stability. We refer to this algorithm as CARRQR.

2.1. The algebra. We consider a block algorithm that partitions the matrix A of size $m \times n$ into panels of size b. In classic QR factorization with column pivoting, at each step i of the factorization, the remaining unselected column of maximum norm is selected and exchanged with the ith column, its subdiagonal elements are annihilated, using for example a Householder transformation, and then the trailing matrix is updated. A block version of this algorithm is described in [28]. The main difficulty in reducing communication in RRQR factorization lies in identifying b pivot columns at each step of the block algorithm. Our communication avoiding algorithm, CARRQR, is based on tournament pivoting and uses a reduction operation on blocks of columns to identify the next b pivot columns at each step of the block algorithm. This idea is analogous to the reduction operation used in CALU [20] to identify the next b pivot rows. The operator used at each node of the reduction tree is an RRQR factorization. Our theoretical analysis presented in section 2.3 is general enough to account for any kind of RRQR factorization, from classical column pivoting to the "strong" RRQR factorization in [22], and gives tighter bound if a strong RRQR factorization is used. The numerical experiments from section 4 will show that using CARRQR is adequate in practice and indeed much better than the bounds derived in this section. This is somewhat similar to using traditional column pivoting for the overall factorization: the average case is much better than the worst case, although the worst case can occur with traditional column pivoting.

To illustrate tournament pivoting, we consider an $m \times n$ matrix A. We use a binary reduction tree and operate on blocks of b_T columns, so there are n/b_T such blocks. In our example $b_T = n/4$, so A is partitioned as $A = [A_{00}, A_{10}, A_{20}, A_{30}]$. Hence our communication avoiding algorithm has two parameters, b which is the number of columns per block in the block factorization, and b_T which is the number of columns per block for the selection of the pivot columns, and hence determines the height of the reduction tree. These two parameters will be discussed in more detail in section 3.

Tournament pivoting starts by computing a (strong) RRQR factorization of each column block A_{i0} to identify b column candidates,

$$A_{i0}\Pi_{i0} = Q_{i0} \begin{bmatrix} R_{i0} & * \\ & * \end{bmatrix} \qquad \text{for } i = 0 \text{ to } 3,$$

where Π_{i0} are permutation matrices of size $b_T \times b_T$, Q_{i0} are orthogonal matrices of size $m \times m$, and R_{i0} are upper-triangular matrices of size $m \times b$. The first subscript i indicates the column block of the matrix, while the second subscript 0 indicates that the operation is performed at the leaves of the binary reduction tree.

At this stage we have n/b_T sets of b column candidates. The final b columns are selected by performing a binary tree (of depth $\log_2(n/b_T) = 2$) of (strong) RRQR factorizations of matrices of size $m \times 2b$. At the first level of the binary tree, we form two matrices by putting together consecutive sets of column candidates.

$$A_{01} = [(A_{00}\Pi_{00})(:, 1:b), (A_{10}\Pi_{10})(:, 1:b)],$$
$$A_{11} = [(A_{20}\Pi_{20})(:, 1:b), (A_{30}\Pi_{30})(:, 1:b)].$$

From each matrix we select a new set of b column candidates by again computing a (strong) RRQR factorization.

$$A_{i1}\Pi_{i1} = Q_{i1}\begin{bmatrix} R_{i1} & * \\ & * \end{bmatrix} \qquad \text{for } i = 0 \text{ to } 1,$$

where Π_{i1} are permutation matrices of size $2b \times 2b$, Q_{i1} are orthogonal matrices of size $m \times m$, and R_{i1} are upper-triangular matrices of size $b \times b$.

At the second (and last) level of the binary tree, the two sets of b column candidates from the first level are combined into a matrix A_{02},

$$A_{02} = [(A_{01}\Pi_{01})(:, 1:b), (A_{11}\Pi_{11})(:, 1:b)].$$

The final b columns are obtained by performing one last (strong) RRQR factorization of A_{02},

$$A_{02}\Pi_{02} = Q_{02}\begin{bmatrix} R_{02} & * \\ & * \end{bmatrix},$$

where Π_{02} is a permutation matrix of size $2b \times 2b$, Q_{02} is an orthogonal matrix of size $m \times m$, and R_{02} is an upper-triangular matrix of size $b \times b$; the final b columns selected are $A_{02}\Pi_{02}(:, 1:b)$.

The matrices Π_{ij}, $i = 0, 1$ and $j = 1, 2$, are partitioned into four blocks of size $b \times b$ as

$$\Pi_{ij} = \begin{bmatrix} \Pi_{ij}^{(1)} & \Pi_{ij}^{(2)} \\ \Pi_{ij}^{(3)} & \Pi_{ij}^{(4)} \end{bmatrix}.$$

Let $\tilde{\Pi}_{ij}$, $i = 0, 1$ and $j = 1, 2$, be permutation matrices obtained by extending Π_{ij} with identity matrices,

$$\tilde{\Pi}_{ij} = \begin{bmatrix} \Pi_{ij}^{(1)} & & \Pi_{ij}^{(2)} & \\ & I_r & & \\ \Pi_{ij}^{(3)} & & \Pi_{ij}^{(4)} & \\ & & & I_r \end{bmatrix},$$

where $r = n/P - b$ for $\tilde{\Pi}_{01}$, $\tilde{\Pi}_{11}$ and $r = n/2 - b$ for $\tilde{\Pi}_{02}$. The tournament pivoting process can be expressed as

$$A\begin{bmatrix} \Pi_{00} & & & \\ & \Pi_{10} & & \\ & & \Pi_{20} & \\ & & & \Pi_{30} \end{bmatrix}\begin{bmatrix} \tilde{\Pi}_{01} & \\ & \tilde{\Pi}_{11} \end{bmatrix}\tilde{\Pi}_{02} = Q_{02}\begin{bmatrix} R_{02} & * \\ & * \end{bmatrix}.$$

In other words, the factorization performed at the root of the binary tree corresponds to the factorization of the first panel of the permuted matrix. The algorithm updates the trailing matrix using Q_{02} and then goes to the next iteration.

Different reduction trees can be used to perform tournament pivoting. The binary tree is presented in the following picture using an arrow notation. At each node of the reduction tree, $f(A_{ij})$ returns the first b columns obtained after performing (strong) RRQR of A_{ij}. The input matrix A_{ij} is obtained by adjoining the input matrices (on the other ends of the arrows pointing towards $f(A_{ij})$):

$$
\begin{tikzcd}
A_{00} \arrow[d] & & A_{10} \arrow[d] & & A_{20} \arrow[d] & & A_{30} \arrow[d] \\
f(A_{00}) \arrow[dr] & & f(A_{10}) \arrow[dl] & & f(A_{20}) \arrow[dr] & & f(A_{30}) \arrow[dl] \\
& f(A_{01}) \arrow[drr] & & & & f(A_{11}) \arrow[dll] & \\
& & & f(A_{02}) & & &
\end{tikzcd}
$$

A flat tree is presented using this arrow notation in the following picture:

$$
\begin{tikzcd}
A_{00} \arrow[d] & A_{10} \arrow[ddl] & A_{20} \arrow[dddll] & A_{30} \arrow[ddddlll] \\
f(A_{00}) \arrow[d] & & & \\
f(A_{01}) \arrow[d] & & & \\
f(A_{02}) \arrow[d] & & & \\
f(A_{03}) & & &
\end{tikzcd}
$$

2.2. Selecting the first b columns from (strong) rank revealing QR factorization. The (possibly strong) RRQR factorization of a matrix A_{ij} is used in tournament pivoting at each node of the reduction tree to select b candidate columns. Suppose that A_{ij} is of dimension $m_1 \times n_1$. When the matrix fits in fast memory on a sequential processor, the b column candidates may be selected by computing the first b steps of QR with column pivoting. When a strong rank revealing factorization is employed, several supplementary operations and swaps are performed, as explained in [22].

When the matrix does not fit in fast memory, or it is distributed over several processors, the b candidate columns are selected by first computing the QR factorization of A_{ij} without pivoting, and then the (strong) QR factorization of the much smaller $(2b \times 2b)$ R factor. The first QR factorization is performed using communication avoiding QR [12] for tall and skinny matrices, referred to as TSQR, which minimizes communication.

2.3. Why QR with tournament pivoting reveals the rank. In this section, we first recall the characterization of a (strong) RRQR factorization from [22], modify it slightly, and then show (with an appropriate choice of bounds) that it describes the result of tournament pivoting. The characterization depends on the particular rank k chosen. Subsection 2.3.1 analyzes the case $k = b$, i.e., the result of a single tournament. Then subsection 2.3.2 extends the analysis to any $1 \leq k \leq \min(m, n)$, i.e., the final output of the algorithm.

To set up the notation needed to explain [22], let $\omega_i(X)$ denote the 2-norm of the

ith row of X^{-1}, and let $\gamma_j(X)$ denote the 2-norm of the jth column of X.

THEOREM 2.1 (Gu and Eisenstat [22]). *Let B be an $m \times n$ matrix and let $1 \le k \le \min(m,n)$. For any given parameter $f > 1$, there exists a permutation Π such that*

$$B\Pi = Q \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix},$$

where R_{11} is $k \times k$ and

$$\left(R_{11}^{-1} R_{12}\right)_{i,j}^2 + \omega_i^2\left(R_{11}\right)\gamma_j^2\left(R_{22}\right) \le f^2. \tag{2.1}$$

The factorization in Theorem 2.1 can be computed in $O(mnk)$ flops. Inequality (2.1) is important because it implies bounds on the singular values of R_{11} and R_{22}.

THEOREM 2.2 (Gu and Eisenstat [22]). *Let the factorization in Theorem 2.1 satisfy inequality (2.1). Then*

$$1 \le \frac{\sigma_i(B)}{\sigma_i(R_{11})}, \frac{\sigma_j(R_{22})}{\sigma_{k+j}(B)} \le \sqrt{1 + f^2 k(n-k)}$$

for any $1 \le i \le k$ and $1 \le j \le \min(m,n) - k$.

In particular, Theorem 2.2 shows that the QR factorization in Theorem 2.1 *reveals the rank* in the sense that the singular values of R_{11} are reasonable approximations of the k largest singular values of B, and the singular values of R_{22} are reasonable approximations of the $\min(m,n) - k$ smallest singular values of B. We call this a *strong* rank revealing factorization because the bound in Theorem 2.2 grows like a low degree polynomial in n. In contrast, traditional column pivoting only guarantees that $f = O(2^n)$. Still, traditional column pivoting often works well in practice, and we will use it as a tool in our numerical experiments later.

To analyze our communication avoiding RRQR algorithm in a more convenient way, we consider the following relaxed version of Theorem 2.1.

COROLLARY 2.3. *Let B be an $m \times n$ matrix and let $1 \le k \le \min(m,n)$. For any given parameter $f > 1$, there exists a permutation Π such that*

$$B\Pi = Q \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix},$$

where R_{11} is $k \times k$ and

$$\sqrt{\gamma_j^2\left(R_{11}^{-1} R_{12}\right) + \left(\gamma_j\left(R_{22}\right)/\sigma_{\min}(R_{11})\right)^2} \le f\sqrt{k} \quad \textit{for} \quad j = 1, \dots, n-k. \tag{2.2}$$

The proof is immediate, as the permutation Π of Theorem 2.1 automatically satisfies inequality (2.2). Below is the analogue of Theorem 2.2 based on Corollary 2.3.

THEOREM 2.4. *Assume that there exists a permutation Π for which the QR factorization*

$$B\Pi = Q \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix},$$

where R_{11} is $k \times k$, satisfies

$$\sqrt{\gamma_j^2\left(R_{11}^{-1} R_{12}\right) + \left(\gamma_j\left(R_{22}\right)/\sigma_{\min}(R_{11})\right)^2} \le F \quad \textit{for} \quad j = 1, \dots, n-k. \tag{2.3}$$

Then

$$1 \leq \frac{\sigma_i(B)}{\sigma_i(R_{11})}, \frac{\sigma_j(R_{22})}{\sigma_{k+j}(B)} \leq \sqrt{1 + F^2(n-k)}$$

for any $1 \leq i \leq k$ *and* $1 \leq j \leq \min(m, n) - k$.

Remark. By Corollary 2.3, there exists a permutation Π for which inequality (2.3) is satisfied with $F = f\sqrt{k}$. For this permutation and with this choice of F, Theorem 2.4 gives the same singular value ratio bounds as those in Theorem 2.2. However, Theorem 2.4 will prove much more convenient for our subsequent analysis and could provide a better practical bound on the singular values, as we can typically expect F to be much smaller than $f\sqrt{k}$.

Proof of Theorem 2.4. Define

$$\alpha = \frac{\sigma_{\max}(R_{22})}{\sigma_{\min}(R_{11})}.$$

Then we can rewrite

$$B\Pi = Q \begin{bmatrix} R_{11} & \\ & R_{22}/\alpha \end{bmatrix} \begin{bmatrix} I & R_{11}^{-1}R_{12} \\ & \alpha I \end{bmatrix}.$$

It follows that

$$\sigma_i(B) \leq \sigma_i\left(\begin{bmatrix} R_{11} & \\ & R_{22}/\alpha \end{bmatrix}\right) \left\| \begin{bmatrix} I & R_{11}^{-1}R_{12} \\ & \alpha I \end{bmatrix} \right\|_2, \quad i = 1, \ldots, k.$$

On the other hand, the largest k singular values of $\left[\begin{smallmatrix} R_{11} & \\ & R_{22}/\alpha \end{smallmatrix}\right]$ are precisely those of the matrix R_{11}, and the 2-norm of the matrix $\left[\begin{smallmatrix} I & R_{11}^{-1}R_{12} \\ & \alpha I \end{smallmatrix}\right]$ is bounded above by

$$\sqrt{1 + \|R_{11}^{-1}R_{12}\|_2^2 + \alpha^2} \leq \sqrt{1 + F^2(n-k)}.$$

In other words,

$$\frac{\sigma_i(B)}{\sigma_i(R_{11})} \leq \sqrt{1 + F^2(n-k)}$$

for $i = 1, \ldots, k$. Conversely, observe that

$$\begin{bmatrix} \alpha R_{11} & \\ & R_{22} \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix} \begin{bmatrix} \alpha I & -R_{11}^{-1}R_{12} \\ & I \end{bmatrix},$$

where the smallest $\min(m, n) - k$ singular values of $\left[\begin{smallmatrix} \alpha R_{11} & \\ & R_{22} \end{smallmatrix}\right]$ are the singular values of R_{22}, and the 2-norm of the matrix $\left[\begin{smallmatrix} \alpha I & -R_{11}^{-1}R_{12} \\ & I \end{smallmatrix}\right]$ can be similarly bounded as

$$\sqrt{1 + \|R_{11}^{-1}R_{12}\|_2^2 + \alpha^2} \leq \sqrt{1 + F^2(n-k)}.$$

This again leads to

$$\frac{\sigma_j(R_{22})}{\sigma_{k+j}(B)} \leq \sqrt{1 + F^2(n-k)}, \quad j = 1, \ldots, \min(m, n) - k.$$

This completes the proof. $\square$

2.3.1. Analyzing one tournament step. Next we apply Theorem 2.4 to analyze one tournament step. Given a subset of b columns of matrix B that reveals its rank (for $k = b$), and another subset of b columns that reveals the rank of a different matrix $\widehat{B}$, we will show that computing a rank revealing decomposition of just these $2b$ columns of B and $\widehat{B}$ will provide b columns that reveal the rank of the combined matrix $[B, \widehat{B}]$ (see Lemma 2.5). Then we will use this as an induction step to analyze an entire tournament, once using a binary tree (Corollary 2.6) and once with a flat tree (Corollary 2.7).

We use the following notation to denote the rank revealing factorizations of B and $\widehat{B}$:

$$B\Pi = Q \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix} \quad \text{and} \quad \widehat{B}\widehat{\Pi} = \widehat{Q} \begin{bmatrix} \widehat{R}_{11} & \widehat{R}_{12} \\ & \widehat{R}_{22} \end{bmatrix}, \tag{2.4}$$

where Π and $\widehat{\Pi}$ are permutation matrices; R_{11} and $\widehat{R}_{11}$ are $b \times b$ upper-triangular matrices. We assume that the factorizations in (2.4) satisfy

$$\gamma_j(N)^2 + \gamma_j(R_{22})^2/\sigma_{\min}(R_{11})^2 \le F^2, \quad \gamma_j(\widehat{N})^2 + \gamma_j(\widehat{R}_{22})^2/\sigma_{\min}\left(\widehat{R}_{11}\right)^2 \le \widehat{F}^2, \tag{2.5}$$

where $N = R_{11}^{-1}R_{12}$ and $\widehat{N} = \widehat{R}_{11}^{-1}\widehat{R}_{12}$. For example, by Theorem 2.1, we can choose $F = \widehat{F} = f\sqrt{b}$ when B and $\widehat{B}$ each consists of $2b$ columns; later on we will use this fact as the basis of our induction. Next we develop similar bounds for the combined matrix $\widetilde{B} = [B \ \ \widehat{B}]$.

Tournament pivoting continues by computing a (strong) RRQR factorization of the form

$$\bar{B}\bar{\Pi} \stackrel{def}{=} \left[Q \begin{bmatrix} R_{11} \\ \end{bmatrix}, \quad \widehat{Q} \begin{bmatrix} \widehat{R}_{11} \\ \end{bmatrix} \right] \bar{\Pi} = \widetilde{Q} \begin{bmatrix} \widetilde{R}_{11} & \bar{R}_{12} \\ & \bar{R}_{22} \end{bmatrix}, \tag{2.6}$$

where

$$\left(\widetilde{R}_{11}^{-1}\bar{R}_{12}\right)_{i,j}^2 + \omega_i^2\left(\widetilde{R}_{11}\right)\gamma_j^2\left(\bar{R}_{22}\right) \le f^2. \tag{2.7}$$

Let

$$\widetilde{\Pi} = \begin{bmatrix} \Pi & \\ & \widehat{\Pi} \end{bmatrix} \begin{bmatrix} I & & & \\ & & I & \\ & I & & \\ & & & I \end{bmatrix} \begin{bmatrix} \bar{\Pi} & \\ & I \end{bmatrix}$$

be the accumulation of all permutations; then we can write $\widetilde{B}$ as

$$\begin{aligned} \widetilde{B}\widetilde{\Pi} &= \left[\widetilde{Q} \begin{bmatrix} \widetilde{R}_{11} & \bar{R}_{12} \\ & \bar{R}_{22} \end{bmatrix}, \ Q \begin{bmatrix} R_{12} \\ R_{22} \end{bmatrix}, \ \widehat{Q} \begin{bmatrix} \widehat{R}_{12} \\ \widehat{R}_{22} \end{bmatrix} \right] \\ &= \widetilde{Q} \left[\begin{bmatrix} \widetilde{R}_{11} & \bar{R}_{12} \\ & \bar{R}_{22} \end{bmatrix}, \ \widetilde{Q}^T Q \begin{bmatrix} R_{12} \\ R_{22} \end{bmatrix}, \ \widetilde{Q}^T \widehat{Q} \begin{bmatrix} \widehat{R}_{12} \\ \widehat{R}_{22} \end{bmatrix} \right] \\ &\stackrel{def}{=} \widetilde{Q} \begin{bmatrix} \widetilde{R}_{11} & \widetilde{R}_{12} \\ & \widetilde{R}_{22} \end{bmatrix}. \end{aligned} \tag{2.8}$$

Our goal is to derive bounds analogous to (2.5) for (2.8). To this end, we need to first identify the matrices $\widetilde{R}_{12}$ and $\widetilde{R}_{22}$. Note that

$$\widetilde{Q}^T Q \begin{bmatrix} R_{12} \\ R_{22} \end{bmatrix} = \widetilde{Q}^T Q \begin{bmatrix} R_{11} N \\ R_{22} \end{bmatrix} = \widetilde{Q}^T Q \begin{bmatrix} R_{11} \\ \end{bmatrix} N + \widetilde{Q}^T Q \begin{bmatrix} \\ R_{22} \end{bmatrix}.$$

Continuing, we may write

$$Q \begin{bmatrix} R_{11} \\ \end{bmatrix} = \widetilde{Q} \begin{bmatrix} \widetilde{R}_{11} \mathcal{N} \\ \mathcal{C} \end{bmatrix}, \tag{2.9}$$

where the $b \times b$ matrices $\mathcal{N}$ and $\mathcal{C}$ are defined as follows: for each $1 \leq t \leq b$, the tth column of the matrix on the left-hand side of (2.9) must be some sth column of $\widetilde{Q}\left[\begin{smallmatrix} \widetilde{R}_{11} & \bar{R}_{12} \\ & \bar{R}_{22} \end{smallmatrix}\right]$. If $s \leq b$, then we set the tth column of $\mathcal{C}$ to be 0, and the tth column of $\mathcal{N}$ to be all 0, except for the sth entry, which will be 1. On the other hand, if $s > b$, then we set the tth columns of $\mathcal{C}$ and $\mathcal{N}$ to be the $(s-b)$th columns of $\bar{R}_{22}$ and $\widetilde{R}_{11}^{-1} \bar{R}_{12}$, respectively. Since $f > 1$, we must have by inequality (2.7) that

$$\mathcal{N}_{i,j}^2 + \omega_i \left(\widetilde{R}_{11} \right)^2 \gamma_j^2 \left(\mathcal{C} \right) \leq f^2 \tag{2.10}$$

for all $1 \leq i, j \leq b$. With the additional notation

$$\widetilde{Q}^T Q \begin{bmatrix} \\ R_{22} \end{bmatrix} \stackrel{def}{=} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} \tag{2.11}$$

we can further rewrite

$$\widetilde{Q}^T Q \begin{bmatrix} R_{12} \\ R_{22} \end{bmatrix} = \begin{bmatrix} \widetilde{R}_{11} \mathcal{N} \\ \mathcal{C} \end{bmatrix} N + \widetilde{Q}^T Q \begin{bmatrix} \\ R_{22} \end{bmatrix} = \begin{bmatrix} \widetilde{R}_{11} \left(\mathcal{N} N + \widetilde{R}_{11}^{-1} C_1 \right) \\ \mathcal{C} N + C_2 \end{bmatrix}. \tag{2.12}$$

Similarly, define matrices $\widehat{\mathcal{N}}, \widehat{\mathcal{C}}, \widehat{C}_1$, and $\widehat{C}_2$ so that

$$\widetilde{Q}^T \widehat{Q} \begin{bmatrix} \widehat{R}_{12} \\ \widehat{R}_{22} \end{bmatrix} = \begin{bmatrix} \widetilde{R}_{11} \left(\widehat{\mathcal{N}} \widehat{N} + \widetilde{R}_{11}^{-1} \widehat{C}_1 \right) \\ \widehat{\mathcal{C}} \widehat{N} + \widehat{C}_2 \end{bmatrix}.$$

All this algebra has finally allowed us to identify

$$\begin{aligned} \widetilde{R}_{12} &= \begin{bmatrix} \bar{R}_{12} & \widetilde{R}_{11} \left(\mathcal{N} N + \widetilde{R}_{11}^{-1} C_1 \right) & \widetilde{R}_{11} \left(\widehat{\mathcal{N}} \widehat{N} + \widetilde{R}_{11}^{-1} \widehat{C}_1 \right) \end{bmatrix}, \\ \widetilde{R}_{22} &= \begin{bmatrix} \bar{R}_{22} & \mathcal{C} N + C_2 & \widehat{\mathcal{C}} \widehat{N} + \widehat{C}_2 \end{bmatrix}. \end{aligned}$$

Below, we derive bounds analogous to (2.5) for (2.8). We do this according to the 1×3 partition in $\widetilde{R}_{12}$ and $\widetilde{R}_{22}$. By inequality (2.7), we have

$$\gamma_j^2 \left(\widetilde{R}_{11}^{-1} \widetilde{R}_{12} \right) + \gamma_j^2 \left(\bar{R}_{22} \right)^2 / \sigma_{\min}^2 \left(\widetilde{R}_{11} \right) \leq b f^2.$$

In addition, we have

$$
\begin{aligned}
(2.13)\qquad & \gamma_j^2\left(\mathcal{N}N+\widetilde{R}_{11}^{-1}C_1\right)+\gamma_j^2\left(\mathcal{C}N+C_2\right)/\sigma_{\min}^2\left(\widetilde{R}_{11}\right)\\
&=\gamma_j^2\left(\begin{bmatrix}\mathcal{N}N\\ \mathcal{C}N/\sigma_{\min}\left(\widetilde{R}_{11}\right)\end{bmatrix}+\begin{bmatrix}\widetilde{R}_{11}^{-1}C_1\\ C_2/\sigma_{\min}\left(\widetilde{R}_{11}\right)\end{bmatrix}\right)\\
&\le 2\left(\gamma_j^2\left(\begin{bmatrix}\mathcal{N}N\\ \mathcal{C}N/\sigma_{\min}\left(\widetilde{R}_{11}\right)\end{bmatrix}\right)+\gamma_j^2\left(\begin{bmatrix}\widetilde{R}_{11}^{-1}C_1\\ C_2/\sigma_{\min}\left(\widetilde{R}_{11}\right)\end{bmatrix}\right)\right)\\
(2.14)\qquad &\le 2\left(\left\|\begin{bmatrix}\mathcal{N}\\ \mathcal{C}/\sigma_{\min}\left(\widetilde{R}_{11}\right)\end{bmatrix}\right\|_F^2\gamma_j^2(N)+\gamma_j^2\begin{bmatrix}C_1\\ C_2\end{bmatrix}/\sigma_{\min}\left(\widetilde{R}_{11}\right)^2\right).
\end{aligned}
$$

It follows from inequality (2.10) that

$$
\left\|\begin{bmatrix}\mathcal{N}\\ \mathcal{C}/\sigma_{\min}\left(\widetilde{R}_{11}\right)\end{bmatrix}\right\|_F^2\le f^2b^2,
$$

and it follows from definition (2.11) that

$$
\gamma_j^2\left(\begin{bmatrix}C_1\\ C_2\end{bmatrix}\right)=\gamma_j^2\left(R_{22}\right).
$$

Furthermore, (2.9) can be rewritten as

$$
R_{11}^TR_{11}=\mathcal{N}^T\widetilde{R}_{11}^T\widetilde{R}_{11}\mathcal{N}+\mathcal{C}^T\mathcal{C},
$$

which implies that

$$
\begin{aligned}
\sigma_{\min}^2\left(R_{11}\right)&\le\sigma_{\min}^2\left(\widetilde{R}_{11}\right)\|\mathcal{N}\|_2^2+\|\mathcal{C}\|_2^2\\
&\le\sigma_{\min}^2\left(\widetilde{R}_{11}\right)\left(\left\|\begin{bmatrix}\mathcal{N}\\ \mathcal{C}/\sigma_{\min}\left(\widetilde{R}_{11}\right)\end{bmatrix}\right\|_F^2\right)\le f^2b^2\sigma_{\min}^2\left(\widetilde{R}_{11}\right),
\end{aligned}
$$

which in turn leads to

$$
1/\sigma_{\min}^2\left(\widetilde{R}_{11}\right)\le f^2b^2/\sigma_{\min}^2\left(R_{11}\right).
$$

Plugging all these results into (2.14), we obtain an upper bound on (2.13):

$$
\begin{aligned}
\gamma_j^2(\mathcal{N}N+\widetilde{R}_{11}^{-1}C_1)+\gamma_j^2\left(\mathcal{C}N+C_2\right)/\sigma_{\min}^2(\widetilde{R}_{11})&\le 2f^2b^2(\gamma_j^2(N)+\gamma_j^2(R_{22})/\sigma_{\min}^2(R_{11}))\\
&\le 2f^2b^2F^2.
\end{aligned}
$$

Similarly, we can derive an upper bound

$$
\gamma_j^2\left(\widehat{\mathcal{N}}\widehat{N}+\widetilde{R}_{11}^{-1}\widehat{C}_1\right)+\gamma_j^2\left(\widehat{\mathcal{C}}\widehat{N}+\widehat{C}_2\right)/\sigma_{\min}^2\left(\widetilde{R}_{11}\right)\le 2f^2b^2\widehat{F}^2.
$$

All these results are now summarized in the following lemma.

LEMMA 2.5. *Suppose we are given two RRQR factorizations of B and $\widehat{B}$, as in* (2.4)*, that reveal their ranks as described in* (2.5)*. Suppose we perform another*

RRQR factorization of the b selected columns of B and b selected columns of $\widehat{B}$, as described in (2.6) *and* (2.7)*. Then the b columns selected by this last QR factorization let us perform a QR factorization of $\widetilde{B} = [B, \widehat{B}]$, as described in* (2.8)*, that reveals the rank of $\widetilde{B}$ with the bound*

$$\sqrt{\gamma_j^2\left(\widetilde{R}_{11}^{-1}\widetilde{R}_{12}\right) + \gamma_j^2\left(\widetilde{R}_{22}\right)/\sigma_{\min}^2\left(\widetilde{R}_{11}\right)} \leq \sqrt{2} f b \max\left(F, \widehat{F}\right). \tag{2.15}$$

We may use Lemma 2.5 as the induction step to analyze the result of any tournament, with any reduction tree. We consider two cases, a binary reduction tree and a flat reduction tree, which are both applied to an $m \times n$ matrix with $m \geq n$.

In the case of a complete binary tree, we can let B and $\widehat{B}$ contain 2^h blocks of b columns each, where $1 \leq h \leq \log_2(n/b) - 1$. Assume that both B and $\widehat{B}$ satisfy relations (2.5) with $F = \widehat{F} \equiv F_h^B$ (the superscript B stands for "binary tree"). By Corollary 2.3, for the base case we can set $F_1^B = f\sqrt{b}$. Lemma 2.5 yields the following recursive relation:

$$(F_{h+1}^B) \leq \sqrt{2} f b F_h^B.$$

Solving this recursion yields

$$F_{h+1}^B \leq \frac{1}{\sqrt{2b}}\left(\sqrt{2} f b\right)^{h+1}. \tag{2.16}$$

For $h = \log_2(n/b) - 1$, i.e., after the entire tournament has completed, we get the following corollary.

Corollary 2.6. *Selecting b columns of the $m \times n$ matrix A using QR with tournament pivoting, with a binary tree, reveals the rank of A in the sense of Theorem* 2.4 *for $k = b$, with bound*

$$F_{\log_2(n/b)}^B \leq \frac{1}{\sqrt{2b}}\left(\sqrt{2} f b\right)^{\log_2(n/b)} = \frac{1}{\sqrt{2b}}\,(n/b)^{\log_2\left(\sqrt{2} f b\right)}. \tag{2.17}$$

The bound in (2.17) can be regarded as a low degree polynomial in n in general for a fixed b and f. Note that the upper bound is a decreasing function of b when $b > \sqrt{n/(\sqrt{2}f)}$.

In the case of a flat tree, we may let B and $\widehat{B}$ contain h blocks and 1 block of b columns, respectively, where $1 \leq h \leq n/b - 1$. Assume that both B and $\widehat{B}$ satisfy relations (2.5) with $F = F_h^F$ and $\widehat{F} = F_1^F = 0$, respectively (the superscript F stands for "flat tree"). Lemma 2.5 now yields the following recursive relation:

$$(F_{h+1}^F) \leq \sqrt{2} f b F_h^F.$$

Solving this recursion yields

$$F_{h+1}^F \leq \frac{1}{\sqrt{2b}}\left(\sqrt{2} f b\right)^{h+1}. \tag{2.18}$$

For $h = n/b - 1$, i.e., after the entire tournament has completed, we get the following corollary.

Corollary 2.7. *Selecting b columns of the $m \times n$ matrix A using QR with tournament pivoting, with a flat tree, reveals the rank of A in the sense of Theorem 2.4 for $k = b$, with bound*

$$F_n^F \leq \frac{1}{\sqrt{2b}} \left(\sqrt{2} f b\right)^{n/b}. \tag{2.19}$$

Bound (2.19) is exponential in n, pointing to the possibility that the QR factorization we compute might not quite reveal the rank in extreme cases. But note that the upper bound is a rapidly decreasing function of b.

Example. $b = 1$ *(traditional column pivoting).* We now evaluate bounds (2.17) and (2.19) when $b = 1$. It is easy to see that the optimal single column to choose to reveal the rank is the one with the largest norm, and that this choice satisfies both Theorem 2.1 with $f = 1$ when $k = 1$, and Theorem 2.4 with $F = 1$, both of which are unimprovable. Furthermore, no matter what kind of reduction tree we use for the tournament, the column with the largest norm will be chosen by the tournament (ties may be broken in different ways), since we always pick the column of largest norm at each step. So when $b = 1$, tournament pivoting is equivalent to classical column pivoting, whose analysis is well known. Comparing our bounds from (2.17) and (2.19) to the optimal value of $F = 1$, we get $F^B_{\log_2 n} \leq \sqrt{n/2}$ and $F^F_n \leq 2^{(n-1)/2}$. So the analysis of the binary tree is reasonably close to the best bound, although the flat tree analysis gives a weaker bound.

2.3.2. Extending the analysis to a full rank revealing QR factorization. In this section we perform a global analysis to extend the one-step analysis of subsection 2.3.1 to a full RRQR factorization.

Corollaries 2.6 and 2.7 in the last section showed that applying tournament pivoting once, to pick the leading b columns of a matrix, provide a column permutation that reveals the rank in the sense of Theorem 2.4, but just for one partition of $R = \left[\begin{smallmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{smallmatrix}\right]$, namely when R_{11} is $b \times b$. The goal of this section is to show that using repeated tournaments to select subsequent groups of b columns can make R rank revealing for R_{11} of *any* dimension $1 \leq k \leq n$.

Since the algorithm described in the last section only chooses groups of b columns at a time, it guarantees nothing about the order of columns within a group. For example the algorithm might do nothing when given b or fewer columns. So to prove a rank revealing property for any k, not just $k = tb$, we must apply a second (lower cost) step where we apply strong RRQR to each $b \times b$ diagonal block of R.

Given this second step, we will derive an upper bound in the form of (2.3). Our approach is to reveal the "least" rank revealed matrix given the one-step results in subsection 2.3.1.

To this end, we first introduce some new notation. Let e be the vector of all 1's of various dimensions. For every matrix X, let $|X|$ be the matrix with each entry the corresponding entry of X in absolute value. Let N and H be two matrices of compatible size; by the relationship

$$N \preceq H,$$

we mean that $H - N$ is a nonnegative matrix. Our global analysis will benefit from the following lemma, the proof of which we omit.

Lemma 2.8 (Theorem 8.12 from [24]). *Let N and H be upper-triangular matrices with unit diagonal, and with nonpositive entries in the upper-triangular part of H.*

Assume that

$$|N| \preceq |H|.$$

Then we have

$$|N^{-1}| \preceq |H^{-1}|.$$

Now let

$$N = \begin{bmatrix} I & N_{12} & \cdots & N_{1t} \\ & I & \cdots & N_{2t} \\ & & \ddots & \vdots \\ & & & I \end{bmatrix}, \tag{2.20}$$

where each N_{ij} is a $b \times b$ matrix with $1 \leq i < j \leq t$, and $\gamma_k(N_{ij}) \leq c_i$ for $1 \leq k \leq b$. Our global analysis will critically depend on tight estimates of $\|N^{-1}\|_2$. As a surrogate, we will instead discuss the choices of all the N_{ij} submatrices to maximize $\|N^{-1}\|_1$. To start, define

$$H = \begin{bmatrix} I & -|N_{12}| & \cdots & -|N_{1t}| \\ & I & \cdots & -|N_{2t}| \\ & & \ddots & \vdots \\ & & & I \end{bmatrix}.$$

In other words, we construct H by flipping the signs of all positive off-diagonal entries of N. It follows that $|N| = |H|$, and from Lemma 2.8 that $|N^{-1}| \preceq |H^{-1}|$, which implies that $\|N^{-1}\|_1 \leq \|H^{-1}\|_1$. Define

$$M = \begin{bmatrix} I & M_{12} & \cdots & M_{1t} \\ & I & \cdots & M_{2t} \\ & & \ddots & \vdots \\ & & & I \end{bmatrix}, \tag{2.21}$$

where $M_{ij} = -\frac{c_i}{\sqrt{b}} ee^T$. It is easy to verify that $\gamma_k(M_{ij}) = c_i$ for all $1 \leq k \leq b$, and hence M satisfies the conditions on the matrix N in (2.20). Straightforward algebra shows that $\|M^{-1}\|_1 = \prod_{j=1}^{t-1}(1 + \sqrt{b}c_j)$. Lemma 2.9 below identifies M as the matrix that maximizes $\|N^{-1}\|_1$.

LEMMA 2.9. *Let matrices N and M be defined by* (2.20) *and* (2.21), *respectively. Then*

$$\|N^{-1}\|_1 \leq \|M^{-1}\|_1.$$

Proof. We only consider the matrix N for which the upper-triangular entries are all nonpositive, so that $|N^{-1}| = N^{-1}$. We prove Lemma 2.9 by induction on t. The lemma is obviously true for $t = 1$. For $t > 1$, we will show that the sum of entries in every column of N^{-1} is bounded above by $\|M^{-1}\|_1$. Let $\widehat{N}$ and $\widehat{M}$ be the first $(t-1) \times (t-1)$ block submatrices of N and M, respectively. By induction, for any $1 \leq k \leq (t-1)b$, the sum of entries in the kth column of N^{-1} is bounded above by $\|\widehat{M}^{-1}\|_1 \leq \|M^{-1}\|_1$. For any $(t-1)b + 1 \leq k \leq tb$, define

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_{t-1} \end{bmatrix} \quad \text{and} \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_{t-1} \end{bmatrix} = -\widehat{N}^{-1} y,$$

where y_i is the $(k-(t-1)b)$th column of N_{it}, with $\|y_i\|_2 \le c_i$. By definition, y and x are the kth columns of N and N^{-1} without the bottom b components, and hence the sum of entries in the kth column of N^{-1} is simply

$$1 + e^T x = 1 + \sum_{j=1}^{t-1} e^T x_j.$$

Since $x_1 = -y_1 + \sum_{j=2}^{t-1} (-N_{1,j})\, x_j$, it follows from the Cauchy–Schwarz inequality that

$$e^T x_1 = -e^T y_1 + \sum_{j=2}^{t-1} e^T (-N_{1,j})\, x_j \le \sqrt{b} c_1 + \sum_{j=2}^{t-1} \sqrt{b} c_1 e^T x_j = \sqrt{b} c_1 \left(1 + \sum_{j=2}^{t-1} e^T x_j \right),$$

and that

$$1 + e^T x \le 1 + \sqrt{b} c_1 + \left(1 + \sqrt{b} c_1\right) \sum_{j=2}^{t-1} e^T x_j = \left(1 + \sqrt{b} c_1\right) \left(1 + \sum_{j=2}^{t-1} e^T x_j \right).$$

To continue with the same argument to the end, we have

$$1 + e^T x \le \prod_{j=1}^{t-1} \left(1 + \sqrt{b} c_j\right) = \|M^{-1}\|_1. \qquad \square$$

We are now ready to derive global upper bounds. Suppose that at least t rounds of tournament pivoting have been computed,

$$B\Pi = Q \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1t} & R_{1,t+1} \\ & R_{22} & \cdots & R_{2t} & R_{2,t+1} \\ & & \ddots & \vdots & \vdots \\ & & & R_{tt} & R_{t,t+1} \\ & & & & R_{t+1,t+1} \end{bmatrix},$$

where R_{ii} is $b \times b$ for $1 \le i \le t$, and $R_{t+1,t+1}$ is $(n-tb) \times (n-tb)$; i.e., the first t tournaments selected the tb columns yielding R_{11} through R_{tt}. In light of (2.3), we need to develop an upper bound on

$$\begin{aligned} \tau^2 \stackrel{def}{=} {} & \gamma_j^2 \left(\begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1t} \\ & R_{22} & \cdots & R_{2t} \\ & & \ddots & \vdots \\ & & & R_{tt} \end{bmatrix}^{-1} \begin{bmatrix} R_{1,t+1} \\ R_{2,t+1} \\ \vdots \\ R_{t,t+1} \end{bmatrix} \right) \\ & + \gamma_j^2 \left(R_{t+1,t+1}\right) / \sigma_{\min}^2 \left(\begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1t} \\ & R_{22} & \cdots & R_{2t} \\ & & \ddots & \vdots \\ & & & R_{tt} \end{bmatrix} \right). \end{aligned}$$

Let N be the matrix defined in (2.20) with $N_{ij} = R_{ii}^{-1} R_{ij}$. Then N satisfies $\gamma_k(N_{ij}) \le c_i$, where the exact value of c_i depends on the reduction tree:

$$c_i = \begin{cases} F^B_{\log_2((n-(i-1)b)/b)} & \text{for binary tree (see Corollary 2.6),} \\ \\ F^F_{n-(i-1)b} & \text{for flat tree (see Corollary 2.7).} \end{cases}$$

Let

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_t \end{bmatrix}$$

be the jth column of the matrix

$$\begin{bmatrix} R_{11}^{-1} R_{1,t+1} \\ \vdots \\ R_{tt}^{-1} R_{t,t+1} \end{bmatrix}.$$

We rewrite τ^2 as

$$\tau^2 = \|N^{-1} y\|_2^2 + \gamma_j^2 \left(R_{t+1,t+1} \right) / \sigma_{\min}^2 \left(\operatorname{diag} \left(R_{11}, \ldots, R_{tt} \right) N \right).$$

By Corollaries 2.6 and 2.7, $\|y_i\|_2$ is bounded above by the same c_i as defined above. Repeating the same arguments made in the proof for Lemma 2.9, it is easy to show that

$$\|N^{-1} y\|_2 \le \|N^{-1} y\|_1 \le \left\| M^{-1} \begin{bmatrix} -\frac{c_1}{\sqrt{b}} e \\ \vdots \\ -\frac{c_t}{\sqrt{b}} e \end{bmatrix} \right\|_1 = \prod_{j=1}^{t} \left(1 + \sqrt{b} c_j \right) - 1 < \prod_{j=1}^{t} \left(1 + \sqrt{b} c_j \right).$$

For the second term in τ^2, we note by Corollaries 2.6 and 2.7 that

$$\gamma_j \left(R_{t+1,t+1} \right) / \sigma_{\min} \left(R_{ii} \right) \le c_i \le c_1$$

for all $1 \le i \le t$. This implies that

$$\gamma_j \left(R_{t+1,t+1} \right) / \sigma_{\min} \left(\operatorname{diag} \left(R_{11}, \ldots, R_{tt} \right) \right) \le c_1.$$

Hence

$$\begin{aligned} &\gamma_j \left(R_{t+1,t+1} \right) / \sigma_{\min} \left(\operatorname{diag} \left(R_{11}, \ldots, R_{tt} \right) N \right) \\ &\le \gamma_j \left(R_{t+1,t+1} \right) / \sigma_{\min} \left(\operatorname{diag} \left(R_{11}, \ldots, R_{tt} \right) \right) \|N^{-1}\|_2 \\ &\le c_1 \sqrt{n} \|N^{-1}\|_1 \le c_1 \sqrt{n} \|M^{-1}\|_1 = \sqrt{n} c_1 \prod_{j=1}^{t-1} \left(1 + \sqrt{b} c_j \right). \end{aligned}$$

Putting it all together, we get

$$\begin{aligned} \tau^2 &\le \left(\prod_{j=1}^{t} \left(1 + \sqrt{b} c_j \right) \right)^2 + \left(\sqrt{n} c_1 \prod_{j=1}^{t-1} \left(1 + \sqrt{b} c_j \right) \right)^2 \\ &= \left(\left(1 + \sqrt{b} c_t \right)^2 + n c_1^2 \right) \left(\prod_{j=1}^{t-1} \left(1 + \sqrt{b} c_j \right) \right)^2 \\ &\le \left(1 + \sqrt{b + n} c_1 \right)^2 \left(\prod_{j=1}^{t-1} \left(1 + \sqrt{b} c_j \right) \right)^2. \end{aligned}$$

To further simplify the upper bound on τ^2, we consider the two special cases of the reduction tree as follows:

Binary tree: In this case, we simply use the relation

$$c_j \leq c_1 = \frac{1}{\sqrt{2b}} \left(\sqrt{2} f b\right)^{\log_2(n/b)}$$

so that

$$\tau^2 \leq (1+\sqrt{b+n} c_1)^2 (1+\sqrt{b} c_1)^{2n/b} = (1+\sqrt{b+n} c_1)^2 \left(1+\frac{1}{\sqrt{2}}(\sqrt{2} f b)^{\log_2(n/b)}\right)^{2n/b}.$$

Flat tree: In this case, we note that

$$\begin{aligned} \tau^2 &\leq \left(1+\sqrt{b+n} c_1\right)^2 \left(\prod_{j=1}^{t-1} \sqrt{b} c_j\right)^2 e^{\sum_{j=1}^{t-1} \frac{2}{\sqrt{b} c_j}} \\ &= \left(1+\sqrt{b+n} c_1\right)^2 b^{t-1} \left(\prod_{j=1}^{t-1} c_j\right)^2 e^{\frac{2}{\sqrt{b}} \sum_{j=1}^{t-1} \frac{1}{c_j}}. \end{aligned}$$

Since

$$\sum_{j=1}^{t-1} \frac{1}{c_j} = \sqrt{2b} \sum_{j=1}^{t-1} \left(\sqrt{2} f b\right)^{-(n/b-j)} \leq \sqrt{2b} / \left(1 - 1/(\sqrt{2} f b)\right) \leq 4\sqrt{b},$$

it follows that

$$\begin{aligned} \tau^2 &\leq \left(1+\sqrt{b+n} c_1\right)^2 b^{n/b} \left(\frac{1}{\sqrt{2b}}\right)^{2n/b} \left(e^{\frac{2}{\sqrt{b}} 4\sqrt{b}}\right) \left(\prod_{j=1}^{n/b} \left(\sqrt{2} f b\right)^{2(n/b-j)}\right) \\ &= e^8 \left(1+\sqrt{b+n} c_1\right)^2 \left(1/\sqrt{2}\right)^{2n/b} \left(\sqrt{2} f b\right)^{n/b(n/b+1)}. \end{aligned}$$

We are now ready to state the main theorem of this section.

THEOREM 2.10. *Let A be $m \times n$ with $m \geq n$, and assume for simplicity that b divides n. Suppose that we do QR factorization with tournament pivoting on A n/b times, each time selecting b columns to pivot to the left of the remaining matrix. Then for ranks k that are multiples of b, this yields an RRQR factorization of A in the sense of Theorem 2.4, with*

$$F = \begin{cases} \left(1+\sqrt{b+n} c_1\right) \left(1+\frac{1}{\sqrt{2}} \left(\sqrt{2} f b\right)^{\log_2(n/b)}\right)^{n/b} & \text{for binary tree,} \\ e^4 \left(1+\sqrt{b+n} c_1\right) \left(1/\sqrt{2}\right)^{n/b} \left(\sqrt{2} f b\right)^{n/b(n/b+1)/2} & \text{for flat tree.} \end{cases}$$

Although the binary tree bound is relatively smaller, we must note that both bounds in Theorem 2.10 are superexponentially large. In contrast, our numerical results in section 4 are much better. As with conventional column pivoting (the special case $b = 1$), the worst case must be exponential, but whether these bounds can be significantly tightened is an open question. The matrix M in (2.21) was constructed to have the largest 1-norm in the inverse among all matrices that satisfy (2.20), which is likely to be a much larger class of matrices than CARRQR actually produces.

Example. $b = 1$ *(traditional column pivoting).* We now evaluate the bound in Theorem 2.10 when $b = 1$, i.e., traditional column pivoting. In this case we know the best bound is $O(2^n)$, which is attained by the upper-triangular Kahan matrix, where $K_{ii} = c^{i-1}$ and $K_{ij} = -sc^{i-1}$ where $j > i$, $s^2 + c^2 = 1$, and s and c are positive. In contrast, our bounds are much larger at $O(n^{n/2})$ and $O(2^{n^2/4})$, respectively.

Finally, we consider the case of k not a multiple of b. We only sketch the derivation of the bounds, since explicit expressions are complicated and not more illuminating. Recall that we must assume that strong RRQR has been independently performed on the $b \times b$ diagonal block

$$R_{ii} = \begin{bmatrix} R_{ii11} & R_{ii12} \\ 0 & R_{ii22} \end{bmatrix}$$

of the final result of tournament pivoting, with analogous notation R_{ij1} and R_{ij2}, with $j > i$, for the subblocks of R_{ij} to the right of R_{ii12} and R_{ii22}, respectively, and R_{ki1} and R_{ki2}, with $k < i$, for the subblocks of R_{ki} above R_{ii11} and R_{ii12}, respectively, yielding

$$\left[\begin{array}{ccc|c||c|ccc}
R_{11} & \cdots & R_{1,i-1} & R_{1i1} & R_{1i2} & R_{1,i+1} & \cdots & R_{1t} \\
 & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & & R_{i-1,i-1} & R_{i-1,i,1} & R_{i-1,i,2} & R_{i-1,i+1} & \cdots & R_{i-1,t} \\ \hline
 & & & R_{ii11} & R_{ii12} & R_{i,i+1,1} & \cdots & R_{it1} \\ \hline\hline
 & & & & R_{ii22} & R_{i,i+1,2} & \cdots & R_{it2} \\ \hline
 & & & & & R_{i+1,i+1} & \cdots & R_{i+1,t} \\
 & & & & & & \ddots & \vdots \\
 & & & & & & & R_{tt}
\end{array}\right]$$
$$\stackrel{def}{=} \left[\begin{array}{c|c||c|c}
\hat{R}_{11} & \hat{R}_{12} & \hat{R}_{13} & \hat{R}_{14} \\ \hline
 & R_{ii11} & R_{ii12} & \hat{R}_{24} \\ \hline\hline
 & & R_{ii22} & \hat{R}_{34} \\ \hline
 & & & \hat{R}_{44}
\end{array}\right].$$

We first need to bound the 2-norm of each column of the matrix

$$\begin{bmatrix} \hat{R}_{11} & \hat{R}_{12} \\ 0 & R_{ii11} \end{bmatrix}^{-1} \cdot \begin{bmatrix} \hat{R}_{13} & \hat{R}_{14} \\ R_{ii12} & \hat{R}_{24} \end{bmatrix}$$
$$= \begin{bmatrix} \hat{R}_{11}^{-1}\hat{R}_{13} - \hat{R}_{11}^{-1}\hat{R}_{12}R_{ii11}^{-1}R_{ii12} & \hat{R}_{11}^{-1}\hat{R}_{14} - \hat{R}_{11}^{-1}\hat{R}_{12}R_{ii11}^{-1}\hat{R}_{24} \\ R_{ii11}^{-1}R_{ii12} & R_{ii11}^{-1}\hat{R}_{24} \end{bmatrix}.$$

If we can bound the 2-norm of every column of all four subblocks in the above expression, then their root-sum-of-squares will bound the overall column 2-norms:

- Column norms of $\hat{R}_{11}^{-1}\hat{R}_{12}$, $\hat{R}_{11}^{-1}\hat{R}_{13}$ and $\hat{R}_{11}^{-1}\hat{R}_{14}$ are all bounded by our previous result on tournament pivoting alone, since $\hat{R}_{11}$ is $(i-1)b \times (i-1)b$.
- $R_{ii11}^{-1}R_{ii12}$ is bounded since we did strong RRQR on R_{ii}.
- To see that columns of $R_{ii11}^{-1}\hat{R}_{24}$ are bounded, we note that columns of $R_{ii}^{-1}R_{ij}$ are bounded (for $j > i$) by our previous result for tournament pivoting alone. Performing strong RRQR on R_{ii} changes R_{ii} to $\hat{Q}R_{ii}\Pi$ and R_{ij} to $\hat{Q}R_{ij}$ for

some permutation Π and orthogonal $\hat{Q}$, so columns of

$$\begin{aligned} R_{ii}^{-1} R_{ij} &= \Pi \cdot (\hat{Q} R_{ii} \Pi)^{-1} (\hat{Q} R_{ij}) \\ &= \Pi \cdot \begin{bmatrix} R_{ii11} & R_{ii12} \\ 0 & R_{ii22} \end{bmatrix}^{-1} \begin{bmatrix} \hat{R}_{24} \\ \hat{R}_{34} \end{bmatrix} \\ &= \Pi \cdot \begin{bmatrix} R_{ii11}^{-1} \hat{R}_{24} - R_{ii11}^{-1} R_{ii12} R_{ii22}^{-1} \hat{R}_{34} \\ R_{ii22}^{-1} \hat{R}_{34} \end{bmatrix} \end{aligned}$$

are bounded by our previous result, and so for each j,

$$\begin{aligned} \gamma_j(R_{ii11}^{-1} \hat{R}_{24}) &\leq \gamma_j(R_{ii11}^{-1} \hat{R}_{24} - R_{ii11}^{-1} R_{ii12} R_{ii22}^{-1} \hat{R}_{34}) + \gamma_j(R_{ii11}^{-1} R_{ii12} R_{ii22}^{-1} \hat{R}_{34}) \\ &\leq \gamma_j(R_{ii}^{-1} R_{ij}) + \|R_{ii11}^{-1} R_{ii12}\|_2 \cdot \gamma_j(R_{ii22}^{-1} \hat{R}_{34}) \\ &\leq \gamma_j(R_{ii}^{-1} R_{ij}) + \|R_{ii11}^{-1} R_{ii12}\|_2 \cdot \gamma_j(R_{ii}^{-1} R_{ij}) \\ &\leq (1 + \|R_{ii11}^{-1} R_{ii12}\|_2) \gamma_j(R_{ii}^{-1} R_{ij}) \end{aligned}$$

is bounded.

- Finally, we can combine these bounds to bound above

$$\gamma_j(\hat{R}_{11}^{-1} \hat{R}_{13} - \hat{R}_{11}^{-1} \hat{R}_{12} R_{ii11}^{-1} R_{ii12}) \leq \gamma_j(\hat{R}_{11}^{-1} \hat{R}_{13}) + \|\hat{R}_{11}^{-1} \hat{R}_{12}\|_2 \cdot \gamma_j \left(R_{ii11}^{-1} R_{ii12}\right)$$

and

$$\gamma_j \left(\hat{R}_{11}^{-1} \hat{R}_{14} - \hat{R}_{11}^{-1} \hat{R}_{12} R_{ii11}^{-1} \hat{R}_{24}\right) \leq \gamma_j \left(\hat{R}_{11}^{-1} \hat{R}_{14}\right) + \|\hat{R}_{11}^{-1} \hat{R}_{12}\|_2 \cdot \gamma_j \left(R_{ii11}^{-1} \hat{R}_{24}\right).$$

Now we must bound from above

$$\gamma_j \left(\begin{bmatrix} R_{ii22} & \hat{R}_{34} \\ 0 & \hat{R}_{44} \end{bmatrix} \right) \Big/ \sigma_{\min} \left(\begin{bmatrix} \hat{R}_{11} & \hat{R}_{12} \\ 0 & R_{ii11} \end{bmatrix} \right).$$

Using the previously established bounds on column norms of $\hat{R}_{11}^{-1} \hat{R}_{12}$ and $R_{ii22}^{-1} \hat{R}_{34}$, it is, as before, enough to bound above

$$\begin{aligned} &\gamma_j \left(\begin{bmatrix} R_{ii22} & 0 \\ 0 & \hat{R}_{44} \end{bmatrix} \right) \Big/ \sigma_{\min} \left(\begin{bmatrix} \hat{R}_{11} & 0 \\ 0 & R_{ii11} \end{bmatrix} \right) \\ &= \gamma_j \left(\begin{bmatrix} R_{ii22} & 0 \\ 0 & \hat{R}_{44} \end{bmatrix} \right) \Big/ \min(\sigma_{\min}(\hat{R}_{11}), \sigma_{\min}(R_{ii11})). \end{aligned}$$

By the strong rank revealing property for $k = (i-1)b$, we know that $\sigma_{\min}(\hat{R}_{11})$ cannot be much smaller than $\gamma_j(R_{ii11})$, so the denominator in the last fraction can be replaced by $\sigma_{\min}(R_{ii11})$. Similarly, the numerator can be replaced by $\gamma_j(R_{ii22})$. This leaves us with $\gamma_j(R_{ii22})/\sigma_{\min}(R_{ii11})$, which is bounded above by the strong rank revealing property of R_{ii}.

3. Performance analysis of QR with tournament pivoting. In this section we analyze the performance of parallel communication avoiding QR with tournament pivoting, and we show that it minimizes communication at the cost of roughly tripling the number of arithmetic operations. Algorithm 1 presents the parallel CARRQR factorization of a matrix A of size $m \times n$. The matrix is distributed block cyclically on a grid of $P = P_r \times P_c$ processors using blocks of size b. For simplicity we suppose n/b is an integer. Consider step j of the factorization, and let $m_b = m - (j-1)b$,

Table 1

Performance models of parallel CAQR and tournament pivoting when factoring an $m \times n$ matrix, distributed in a 2-D block cyclic layout on a $P_r \times P_c$ grid of processors with square $b \times b$ blocks. All terms are counted along the critical path. We generally assume $m \geq n$. The cost of CARRQR is equal to the cost of tournament pivoting plus the cost of CAQR. In the table, $f(m,n,b,P_r,P_c) = \frac{4(2mnb-n^2b)}{P_r}\log_2 P_c + \frac{16nb^2}{3}\log_2 P_r \log_2 P_c + 11nb^2 \log_2 P_c$.

	Parallel CAQR
# flops	$\frac{2mn^2-2n^3/3}{P} + \frac{bn^2}{2P_c} + \frac{3bn(2m-n)}{2P_r} + \left(\frac{4b^2n}{3} + \frac{n^2(3b+5)}{2P_c}\right)\log_2 P_r - b^2 n$
# words	$\left(\frac{n^2}{P_c} + \frac{bn}{2}\right)\log_2 P_r + \left(\frac{mn-n^2/2}{P_r} + 2n\right)\log_2 P_c$
# messages	$\frac{3n}{b}\log_2 P_r + \frac{2n}{b}\log_2 P_c$
	Tournament pivoting with $b_T = 2b$ (excluding cost of QR factorization)
# flops	$\frac{4mn^2-4n^3/3}{P} + \frac{8n^2b}{3P_c}(\log_2 P_r + 2) + f(m,n,b,P_r,P_c)$
# words	$\frac{n^2}{P_c}\log_2 P_r + \frac{mn-n^2/2}{P_r}(\log_2 P_c + 1)$
# messages	$\frac{n^2}{2b^2P_c}\log_2 P_r + \frac{n}{b}\log_2 P_c(\log_2 P_r + 1)$
	Tournament pivoting with $b_T = n/P_c$ (excluding cost of QR factorization)
# flops	$\frac{2}{3}\frac{mn^2-n^3/4}{P}\frac{n}{bP_c} + \frac{1}{6}\frac{n^3}{P_c^2}\frac{n}{bP_c}(\log_2 P_r + 2) + f(m,n,b,P_r,P_c)$
# words	$\frac{1}{6}\frac{n^2}{P_c}\frac{n}{bP_c}\log_2 P_r + \frac{mn-n^2/2}{P_r}(\log_2 P_c + 1) + 2nb\log_2 P_r \log_2 P_c$
# messages	$\frac{n}{b}(\log_2 P_r + 2\log_2 P_c + \log_2 P_r \log_2 P_c)$

$n_b = n-(j-1)b$. The size of the matrix on which the algorithm operates at this step is $m_b \times n_b$. First, tournament pivoting is used to identify b pivot columns, using a binary tree of depth $\log_2 n_b/b_T$. For the ease of analysis, we consider that tournament pivoting is performed as an all-reduce operation; that is, all processors participate at all the stages of the reduction, and the final result is available on all processors.

Depending on the size of b_T, a processor can be involved in operations at more than one node at each level of the binary tree. At the leaves, the b candidate columns are selected from blocks of size $m_b \times b_T$. For this, the processors in the same process column perform the QR factorization of their blocks of columns, using TSQR [12]. The R factors obtained from this factorization are available on all processors. Each processor selects b column candidates by performing QR with column pivoting on its R factor.

After this step, there are nb/b_T candidate columns. The subsequent steps of the reduction operate on blocks of $2b$ columns, where the new column candidates are chosen similarly by computing TSQR followed by QR with column pivoting on the R factor. In the first $\log_2(n/(bP_c))$ levels of the reduction tree, a processor is involved in the computation of several nodes per level. In other words, it is the owner of several sets of candidate columns. Hence it can form with no communication the matrix of $2b$ column candidates of the next level. At the last $\log_2 P_c$ levels of the reduction tree, a processor is involved in the computation performed at only one node per level. Hence the processors in the same process row need to exchange their local parts of the candidate columns.

To study the theoretical performance of CARRQR, we use a simple model to describe a machine architecture in terms of speed, network latency, and bandwidth. The cost of performing parallel CARRQR of an $m \times n$ matrix is given in Table 1. We display separately the cost of performing communication avoiding QR factorization and the cost of performing tournament pivoting, with $b_T = 2b$ and $b_T = n/P_c$. The total cost of CARRQR is the cost of performing CAQR plus the cost of performing

Algorithm 1 Parallel QR with tournament pivoting.

Input matrix A of size $m \times n$, block size b, b_T
for $j = 1$ to n/b **do**
  Let $m_b = m - (j-1)b$, $n_b = n - (j-1)b$
  /* Perform tournament pivoting to choose b pivot columns */
  for $k = 1$ to $n_b/(2bP_c)$ **do**
    Let A_{0k} be the kth column block of size $m_b \times 2b$ that belongs to the process column of my processor.
    Processors in the same process column select b column candidates by performing TSQR of their block A_{0k} followed by strong RRQR of the R factor.
  end for
  for $i = 1$ to $log_2(n_b/b_T)$ **do**
    for each node $k = 1$ to $n_b/(2bP_c2^i)$ in the current level assigned to my processor **do**
      if at most one node is assigned per processor **then**
        Each of the two processors in the same process row exchanges their local parts of the b column candidates selected at the sons of their current node k.
      end if
      Let A_{ik} be the matrix obtained by putting next to each other the two sets of b column candidates selected at the sons of the current node k.
      Processors in the same process column select b column candidates by performing TSQR of their block A_{ik} followed by strong RRQR of the R factor.
    end for
  end for
  Swap the b pivot columns to jth column block: $A(:, j_0 : end) = A(:, j_0 : end)\Pi_j$, where $j_0 = (j-1)b+1$ and Π_j is the permutation matrix returned by tournament pivoting.
  TSQR factorization of the jth column block $A(j_0 : end, j_0 : j_1) = Q_j R_j$, where $j_1 = jb$, R_j is an upper-triangular matrix.
  Update of the trailing matrix $A(j_0 : end, j_1 + 1 : end) = Q_j^T A(j_0 : end, j_1 + 1 : end)$.
end for

tournament pivoting. The parallel CARRQR factorization based on tournament pivoting with $b_T = 2b$ requires three times more flops than the QR factorization. However, for $b_T = n/P_c$, the parallel CARRQR factorization performs a factor of $n/(bP_c)$ more flops than the QR factorization. Hence the former choice of $b_T = 2b$ should lead to a faster algorithm in practice.

We recall now briefly the lower bounds on communication from [3], which apply to QR under certain hypotheses. On a sequential machine with fast memory of size M and slow memory, a lower bound on the volume of data and on the number of messages transferred between fast and slow memory during the QR factorization of a matrix of size $m \times n$ is

$$\# \text{ words} \geq \Omega\left(\frac{mn^2}{\sqrt{M}}\right), \quad \# \text{ messages} \geq \Omega\left(\frac{mn^2}{M^{3/2}}\right). \tag{3.1}$$

When the matrix is distributed over P processors, the size of the memory per processor is on the order of $O(mn/P)$, and the work is balanced among the P

processors, then a lower bound on the volume of data and the number of messages that at least one of the processors must transfer is

$$\# \text{ words} \geq \Omega\left(\sqrt{\frac{mn^3}{P}}\right), \quad \# \text{ messages} \geq \Omega\left(\sqrt{\frac{nP}{m}}\right). \tag{3.2}$$

To minimize communication in parallel CARRQR, we use an optimal layout, with the same values as in [11], $P_r = \sqrt{mP/n}$, $P_c = \sqrt{nP/m}$, and $b = B \cdot \sqrt{mn/P}$. The number of flops required by tournament pivoting with $b_T = 2b$, which does not include the number of flops required for computing the QR factorization once the pivot columns have been identified, is

$$\begin{aligned}\#\mathit{flops} = {} & \frac{4mn^2 - 4n^3/3}{P} \\ & + \frac{mn^2}{P}\left(8B\left(\frac{1}{3}\log_2 P_r + \log_2 P_c + \frac{2}{3}\right) + 32B^2\left(\frac{1}{6}\log_2 P_r \log_2 P_c + \frac{1}{3}\log_2 P_c\right)\right).\end{aligned}$$

By choosing $B = 8^{-1}\log_2^{-1}(P_r)\log_2^{-1}(P_c)$, the first term in $\#\mathit{flops}$ dominates the redundant computation due to tournament pivoting. This is a term we cannot decrease. After dropping some of the lower order terms, the counts of the entire parallel CARRQR factorization become

$$\begin{aligned}\#\mathit{flops} &\approx \frac{6mn^2 - 6n^3/3}{P} + cmn^2, \quad c < 1, \\ \#\mathit{words} &\approx 2\frac{\sqrt{mn^3}}{\sqrt{P}}\left(\log_2\sqrt{\frac{mP}{n}} + \log_2\sqrt{\frac{nP}{m}}\right), \\ \#\mathit{messages} &\approx 2^7\sqrt{\frac{nP}{m}}\log_2^2\sqrt{\frac{mP}{n}}\log_2^2\sqrt{\frac{nP}{m}},\end{aligned}$$

and this shows that parallel CARRQR is communication optimal, modulo polylogarithmic factors.

Appendix B in the technical report [10] on which this paper is based describes briefly the performance model of a sequential communication avoiding QR. It shows that sequential CARRQR performs three times more flops than QRCP, transfers $\Theta(mn^2/M^{1/2})$ number of words, and exchanges $\Theta(mn^2/M^{3/2})$ number of messages between the slow memory and the fast memory of size M of the sequential computer. Thus sequential QR attains the lower bounds on communication. As explained in the introduction, neither sequential QRCP nor parallel QRCP is communication optimal. We note, however, that parallel QRCP minimizes the volume of communication, but not the number of messages.

4. Experimental results. In this section we discuss the numerical accuracy of our CARRQR and compare it with the classic QR factorization with column pivoting and the singular value decomposition. We focus in particular on the value of the elements obtained on the diagonal of the upper-triangular factor R (referred to as R-values) of the factorization $A\Pi = QR$, and compare them with the singular values of the input matrix. For the CARRQR factorization, we test binary tree based CARRQR and flat tree based CARRQR, denoted in the figures as CARRQR-B and CARRQR-F, respectively. The singular values are computed by first performing a QR factorization with column pivoting of A, and then computing the singular values of the upper-triangular factor R with the highly accurate routine `dgesvj` [14, 15]. We use this approach to compute the singular values since given a matrix $A = DY$ (or $A = YD$), where D is diagonal and Y is reasonably well-conditioned, the Jacobi singular value decomposition (SVD) algorithm in `dgesvj` computes the singular values with relative error of at most $O(\epsilon)\kappa(Y)$, whereas the SVD algorithm based on the QR iteration has a relative error of at most $O(\epsilon)\kappa(A)$. Here $\kappa(A)$ is the condition number of A, $\kappa(A) = ||A||_2 \cdot \left|\left|A^{-1}\right|\right|_2$. This choice affects in particular the accuracy of the small singular values. Not all our input matrices A have the scaling property that A can be expressed as the product of a diagonal matrix and a well-conditioned matrix, but after computing $A\Pi = QR$ by using an RRQR factorization and $R = DY$, we expect to obtain a well-conditioned Y. Even when Y is not well-conditioned, it is still expected that `dgesvj` of R is more accurate than SVD of R.

In the plots displaying R-values and singular values, we also display bounds for trustworthiness, computed as

$$\epsilon \min\{||(A\Pi_0)(:,i)||_2\,, ||(A\Pi_1)(:,i)||_2\,, ||(A\Pi_2)(:,i)||_2\}, \tag{4.1}$$

$$\epsilon \max\{||(A\Pi_0)(:,i)||_2\,, ||(A\Pi_1)(:,i)||_2\,, ||(A\Pi_2)(:,i)||_2\} \tag{4.2}$$

where $\Pi_j (j = 0, 1, 2)$ are the permutation matrices obtained by QRCP, CARRQR-B, and CARRQR-F (represented by the subscripts $j = 0, 1, 2$, respectively), $(A\Pi)(:, i)$ is the ith column of the permuted matrix $A\Pi$, and ϵ is the machine precision. Since the algorithm can be interpreted as applying orthogonal transformations to each column separately, machine epsilon times the norm of column i is a reasonable estimate of the uncertainty in any entry in that column of R, including the diagonal, our estimate of σ_i. Therefore the quantities in (4.1) and (4.2) describe the range of uncertainties in σ_i, for all three choices of column i, from the three pivoting schemes tested.

For each matrix in our test set we display the ratio $R(i, i)/\sigma_i$, where R is the upper-triangular factor obtained by QRCP, CARRQR-B, or CARRQR-F, $R(i, i)$ denotes the ith diagonal element of R, assumed to be nonnegative, and σ_i is the ith singular value computed as described above. Consider the factorization $A\Pi = QR$ obtained by using QRCP, CARRQR-B, or CARRQR-F. Let $D = \mathtt{diag}(\mathtt{diag}(R))$ and define Y by $R = DY^T$. Then we have $A\Pi = QDY^T$. The R-values of QRCP decrease monotonically, and it follows straightforwardly from the minimax theorem that the ratio $R(i, i)/\sigma_i$ can be bounded as

$$\frac{1}{||Y||} \leq \frac{R(i,i)}{\sigma_i} \leq ||Y^{-1}||, \tag{4.3}$$

and these lower and upper bounds are also displayed in the corresponding plots.

The entire set of matrices is presented in Table 2. Unless otherwise specified, the matrices are of size 256×256 and the block size is $b = 8$. For these matrices we test QRCP, CARRQR-B, and CARRQR-F. In addition, for two challenging matrices for rank revealing factorizations, the devil's stairs and Kahan matrix, we also test the QLP factorization which approximates the SVD by two calls to QR factorization with pivoting (see [29] for more details on the QLP factorization). The obtained QLP factorization is of the form $A = Q\Pi_1 L Q_1^T \Pi^T$, where Q and Q_1 are orthogonal matrices and L is a lower triangular matrix. We refer to the diagonal elements of L which approximate the singular values of A as L-values.

The binary tree version of CARRQR uses a tournament that has $2b$ columns at the leaves of the reduction tree. The matrices in our set were used in several previous papers focusing on rank revealing factorizations [4, 22, 29, 26]. A short

Table 2
Test matrices.

No.	Matrix	Descriptions
1	Baart	Discretization of the 1st kind Fredholm integral equation [23].
2	Break-1	Break 1 distribution, matrix with prescribed singular values; see description in the text and [4].
3	Break-9	Break 9 distribution, matrix with prescribed singular values; see description in the text and [4].
4	Deriv2	Computation of second derivative [23].
5	Exponential	Exponential distribution, $\sigma_1 = 1$, $\sigma_i = \alpha^{i-1}$ $(i = 2, \ldots, n)$, $\alpha = 10^{-1/11}$ [4].
6	Foxgood	Severely ill-posed test problem of the 1st kind Fredholm integral equation used by Fox and Goodwin [23].
7	Gks	An upper-triangular matrix whose jth diagonal element is $1/\sqrt{j}$ and whose (i, j) element is $-1/\sqrt{j}$ for $j > i$ [19, 22].
8	Gravity	One-dimensional (1D) gravity surveying problem [23].
9	H-C	Matrix with prescribed singular values; see description in the text and [26].
10	Heat	Inverse heat equation [23].
11	Phillips	Phillips' famous test problem [23].
12	Random	Random matrix `A = 2* rand(n) - 1` [22].
13	Scale	Scaled random matrix, a random matrix whose ith row is scaled by the factor $\eta^{i/n}$ [22]. We choose $\eta = 10 \cdot \epsilon$.
14	Shaw	1D image restoration model [23].
15	Spikes	Test problem with a "spiky" solution [23].
16	Stewart	Matrix $\mathtt{A = U}\ \Sigma\ \mathtt{V}^T \mathtt{ + 0.1}\ \sigma_m \mathtt{ * rand(n)}$, where σ_m is the smallest nonzero singular values; see description in the text and [29].
17	Ursell	Integral equation with no square integrable solution [23].
18	Wing	Test problem with a discontinuous solution [23].
19	Kahan	Kahan matrix; see (4.4).
20	Devil	The devil's stairs, a matrix with gaps in its singular values; see [29] or Algorithm 2 in Appendix A of [10].
21 ⋮ 281	SJSU Singular	A subset of matrices from the San Jose State University Singular Matrix Database with more than 32 but less than 2048 columns and less than 1024 rows. These 261 numerically singular matrices are sorted by the number of columns.

description is given in the table. In addition, we describe in more detail here matrices Break-1, Break-9, H-c, and Stewart, which are random matrices of size $n \times n$ with prescribed singular values $\{\sigma_i\}$. The first three matrices are of the form $A = U\Sigma V^T$, where U, V are random orthogonal matrices and Σ is a diagonal matrix. For Break-1, Σ has the following diagonal entries $\sigma_1 = \cdots = \sigma_{n-1} = 1, \sigma_n = 10^{-9}$ [4]. For Break-9, the diagonal entries of Σ are $\sigma_1 = \cdots = \sigma_{n-9} = 1, \sigma_{n-8} = \cdots = \sigma_n = 10^{-9}$ [4]. For H-c, Σ has diagonal entries 100, 10, and the following $n - 2$ are evenly spaced between 10^{-2} and 10^{-8} [26]. For the matrix Stewart, $A = U\Sigma V^T + 0.1\sigma_m E$ [29], where Σ is a diagonal matrix with the first half of the diagonals decreasing geometrically from 1 to $\sigma_m = 10^{-3}$ and the last half of the diagonals being set to zero, U and V are random orthogonal matrices, and E is a matrix with random entries chosen from a uniform distribution in the interval (0, 1). In MATLAB notation, `smax = 1; smin = 1e-3; nhalf = floor(n/2); v = zeros(n,1); v(1:nhalf) = fliplr(logspace( log10(smin), log10(smax), nhalf) ); A = orth(rand(n)) * diag(v) * orth(rand(n)) + 0.1 * smin * rand(n).` We also test numerically singular matrices from the SJSU Singular Matrix Database; for more details on how to obtain them see [16]. These matrices either are from real applications or represent problems from real applications. We have selected all matrices

TABLE 3

Kahan-like matrix (of size $n = 128$) with the parameter $\tau = 10^{-7}$, comparison between last two singular values, R*-values, and* L*-values. In the table, r_{n-1}, r_n are the last two* R*-values, and l_{n-1}, l_n are the last two* L*-values. $\epsilon = ulp \approx 2.22E-16$, i.e., the eps in MATLAB.*

c	$\epsilon\|\|A\|\|_2$	Singular values		R-values		QRCP + QLP		CARRQR-B + QLP		CARRQR-F + QLP	
		σ_{n-1}	σ_n	r_{n-1}	r_n	l_{n-1}	l_n	l_{n-1}	l_n	l_{n-1}	l_n
0.1	1.44E-15	5.57E-01	5.71E-06	5.31E-01	5.28E-01	4.13E-01	1.34E-05	4.13E-01	1.34E-05	4.13E-01	1.34E-05
0.2	2.11E-15	8.37E-02	1.26E-11	7.64E-02	7.49E-02	6.48E-02	2.18E-11	6.48E-02	2.18E-11	6.48E-02	2.18E-11
0.3	2.32E-15	3.00E-03	1.68E-17	2.63E-03	2.51E-03	2.42E-03	2.30E-17	2.42E-03	2.37E-17	2.42E-03	2.34E-17
0.4	2.41E-15	2.01E-05	4.63E-23	1.70E-05	1.55E-05	1.68E-05	0.00E+00	1.68E-05	5.08E-21	1.68E-05	3.39E-21
0.5	2.44E-15	1.65E-08	7.35E-26	1.35E-08	1.17E-08	1.43E-08	2.48E-24	1.43E-08	1.65E-24	1.43E-08	1.65E-24
0.6	2.47E-15	7.79E-13	1.19E-29	6.16E-13	4.93E-13	6.97E-13	0.00E+00	6.97E-13	4.42E-29	6.97E-13	0.00E+00

that have more than 32 but less than 2048 columns and less than 1024 rows, and there are 261 such numerically singular matrices in the collection. The index of the test matrices in the database are obtained as follows. `ind = SJget; index = find ( index.ncols>32 & ind.ncols<=2048 & ind.nrows<=1024 ); [∼, k] = sort ( ind.ncols (index) ); index = index(k).`

We first discuss the Kahan matrix and the devil's stairs. The Kahan matrix is presented in (4.4) where $c^2 + s^2 = 1$. For $c = 0$, the singular values are all 1's. An increasing gap between the last two singular values is obtained when the value of c is increased. Since $\sigma_{\min}(R_{11}) \leq \sigma_k(A)$ in (1.1), we would like to find Π such that $\sigma_{\min}(R_{11})$ is sufficiently large. For the $n \times n$ Kahan matrix with the decomposition (1.1), it is known that $\sigma_k(A)/\sigma_{\min}(R_{11}) \geq \frac{1}{2}c^3(1+c)^{n-4}/s$ for $k = n-1$, and $\sigma_{\min}(R_{11})$ can be much smaller than $\sigma_k(A)$ [22]. Traditional QR with column pivoting does not permute the columns of A in exact arithmetic and fails to reveal the gap between the last two singular values. It is easy to notice that CARRQR does not permute the columns in exact arithmetic either, if we assume that during tournament pivoting, ties are broken by choosing the leftmost column when multiple columns have the same norm. This results in poor rank revealing, similarly to QRCP. However, in finite precision, both QRCP and CARRQR might permute the columns of the matrix, and in this case both reveal the rank. To avoid a possible nontrivial permutation in finite precision (a well-known phenomenon [13] of the Kahan matrix), we multiply the jth column of the Kahan matrix by $(1-\tau)^{j-1}$ for all j and $1 \gg \tau \gg \epsilon$. The additional numerical experiments we have performed revealed that when τ is small, for example, for $c = 0.6$ and $\tau = 10^{-15}$, all three algorithms, QRCP, CARRQR-B, and CARRQR-F, pivot the columns of A and are effective in revealing the rank. However, when the parameter τ is increased, for example, for $\tau = 10^{-7}$, the three algorithms do not perform any pivoting, and result in poor rank revealing. This can be seen in the results displayed in Table 3, where we compare the last two singular values with the last two L-values and R-values obtained from QRCP, CARRQR-B, and CARRQR-F.

$$
A = \begin{pmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & s & 0 & \cdots & \cdots & 0 \\ 0 & 0 & s^2 & \ddots & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & \cdots & 0 & s^{n-1} \end{pmatrix} \begin{pmatrix} 1 & -c & -c & \cdots & \cdots & -c \\ 0 & 1 & -c & \cdots & \cdots & -c \\ 0 & 0 & 1 & \ddots & \cdots & -c \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \ddots & -c \\ 0 & 0 & \cdots & \cdots & 0 & 1 \end{pmatrix}. \tag{4.4}
$$

The devil's stairs [29] is a matrix with multiple gaps in its singular values, generated by the MATLAB code given in Algorithm 2, Appendix A of the technical report

[10]. In the results presented in Figure 1, the gap in the singular values of this matrix is nearly 4. Precisely speaking, $\max_i\{\sigma_i/\sigma_{i+1}\} = 10^{0.6} = 3.98$, where $1 \leq i \leq n-1$. In this case, we can see that the L-values, that is, the singular value estimates obtained from QLP and displayed in Figure 1(c), reveal the gaps in the singular values. However, the R-values, that is, the diagonal elements of the R factor obtained after one QR factorization and displayed in Figure 1(a), do not reveal the gap. Both our versions of CARRQR factorization provide a good first step for the QLP factorization, similar to the traditional QR with column pivoting.

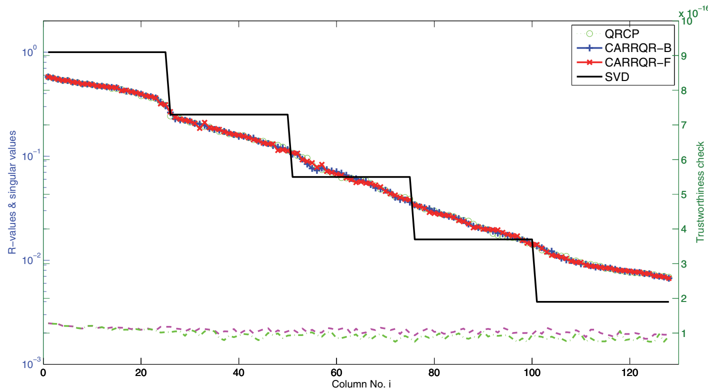
We now discuss the first 18 matrices in our test set, given in alphabetical order in Table 2. In the technical report [10] we present detailed results for each matrix, while here we summarize these results in Figures 2 and 3. Figure 2 presents the ratios of the R-values obtained from the different QR factorizations to the singular values. Let r be the vector of R-values obtained from QRCP/CARRQR, and let s be the vector of singular values. The R-values obtained from CARRQR are not in descending order and we do not sort them. The values displayed in Figure 2 are the minimum of the ratios $\mathtt{min}(r./s)$, the maximum of the ratios $\mathtt{max}(r./s)$, and the median of the ratios $\mathtt{median}(r./s)$. For all the test cases, we can see that the ratios are close to 1, and are well bounded as in (4.3). We conclude that the R-values obtained by CARRQR reveal the rank for all the matrices in our test set.

For the purpose of clarity, we display in the fourth plot of Figure 2 the ratio $\min_i\{\frac{R(i,i)}{\epsilon||(A\Pi)(:,i)||_2}\}$ for the first 18 matrices in our test set. The R factor is obtained from QRCP, CARRQR-B, and CARRQR-F. It can be seen that for the matrices numbered 1, 5–8, 10, 14, 15, and 18, this ratio is smaller than 1. But as displayed in Figure 2, the ratios $R(i,i)/\sigma_i(R)$ are close to 1 (usually within a factor of 10), and well bounded by (4.3). In other words, even when $\frac{R(i,i)}{\epsilon||(A\Pi)(:,i)||}$ is small and we do not expect an accurate computation of the R-values due to round-off error, for the matrices presented here the computed R-values are still very close to the accurately computed singular values of the R matrix. However, this is not true in general.

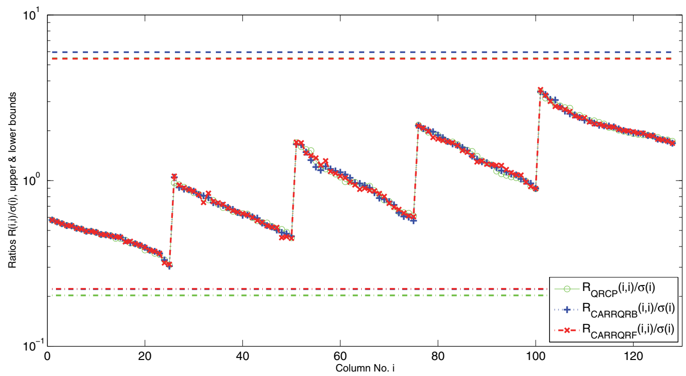
As explained earlier, tournament pivoting used in CARRQR does not guarantee that the R-values decrease monotonically, while QR with column pivoting does. The formula (4.3) should be modified for CARRQR as

$$\frac{1}{||Y||} \leq \frac{\rho_i}{\sigma_i} \leq ||Y^{-1}||,$$

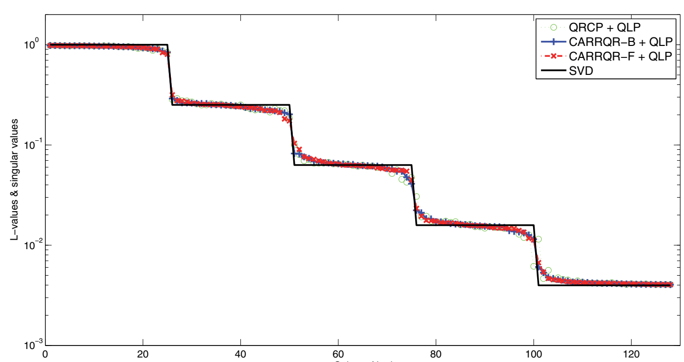
where ρ_i is the ith largest diagonal of the R factor of CARRQR, that is, the ith value of the sorted R-values. Since the CARRQR factorizations have good rank revealing properties in practice, we can expect that (4.3) still holds approximately for CARRQR, even without this modification. And this is indeed verified by the numerical results in Figure 2, where the ratios $R(i,i)/\sigma_i$ are bounded by the bounds in (4.3) for all our test cases. To check the monotonicity of the R-values, Figure 3 displays the minimum, the maximum, and the median of the rations $R(i+1, i+1)/R(i,i)$, where $i = 1, \ldots, n-1$ and n is the size of the input matrix. The factor R is obtained from RRQR with column pivoting (top plot), CARRQR-B (middle plot), and CARRQR-F (bottom plot). It can be seen that for both CARRQR-B and CARRQR-F, the ratios are well below 1, except for a very few cases, and are never more than 2.



(a) R-values of QRCP and CARRQR.



(b) Ratios $|R(i,i)|/\sigma_i$.



(c) L-values of QRCP and CARRQR.

FIG. 1. *The devil's stairs, matrix of size* 128×128*. The roughly horizontal dotted lines in* (a) *stand for the upper and lower bounds given in* (4.1) *and* (4.2)*; the horizontal dotted lines in* (b) *denote the upper and lower bounds from* (4.3)*, where the* Y *factors are obtained from QRCP, CARRQR-B, and CARRQR-F, respectively.*

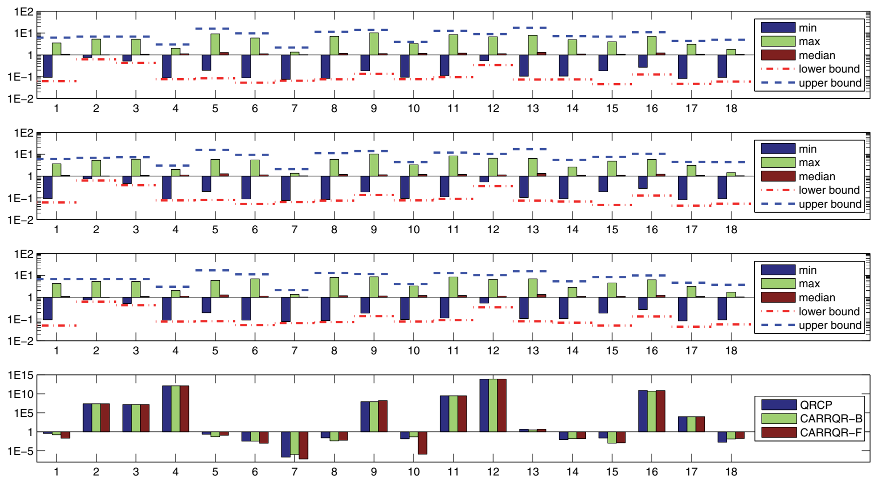


Fig. 2. *The first three plots display minimum, maximum, and median of the ratios* $|R(i,i)|/\sigma_i(R)$ *for the first* 18 *matrices in our test set, where* $i = 1, \ldots, n$ *and* n *is the size of the input matrix. The dotted horizontal lines represent the upper and lower bounds from* (4.3)*. The R factor is obtained from QRCP (top plot), CARRQR-B (second plot), and CARRQR-F (third plot). The number along the x-axis represents the index of test matrices in Table* 2*. The fourth plot displays the ratios* $\min_{i=1:n}\{\frac{|R(i,i)|}{\epsilon||(A\Pi)(:,i)||_2}\}$ *for the first* 18 *matrices in our test set, where* n *is the size of the input matrix. In the bottom row, the R factor is obtained from QRCP (left column), CARRQR-B (middle column), and CARRQR-F (right column).*

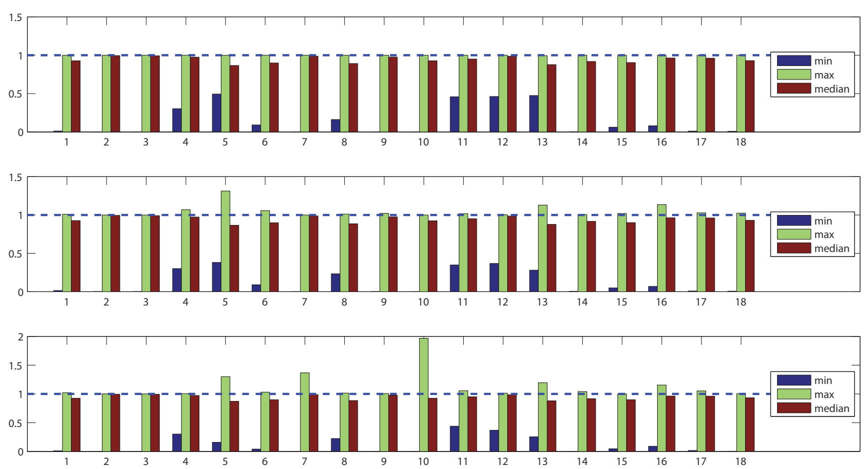


Fig. 3. *Ratios of successive R-values,* $|R(i+1,i+1)|/|R(i,i)|$*, for* $i = 1, \ldots, n-1$*, and* n *is the size of the matrix. The R factor is obtained from QRCP (top plot), CARRQR-B (middle plot), and CARRQR-F (bottom plot). These results are for the first* 18 *matrices in our test set.*

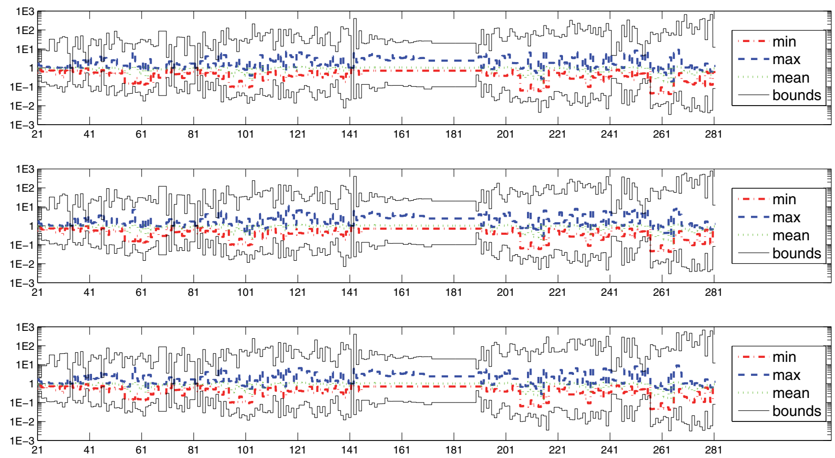


FIG. 4. *Minimum, maximum, and median of the ratios $|R(i,i)|/\sigma_i(R)$, where $i = 1, \ldots, n_{rk}$ and n_{rk} is the numerical rank of input matrix, which comes from the SJSU Singular Matrix Database. The two solid lines represent the upper and lower bounds from* (4.3). *The R factor is obtained from QRCP (top plot), CARRQR-B (middle plot), and CARRQR-F (bottom plot). The x-axis denotes the index of* 261 *matrices.*

The results for the 261 matrices from SJSU Singular Matrix Database are summarized in Figure 4 and Table 4. Here we set $b = 16$ for all test cases. To check the ratios $R(i,i)/\sigma_i$ for $i = 1, \ldots, n_{rk}$, where n_{rk} is the numerical rank of A provided by the database, we need to modify the formula (4.3). Suppose that we have the decomposition (1.1) with the R factor's (1,1) block R_{11} of the size $n_{rk} \times n_{rk}$ and the (2,2) block R_{22} where $||R_{22}||_2 = O(\epsilon)$. Then the R factor can be expressed as

$$R = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Y & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & X \\ 0 & I \end{bmatrix} + O(\epsilon),$$

where $D = \texttt{diag}(\texttt{diag}(R_{11}))$ is assumed to be nonnegative, $Y = D^{-1}R_{11}$, and $X = R_{11}^{-1}R_{12}$. Using the minimax theorem, we obtain the following approximate estimate:

$$\frac{1}{||Y||(1 + ||X||)} \leq \frac{R(i,i)}{\sigma_i} \leq ||Y^{-1}||(1 + ||X||) \tag{4.5}$$

for $1 \leq i \leq n_{rk}$. This is the slight modification of the formula (4.3).

Figure 4 presents the ratios of the R-values to the singular values, $R(i,i)/\sigma_i$ for $1 \leq i \leq n_{rk}$, where the R-values are obtained from QRCP or CARRQR. All these ratios are well bounded by (4.5), and the statistical results of the ratios of these three factorizations are very similar. Please note that the matrices numbered 34, 73, 82, and 142 (with the matrix names Bcsstm01, Bcsstm03, Bcsstm04, and Odepb400, respectively) are singular diagonal matrices. And the bounds for these four matrices are equal to one.

The maximum and minimum of these ratios $R(i,i)/\sigma_i$ ($i \leq n_{rk}$) for all 261 test cases are also given on the left in Table 4 (each number is obtained from the results of 74195 ratios). We also display on the right in Table 4 the maximum and minimum of the ratios $\max\{R(i,i), \epsilon\sigma_{\max}(A)\}/\max\{\sigma_i(A), \epsilon\sigma_{\max}(A)\}$ for $i > n_{rk}$ (each number is obtained from the results of 22422 ratios). Since the singular values and the diagonal

TABLE 4

Maximum and minimum of the ratios $|R(i,i)|/\sigma_i(A)$ for $1 \le i \le n_{rk}$ (left) and maximum and minimum of the ratios $\max\{|R(i,i)|, \epsilon\sigma_{\max}(A)\}/\max\{\sigma_i(A), \epsilon\sigma_{\max}(A)\}$ for $n_{rk} < i \le$ `min(size(`A`))` (right) for 261 matrices from the SJSU Singular Matrix Database.

	$\|R(i,i)\|/\sigma_i(A)(1 \le i \le n_{rk})$			$\max\{\|R(i,i)\|, \epsilon\sigma_1\}/\max\{\sigma_i, \epsilon\sigma_1\}(i > n_{rk})$		
	QRCP	CARRQR-B	CARRQR-F	QRCP	CARRQR-B	CARRQR-F
max	8.957E+00	1.138E+01	9.054E+00	7.416E+00	7.666E+00	7.416E+00
min	4.169E-02	4.169E-02	4.169E-02	1.348E-01	1.360E-01	1.351E-01

entries of R are very small for $i > n_{rk}$, these ratios are computed differently to account for round-off errors. These results show that the CARRQR algorithms successfully reveal the rank for the matrices in this data set.

We next examine the permutation vectors of the three methods on the 261 matrices from the SJSU Singular Matrix Database. Let $p_j (j = 0, 1, 2)$ be the permutation vectors obtained by QRCP, CARRQR-B, and CARRQR-F, respectively. We are concerned about the first n_{rk} elements and define the row vectors $\pi_j = p_j(1 : n_{rk}), (j = 0, 1, 2)$. Then we check the number of different elements between two permutation vectors. For example, m_{10} `= size( setdiff(`π_1, π_0`), 2 )` returns the number of different elements in the first n_{rk} entries of the permutation vectors of CARRQR-B and QRCP, and similarly we can define m_{20} and m_{12} for each test case. We find that there are 43 cases with $m_{10} = 0$, 48 cases with $m_{20} = 0$, and 45 cases with $m_{12} = 0$. About half of the test cases yield the results with $m_i \le 6$ ($i = 10$, 20, or 12).

Again we check in more detail the R-factors in Figures 5–7. The gaps in R-values, the diagonals of R factors, are checked in Figure 5. Two metrics are used here, $R(n_{rk}, n_{rk})/R(1,1)$ and $R(n_{rk}+1, n_{rk}+1)/R(n_{rk}, n_{rk})$. The ratios of singular values $\sigma(n_{rk})/\sigma(1)$ and $\sigma(n_{rk}+1)/\sigma(n_{rk})$ are also plotted for comparison with the corresponding ratios between R-values, where the singular values are obtained by `svd` on the R factor of QRCP, CARRQR-B, or CARRQR-F. Since the singular value ratios of these three methods are indistinguishable, we just present the ratios of singular values of QRCP's R factor for comparison. We can observe that there exists a gap between the n_{rk}th and the $(n_{rk}+1)$th entries of the R-values or the singular values for most cases. For the cases where there is no obvious gap between $R(n_{rk}+1, n_{rk}+1)$ and $R(n_{rk}, n_{rk})$, the n_{rk}th entry $R(n_{rk}, n_{rk})$ is already very tiny compared with $R(1,1)$. It seems that the numerical rank n_{rk} provided by the online database is a bit arbitrary, for example, when there is no obvious gap in the singular values, but we still use this n_{rk} for consistency with the database. Please note that the ratios $R(n_{rk}+1, n_{rk}+1)/R(n_{rk}, n_{rk})$ for seven matrices numbered 34, 46, 73, 82, 142, 253, and 254 are zeros, and they are left blank in the bottom plot of Figure 5. The matrices numbered 46, 253, 254 are CH7-7-B1, DWG961A, IG5-10, respectively; the other four are given before.

To derive the estimate (4.5), we assume that $R_{22} = O(\epsilon)$. This is checked in the top plot of Figure 6, where we can see that $||R_{22}||/||R||$ is of the order $O(10^{-15})$ for most cases. The formula (4.5) is slightly modified by a factor $1 + ||X||$, where $X = R_{11}^{-1} R_{12}$. The norm of X is checked in the middle plot of Figure 6. The bounds for trustworthiness $\min_{i=1:n_{rk}}\{\frac{|R(i,i)|}{\epsilon||(A\Pi)(:,i)||_2}\}$ for each case are displayed in the bottom plot of Figure 6.

The monotonicities of the R-values for these 261 test cases are checked in Figure 7; that is, for each case we use three methods (QRCP, CARRQR-B, and CARRQR-F) to obtain the R-factors and compute the ratios $R(i+1, i+1)/R(i,i)$, where

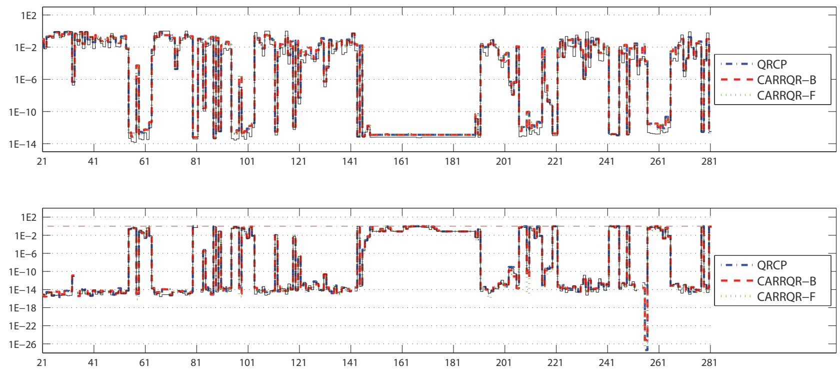


FIG. 5. *The gaps in R-values and singular values. Top:* $|R(n_{rk}, n_{rk})|/|R(1,1)|$*, where the R-factors are obtained by QRCP, CARRQR-B, and CARRQR-F, respectively. The solid black line stands for the ratio* $\sigma(n_{rk})/\sigma(1)$*. Bottom:* $|R(n_{rk}+1, n_{rk}+1)|/|R(n_{rk}, n_{rk})|$ *and* $\sigma(n_{rk}+1)/\sigma(n_{rk})$ *(represented by the solid line). The x-axis denotes the index of* 261 *matrices from the SJSU Singular Matrix Database.*

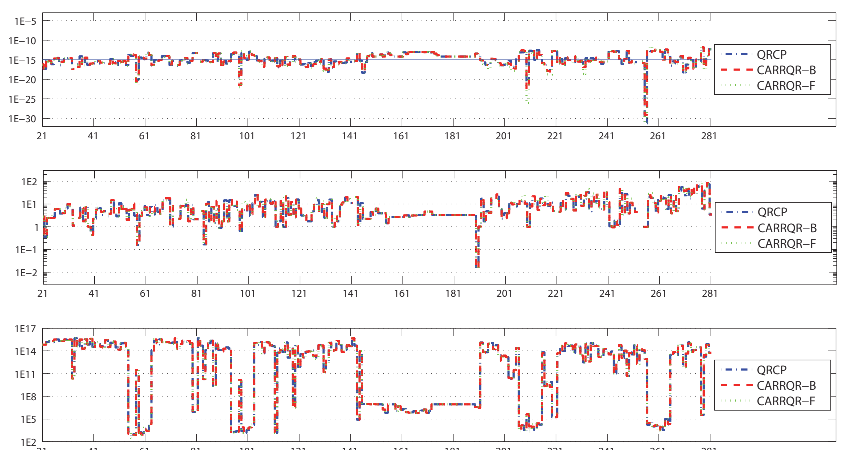


FIG. 6. *Top:* $||R_{22}||/||R||$*, where R is the R factor obtained from QRCP, CARRQR-B, or CARRQR-F, and* R_{22} *is its* (2,2) *block as defined by* (1.1)*. Middle:* $||X||$ *in* (4.5)*, where* $X = R_{11}^{-1}R_{12}$*. Bottom:* $\min_{i=1:n_{rk}}\{\frac{|R(i,i)|}{\epsilon||(A\Pi)(:,i)||_2}\}$*. The x-axis denotes the index of* 261 *matrices from the SJSU Singular Matrix Database.*

$i = 1, \ldots, n_{rk} - 1$. We note that there are very few ratios larger than 1 in Figure 7. The largest ratio appears in CARRQR-F and is 1.58, which corresponds to the matrix HEAT_1000.

5. Tournament pivoting for other factorizations. In this section we describe very briefly how the tournament pivoting can be extended to other factorizations that require some form of pivoting.

Cholesky with diagonal pivoting. Since QR with column pivoting applied to A is mathematically equivalent to Cholesky with diagonal pivoting applied to A^TA (in exact arithmetic), the same general techniques as for RRQR can be used in this

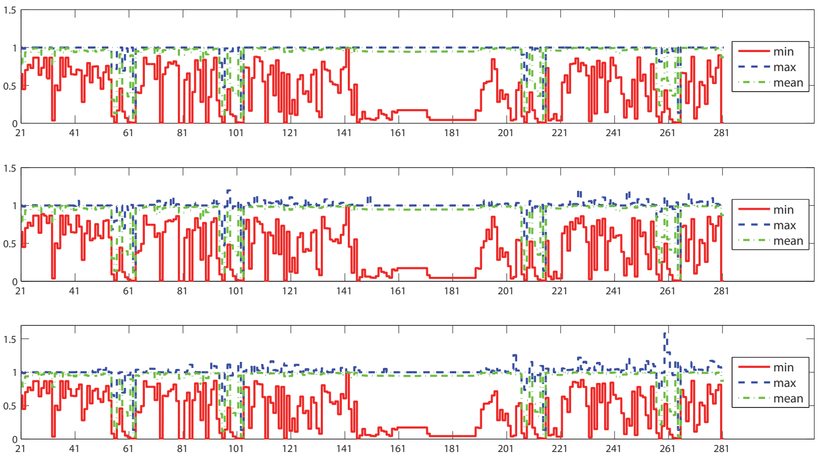


FIG. 7. *Minimum, maximum, and median of the ratios of successive R-values* $|R(i+1,i+1)|/|R(i,i)|$ *for* $i = 1, \ldots, n_{rk} - 1$*, and* n_{rk} *is the numerical rank of the matrix, which comes from the SJSU Singular Matrix Database. The R factor is obtained from QRCP (top plot), CARRQR-B (middle plot), and CARRQR-F (bottom plot).*

context. But now the leaves in our reduction tree are $b \times b$ diagonal subblocks of the symmetric positive-definite matrix H to which we want to apply Cholesky with pivoting, and at each internal node of the (binary) reduction tree we take the $2b \times 2b$ diagonal submatrix enclosing the two $b \times b$ matrices from the child nodes, and perform some kind of Cholesky with diagonal pivoting on this $2b \times 2b$ matrix to select the best $b \times b$ submatrix to pass up the tree.

Rank revealing decompositions of products/quotients of matrices. The goal is to compute an RRQR-like decomposition of an arbitrary product $P = A_1^{\pm 1} \cdot A_2^{\pm 1} \cdots A_k^{\pm 1}$ without actually multiplying or inverting any of the factors A_i. This problem arises, for example, in algorithms for eigenproblems and the SVD that either run asymptotically as fast as fast matrix multiplication ($O(n^\omega)$ for some $\omega < 3$) or minimize communication.

When $P = A_1$, the communication avoiding RRQR algorithm discussed in this paper can be used. But when $P = A_1^{-1}$, or $k > 1$ matrices are involved, the only solution available so far involves randomization, i.e., computing the regular QR decomposition of PV where V is a random orthogonal/unitary matrix. This can be obtained by computing only QR factorizations and multiplying by orthogonal matrices, and without multiplying or inverting other matrices, and so it is stable. The resulting factorization is of the form $P = Q\hat{R}V$ where V is random orthogonal, Q is orthogonal, and $\hat{R}$ is represented as a product of R factors and their inverses. The useful property is that the leading columns of Q do indeed span the desired subspaces with high probability. This approach is used for designing communication avoiding eigendecompositions and SVDs [2].

GECP - LU with complete pivoting. An approach for extending tournament pivoting to GECP is to perform each panel factorization as following. Tournament pivoting uses RRQR to pick the next best b columns to use, and then uses TSLU on these columns to pick their best b rows. Then the resulting $b \times b$ submatrix is permuted to the upper left corner of the matrix, and b steps of LU with no pivoting are performed. Then the process repeats on the trailing submatrix. The intuition is that by picking the best b columns, and then the best b rows from these columns, we are in effect picking the best $b \times b$ submatrix overall, which is then permuted to the upper left corner. The communication costs are clearly minimal, since the process just uses previously studied components.

LDL^T factorization with pivoting. The challenge here is preserving symmetry. A possible usage of tournament pivoting is the following:

1. Use the approach for GECP above to find the "best" $b \times b$ submatrix S of the symmetric matrix A, whether or not it is a principal submatrix (i.e., lies in the same set of b rows and b columns of A). If S is a principal submatrix, symmetrically permute it to lie in the first b rows and columns of A, and use it to perform b steps of symmetric LU without pivoting; otherwise continue to step 2.
2. Expand S to be a smallest-possible principal submatrix of A, called T. The dimension of T can be from $b+1$ up to $2b$, depending on how much S overlaps the diagonal of A.
3. Find a well-conditioned principal submatrix W of T of dimension d where $b \leq d \leq 2b$, permute it into the top left corner of A, and perform d steps of symmetric LU as above.

The conjecture is that such a well-conditioned principal submatrix W of T must exist. Here is a sketch of an algorithm for finding W. The b largest singular values of T are at least as large as the b singular values of S, by the interlacing property. Write the eigendecomposition $T = Q\Lambda Q^T = [Q_1, Q_2]\mathrm{diag}(\Lambda_1, \Lambda_2)[Q_1, Q_2]^T$ where Λ_1 has the large eigenvalues and Λ_2 has the small ones. Do GEPP on Q_1 to identify the most independent rows, and choose these as pivot rows determining W. The above sketch may serve to prove that a well-conditioned principal submatrix W exists, under the condition that there is a big enough gap in the eigenvalues of T. But we may prefer to simply do more conventional LDL^T factorization with pivoting to find it, instead of using an eigendecomposition as above.

Of course one reason for using LDL^T factorization instead of LU is that it traditionally takes half the storage and half the flops. It is not clear whether we can retain either of these advantages, or even how much the latter one still matters.

6. Conclusions. In this paper we introduce CARRQR, a communication optimal rank revealing QR factorization based on tournament pivoting. CARRQR does asymptotically less communication than the classic RRQR factorization based on column pivoting, at the cost of performing a factor of 3 more floating point operations. We have shown through extensive numerical experiments on challenging matrices that the CARRQR factorization reveals the rank similarly to the QR factorization with column pivoting and provides results close to the singular values computed with the highly accurate routine `dgesvj`. Our future work will focus on implementing CARRQR and studying its performance with respect to current implementations of QR with column pivoting available in LAPACK and ScaLAPACK. We have also outlined how tournament pivoting extends to a variety of other pivoted matrix factorizations, such as Cholesky with diagonal pivoting, LU with complete pivoting, or LDL^T factorization with pivoting.

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