Rank Revealing Gaussian Elimination by the
Maximum Volume Concept

Lukas Schork∗ Jacek Gondzio†

School of Mathematics, University of Edinburgh, Edinburgh EH9 3FD, Scotland, UK

Abstract

A Gaussian elimination algorithm is presented that reveals the numerical rank of
a matrix by yielding small entries in the Schur complement. The algorithm uses
the maximum volume concept to find a square nonsingular submatrix of maximum dimen-
sion. The bounds on the revealed singular values are similar to the best known bounds
for rank revealing $LU$ factorization, but in contrast to existing methods the algorithm
does not make use of the normal matrix. An implementation for dense matrices is de-
scribed whose computational cost is roughly twice the cost of an $LU$ factorization with
complete pivoting. Because of its flexibility in choosing pivot elements, the algorithm
is amenable to implementation with blocked memory access and for sparse matrices.

1 Introduction

This paper is concerned with the problem to determine the rank of a matrix in the numerical
sense. Given $A \in \mathbb{R}^{m \times n}$ and a tolerance $\varepsilon$, the task is to determine an index $r$ such that
$\sigma_r \geq \varepsilon$ and $\sigma_{r+1} = O(\varepsilon)$, where $\sigma_1 \geq \ldots \geq \sigma_d \geq \sigma_{d+1} := 0$ ($d = \min(m, n)$) are the singular
values of $A$. Our definition of numerical rank relaxes the condition $\sigma_r \geq \varepsilon > \sigma_{r+1}$ since the
latter can only be achieved by computing the singular values. Additionally to the rank $r$,
we want to identify an $r \times r$ submatrix of $A$ whose minimum singular value is not too much
smaller than $\sigma_r$.

It is well known that Gaussian elimination with complete pivoting may not detect a near
singularity. For the example from [7],

$$A = \begin{bmatrix}
1 & -1 & \cdots & -1 & -1 \\
1 & 1 & \cdots & \cdots & \cdots \\
\vdots & & 1 & -1 & 1 \\
1 & & & & 1
\end{bmatrix} \in \mathbb{R}^{m \times m}, \quad (1)
$$

complete pivoting allows to choose the diagonal elements as pivots, so that no eliminations
are needed and $A$ is determined to be of full rank. It is not revealed that $\sigma_m(A) = O(2^{-m})$
(see [6] Section 5) and the numerical rank of $A$ to be $m - 1$ for $m$ moderately large.

∗L.Schork@ed.ac.uk
†J.Gondzio@ed.ac.uk
The algorithm presented in this paper is based on Gaussian elimination and is rank revealing in the above definition. It finds a nonsingular submatrix $A_{11}$ of $A$ such that

$$\|A/A_{11}\|_C \leq \beta \quad \text{and} \quad \|A_{11}^{-1}\|_C \leq \beta^{-1}$$

for a given parameter $\beta > 0$. Here $\|\cdot\|_C$ is the maximum absolute entry of a matrix and $A/A_{11}$ is the Schur complement of $A_{11}$ in $A$. It will be shown that for $\beta = \max(m, n)\varepsilon$ the dimension of $A_{11}$ reveals the numerical rank of $A$. A lower bound on the minimum singular value of $A_{11}$ will be derived in terms of $\sigma_r(A)$. Applied to the matrix (1), the algorithm selects the upper right $(m-1) \times (m-1)$ block as $A_{11}$ for which $\|A/A_{11}\|_C = O(2^{-m})$ and $\sigma_{\min}(A_{11}) \approx \sigma_{m-1}(A)$.

To find $A_{11}$, the algorithm selects an $m \times m$ basis matrix $A_B$ of local maximum volume in $A = \begin{bmatrix} A & \beta I_m \end{bmatrix}$, where $I_m$ is the identity matrix of dimension $m$. The concept of maximum volume has been used before in rank revealing factorizations and related topics, see [6, 5, 4] and the references therein. The novelty of our algorithm is to work on the matrix $A_B$ rather than $A$ itself. $A_{11}$ will be defined by means of the columns of $A$ and the columns of $\beta I_m$ which compose $A_B$. It will be shown that $\|A/A_{11}\|_2$ and $\sigma_{\min}(A_{11})$ satisfy bounds in terms of the singular values of $A$ that are very similar to the best known bounds for the rank revealing $LU$ factorization [6].

A rank revealing factorization based on the maximum volume concept that yields a square nonsingular submatrix has also been derived by Pan [6]. Pan’s method first chooses a column subset of $A$ by utilizing the normal matrix $A^TA$, and then chooses a square submatrix within these columns. A detailed comparison to our method is given. While the resulting submatrices have the same rank revealing properties, an advantage of our method is not to use the normal matrix but instead to use pivot operations on $A_B$ only. This is particularly relevant with regard to an implementation for sparse matrices.

An implementation of the proposed algorithm for dense matrices is described. It requires roughly twice the computational cost than an $LU$ factorization of $A_B$ with complete pivoting. Comparisons to the singular value decomposition on a set of rank deficient matrices show that the rank detection is reliable and that the condition number of the selected submatrices is close to $\sigma_1(A)/\sigma_r(A)$.

Throughout the paper $A$ is an $m \times n$ matrix and $A_{11}$ is a square nonsingular submatrix. It is assumed that $A$ has been permuted so that

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

(2)

The Schur complement of $A_{11}$ in $A$ is

$$A/A_{11} = A_{22} - A_{21}A_{11}^{-1}A_{12}.$$  

$\sigma_k(\cdot)$ denotes the $k$-th singular value of a matrix, where the singular values are ordered nonincreasingly. $\|\cdot\|_2$ and $\|\cdot\|_C$ are the maximum singular value and the maximum absolute entry norm of a matrix. They satisfy the relation

$$\|A\|_C \leq \|A\|_2 \leq \sqrt{mn} \|A\|_C.$$  

For an index set $J$, $A_J$ is the matrix composed of the columns of $A$ indexed by $J$. A basis $B$ for $A \in \mathbb{R}^{m \times (n+m)}$ is an index set such that the basis matrix $A_B$ is square and nonsingular (requiring that $A$ has rank $m$). Associated with $B$ is the nonbasic set $N = \{1, \ldots, n+m\} \setminus B$. Vectors are notated in bold lower case, where $e_j$ is the $j$-th unit vector. Expression like $|A|$ and $|b|$ are meant componentwise.
2 Maximum Volume Concept

The volume of a matrix of arbitrary dimension and rank is introduced in [1]. This paper uses the definition from [6], which differs in that the volume of a rank deficient matrix is zero.

**Definition 2.1.** For $A \in \mathbb{R}^{m \times n}$ with singular values $\sigma_1 \geq \ldots \geq \sigma_d \geq 0$ $(d = \min(m, n))$, the volume of $A$ is defined by

$$\text{vol}(A) = \sigma_1 \cdots \sigma_d.$$ 

In particular, the volume of a square matrix is the absolute value of its determinant.

**Definition 2.2.** Let $A \in \mathbb{R}^{m \times n}$ and $\rho \geq 1$.

(i) Let $B$ be a $k \times k$ submatrix of $A$. $\text{vol}(B) (\neq 0)$ is said to be a **global $\rho$-maximum volume** in $A$ if

$$\rho \text{vol}(B) \geq \text{vol}(B')$$

for all $k \times k$ submatrices $B'$ of $A$.

(ii) Let $B$ be formed by $k$ columns (rows) of $A$. $\text{vol}(B) (\neq 0)$ is said to be a **local $\rho$-maximum volume** in $A$ if (3) holds for any $B'$ that is obtained by replacing one column (row) of $B$ by a column (row) of $A$ which is not in $B$.

(iii) Let $B$ be a $k \times k$ submatrix $(k < \min(m, n))$ of $A$. $\text{vol}(B) (\neq 0)$ is said to be a **local $\rho$-maximum volume** in $A$ if it is a global $\rho$-maximum volume in all $(k + 1) \times (k + 1)$ submatrices of $A$ which contain $B$.

The important concept in the theory of rank revealing factorizations is the local maximum volume. The definition 2.2(ii) is from [6] and 2.2(iii) is the natural extension to square submatrices of any dimension. It is equivalent to saying that $A_{11}$ has local $\rho$-maximum volume in (2) if the volume of the $(1, 1)$ block cannot be increased by more than a factor $\rho$ by interchanging two columns and/or two rows.

Finding a submatrix of local maximum volume will make use of column and row exchanges. The following lemmas provide formulas for the change of volume when a column and/or row is replaced in a square nonsingular matrix.

**Lemma 2.3.** Let $A_{11}$ be $k \times k$ nonsingular and $A'_{11}$ be obtained by replacing column $j$ by the vector $b$. Then

$$\frac{\text{vol}(A'_{11})}{\text{vol}(A_{11})} = |A_{11}^{-1}b|_j.$$

In particular, $A_{11}$ in (2) has local $\rho$-maximum volume in its block row and block column if and only if $\|A_{11}^{-1}A_{12}\|_C \leq \rho$ and $\|A_{21}A_{11}^{-1}\|_C \leq \rho$, respectively.

**Proof.**

$$A'_{11} = A_{11} - A_{11}e_j e_j^T + be_j^T = A_{11}(I_k - e_j e_j^T + A_{11}^{-1}be_j^T).$$

The expression in parenthesis is the identity matrix with column $j$ replaced by $A_{11}^{-1}b$. Therefore

$$\det(A'_{11}) = \det(A_{11}) \det(I_k - e_j e_j^T + A_{11}^{-1}be_j^T) = \det(A_{11})(A_{11}^{-1}b)_j$$

and taking absolute values completes the proof.

Lemma 2.4. Let $\hat{A}$ be square and nonsingular and $B$ be obtained by removing row $i$ and column $j$. Then
\[
\frac{\text{vol}(B)}{\text{vol}(\hat{A})} = |\hat{A}^{-1}|_{j,i}.
\]
In particular, $B$ has $\rho$-maximum volume in $\hat{A}$ if and only if $\rho |\hat{A}^{-1}|_{j,i} \geq \|\hat{A}^{-1}\|_C$.

Proof. By Cramer’s rule
\[
(\hat{A}^{-1})_{j,i} = \frac{\det(\hat{A} - \hat{A}e_j e_i^T + e_i e_j^T)}{\det(\hat{A})}.
\]
Since the matrix whose determinant is taken in the numerator has unit column $e_i$ in position $j$, by Laplace’s formula
\[
\det(\hat{A} - \hat{A}e_j e_i^T + e_i e_j^T) = (-1)^{i+j} \det(B).
\]
Substituting into the previous expression and taking absolute values completes the proof. 

Lemma 2.5. Let $A_{11}$ be $k \times k$ nonsingular and
\[
\hat{A} = \begin{bmatrix} A_{11} & b \\ c^T & \alpha \end{bmatrix}.
\] (4)

Let $\gamma = \hat{A}/A_{11}$ and $A''_{11}$ be the leading $k \times k$ block of $\hat{A}$ after interchanging columns $k+1$ and $j$ ($1 \leq j \leq k$) and rows $k+1$ and $i$ ($1 \leq i \leq k$). Then
\[
\frac{\text{vol}(A''_{11})}{\text{vol}(A_{11})} = |\gamma (A^{-1}_{11})_{j,i} + (A^{-1}_{11} b)_j (A^{-T}_{11} c)_i|.
\] (5)

Proof. Firstly consider that $\hat{A}$ is singular, in which case $\text{rank}(\hat{A}) = k$ and $\gamma = 0$. If $|A^{-1}_{11} b|_j = 0$, then the first $k$ columns of $\hat{A}$ after the interchanges have rank $k-1$. Hence $A''_{11}$ must be singular and both sides of (5) are zero. Otherwise let $A'_{11}$ be obtained from $A_{11}$ by replacing column $j$ by the vector $b$. Then, by Lemma 2.4
\[
\text{vol}(A'_{11}) = \text{vol}(A_{11}) |A^{-1}_{11} b|_j.
\]
Let $c'$ be obtained from $c$ by replacing the $j$-th entry by $\alpha$. Because $\hat{A}$ is singular,
\[
(A'_{11})^{-T} c' = A^{-T}_{11} c.
\]
Therefore, by Lemma 2.8
\[
\text{vol}(A''_{11}) = \text{vol}(A'_{11}) |(A'_{11})^{-T} c'|_i
= \text{vol}(A_{11}) |A^{-1}_{11} b|_j |A^{-T}_{11} c|_i.
\]

Secondly consider that $\hat{A}$ is nonsingular, in which case $\gamma \neq 0$. Then
\[
\hat{A}^{-1} = \begin{bmatrix} H & f \\ g^T & \gamma^{-1} \end{bmatrix},
\] (6)
where
\[
f = -\gamma^{-1} A^{-1}_{11} b,
\]
\[
g = -\gamma^{-1} A^{-T}_{11} c,
\]
\[
H = A^{-1}_{11} + \gamma fg^T.
\]
It follows from Lemma 2.4 that
\[
\text{vol}(A_{11}) = |\gamma^{-1}| \text{vol}(\hat{A}),
\]
\[
\text{vol}(A''_{11}) = |H_{j,i}| \text{vol}(\hat{A}).
\]

Therefore
\[
\frac{\text{vol}(A''_{11})}{\text{vol}(A_{11})} = \frac{|(A_{11}^{-1})_{j,i} + \gamma^{-1}(A_{11}^{-1}b_j)(A_{11}^{-1}Tc)_i|}{|\gamma^{-1}|} = |(A_{11}^{-1})_{j,i} + (A_{11}^{-1}b_j)(A_{11}^{-1}Tc)_i|.
\]

\[\blacksquare\]

3 Rank Revealing Algorithm

This section presents the algorithm for selecting the submatrix $A_{11}$ whose dimension reveals the numerical rank of $A$. Instead of selecting the row and column subsets directly, the algorithm selects a basis matrix of $A = [A \ \beta I_m]$. The columns of $A$ and $\beta I_m$ in $A$ are termed structural and logical, respectively. Assume that $B, N$ is a basic-nonbasic partitioning of the columns of $A$ and

\[
A_B = \begin{bmatrix} A_{11} & 0 \\ A_{21} & \beta I_{m-k} \end{bmatrix}, \quad A_N = \begin{bmatrix} A_{12} & \beta I_k \\ A_{22} & 0 \end{bmatrix},
\]

(7)

where the rightmost $m - k$ and $k$ columns of $A_B$ and $A_N$ are logical (the indices in $B$ and $N$ can always be permuted to obtain that form). The partitioning uniquely determines $A_{11}$. Therefore any basis for $A$ determines a square nonsingular $A_{11}$.

To obtain $A_{11}$ with the desired properties, it will turn out that $A_B$ must have local $\rho$-maximum volume in $A$. An algorithm for finding a basis matrix of local maximum volume is given in [4]. Algorithm 1 is a generic version that leaves some flexibility to the implementation by not specifying how to choose $(p, q)$ in line 8 in case there is more than one candidate. In particular, it is not necessary to scan the entire matrix $A_B^{-1}A_N$ in every iteration or even to compute it explicitly.

Algorithm 1 find_submatrix

Require: $A \in \mathbb{R}^{m \times n}$, $\rho \geq 1$, $\beta > 0$
1: Build $A = [A \ \beta I_m]$
2: Initialize $B = \{n + 1, \ldots, n + m\}$, $N = \{1, \ldots, n\}$
3: loop
4: Let $M = A_B^{-1}A_N$
5: if $\|M\|_C \leq \rho$ then
6: Stop
7: end if
8: Choose $(p, q)$ such that $|M|_{p,q} > \rho$
9: $B_p \leftarrow N_q$
10: end loop
11: Build $A_{11}$ from (7)
12: Let $r$ be the dimension of $A_{11}$
Lemma 3.1. Algorithm \[ \text{[1]} \] terminates in a finite number of iterations. The resulting \( A_{11} \)
has local \((2\rho^2)\)-maximum volume in \( A \) and
\[
\|A/A_{11}\|_C \leq \rho \beta, \quad \|A_{11}^{-1}\|_C \leq \rho \beta^{-1}. \tag{8}
\]

Proof. Each basis update in Algorithm \[ \text{[1]} \] increases the volume of \( A_B \) by a factor greater than 1. Therefore a basis cannot repeat and the algorithm terminates in a finite number of iterations. When the algorithm terminates, all entries of
\[
A_B^{-1} A_N = \begin{bmatrix}
A_{11}^{-1} A_{12} & \beta A_{11}^{-1} \\
\beta^{-1} A/A_{11} & -A_{21} A_{11}^{-1}
\end{bmatrix}
\]
are bounded by \( \rho \) in absolute value. This means that \( A_{11} \) has local \( \rho \)-maximum volume in its block row and block column, and \( \|A/A_{11}\|_C \leq \rho \beta \) and \( \|A_{11}^{-1}\|_C \leq \rho \beta^{-1} \). If \( r = m \) (i.e. \( B \) contains only structural columns), then \( A_{11} \) has local \( \rho \)-maximum volume in \( A \). Otherwise consider any submatrix of \( A \) of the form \[ \text{[4]} \]. The right-hand side in \[ \text{[5]} \] is bounded by
\[
|\gamma (A_{11}^{-1})_{j,i} + (A_{11}^{-1} b_j) (A_{11}^{-T} c)_i| \leq \rho \beta \rho \beta^{-1} + \rho = \rho^2.
\]
Therefore \( A_{11} \) has local \((2\rho^2)\)-maximum volume in \( A \). \[ \square \]

The numerical rank of \( A \) is determined by Algorithm \[ \text{[1]} \] as the dimension of \( A_{11} \). It follows from the interlacing property of the singular values \[ \text{[3]} \] Corollary 8.6.3 that for any \( k \times k \) submatrix \( B \) of \( A \),
\[
\|B^{-1}\|_C \geq \frac{1}{k} \|B^{-1}\|_2 = \frac{1}{k \sigma_{\min}(B)} \geq \frac{1}{k \sigma_k(A)}.
\]
If we choose \( \beta \geq \max(m, n) \varepsilon \rho \) in Algorithm \[ \text{[1]} \] then it is guaranteed that
\[
\frac{1}{r \sigma_r(A)} \leq \|A_{11}^{-1}\|_C \leq \frac{1}{\max(m, n) \varepsilon}
\]
and therefore \( \sigma_r(A) \geq \varepsilon \) as desired. (Using \( \min(m, n) \) instead of \( \max(m, n) \) would be sufficient.) On the other hand, from \[ \text{[6]} \] Theorem 2.7,
\[
\|A/B\|_2 \geq \sigma_{k+1}(A)
\]
for any \( k \times k \) submatrix \( B \) of \( A \). Therefore
\[
\sigma_{k+1}(A) \leq \|A/A_{11}\|_C \sqrt{(m-r)(n-r)} = \beta \rho \sqrt{(m-r)(n-r)}.
\]
In contrast to the singular value decomposition, Algorithm \[ \text{[1]} \] cannot determine \( r \) such that \( \sigma_r(A) \geq \varepsilon > \sigma_{r+1}(A) \). It can only guarantee the first inequality and a bound on \( \sigma_{r+1}(A) \) in terms of \( \varepsilon \) and the dimension of \( A \). In our definition this is sufficient for a rank revealing factorization. In practice, a reasonable choice for \( \beta \) might be
\[
\beta = \max(m, n) \varepsilon_{\text{mach}} \|A\|_C,
\tag{10}
\]
where \( \varepsilon_{\text{mach}} \) is the relative machine precision.

4 Bounds on \( \sigma_{\min}(A_{11}) \) and \( \|A/A_{11}\|_2 \)

The discussion so far has shown that \( A_{11} \) that satisfies \[ \text{[8]} \] reveals the numerical rank of \( A \). It remains to be shown that the minimum singular value of \( A_{11} \) is close to \( \sigma_r(A) \) for \( A_{11} \) obtained from Algorithm \[ \text{[1]} \] this section derives bounds on \( \sigma_{\min}(A_{11}) \) and \( \|A/A_{11}\|_2 \) in terms of the singular values of \( A \) that hold for any local maximum volume submatrix. More specifically, the following theorem is proved.
Theorem 4.1. Let $A_{11}$ be $k \times k$ nonsingular and have local $(2\rho^2)$-maximum volume in $A$. Then
\[
\sigma_k(A) \geq \sigma_{\min}(A_{11}) \geq \frac{1}{2\rho^2 k \sqrt{(m-k+1)(n-k+1)}} \sigma_k(A),
\]
\[
\sigma_{k+1}(A) \leq \|A/A_{11}\|_2 \leq 2\rho^2(k+1)\sqrt{(m-k)(n-k)}\sigma_{k+1}(A).
\]

The first inequalities in (11) and (12) hold true for any $k \times k$ submatrix of $A$, whereas the second inequalities require the maximum volume property. (12) is proved in [5] under the assumption that $A_{11}$ has global $\rho$-maximum volume in $A$. Interestingly, the proof given there goes through unchanged if $A_{11}$ has local $\rho$-maximum volume as defined in this paper. The proof is given for completeness. The proof for (11) is new to the authors.

Lemma 4.2. Let $A \in \mathbb{R}^{m \times n}$ and $A_{11}$ be a nonsingular $k \times k$ submatrix ($k < \min(m,n)$) of local $\rho$-maximum volume. Then
\[
\|A/A_{11}\|_C \leq \rho(k+1)\sigma_{k+1}(A).
\]

Proof (from [5]). Consider any $(k+1) \times (k+1)$ submatrix of $A$ of the form
\[
\hat{A} = \begin{bmatrix} A_{11} & b \\ c^T & \alpha \end{bmatrix}.
\]

Then $\gamma = \alpha - c^T A_{11}^{-1} b$ is an entry of $A/A_{11}$ and each entry of $A/A_{11}$ has this form for a particular $\hat{A}$. Therefore it suffices to show that $|\gamma| \leq \rho(k+1)\sigma_{k+1}(A)$.

If $\hat{A}$ is singular, then $\gamma = 0$ and the claim is trivial. Otherwise, because $A_{11}$ has $\rho$-maximum volume in $\hat{A}$, by Lemma 2.4 and (11),
\[
\rho|\gamma^{-1}| \geq \|\hat{A}^{-1}\|_C.
\]

It follows that
\[
|\gamma| \leq \rho \frac{1}{\|\hat{A}^{-1}\|_C} \leq \rho \frac{k+1}{\|\hat{A}^{-1}\|_2} = \rho(k+1)\sigma_{k+1}(\hat{A}) \leq \rho(k+1)\sigma_{k+1}(A),
\]
where the last inequality comes from the interlacing property of singular values [3 Corollary 8.6.3].

Corollary 4.3. Let $A \in \mathbb{R}^{m \times n}$ and $A_{11}$ be a nonsingular $k \times k$ submatrix ($k < \min(m,n)$) of local $\rho$-maximum volume. Then
\[
\sigma_{k+1}(A) \leq \|A/A_{11}\|_2 \leq \rho(k+1)\sqrt{(m-k)(n-k)}\sigma_{k+1}(A).
\]

Proof. The first inequality is proved in [5] Theorem 2.7. The second inequality follows from Lemma 4.2.

Lemma 4.4. Let $A \in \mathbb{R}^{m \times n}$ and $A_{11}$ be a nonsingular $k \times k$ submatrix of local $\rho$-maximum volume. Then
\[
\sigma_k(A) \leq \rho k \sqrt{(m-k+1)(n-k+1)}\sigma_k(A_{11}).
\]

Proof. If $k = 1$, then $A_{11}$ is scalar and because of local $\rho$-maximum volume it satisfies $\rho|A_{11}| \geq \|A\|_C$. Therefore
\[
\sigma_1(A) \leq \sqrt{mn} \|A\|_C \leq \sqrt{mn}\rho|A_{11}| = \rho\sqrt{mn}\sigma_1(A_{11}).
\]
If $k > 1$, let $B$ be a $(k - 1) \times (k - 1)$ submatrix of $A_{11}$ with maximum volume in $A_{11}$. In particular $B$ is nonsingular. Consider any $k \times k$ submatrix of $A$ of the form

$$A''_{11} = \begin{bmatrix} B & b \\ c^T & \alpha \end{bmatrix}.$$ 

Because $A''_{11}$ differs from $A_{11}$ by at most one row and one column, and because $A_{11}$ has local $\rho$-maximum volume in $A$,

$$\rho \text{vol}(A_{11}) \geq \text{vol}(A''_{11}).$$

From the determinant property of the Schur complement,

$$\det(A_{11}) = \det(B) \det(A_{11}/B),$$

it follows that

$$\rho |A_{11}/B| = \rho \frac{\text{vol}(A_{11})}{\text{vol}(B)} \geq \frac{\text{vol}(A''_{11})}{\text{vol}(B)} = |A''_{11}/B|.$$ 

Since $A''_{11}/B$ is an entry of $A/B$ and each entry of $A/B$ has this form for a particular $A''_{11}$, it follows that

$$\rho |A_{11}/B| \geq \|A/B\|_C.$$ 

Therefore

$$\sigma_k(A) \leq \|A/B\|_2 \leq \sqrt{(m - k + 1)(n - k + 1)} \|A/B\|_C$$

$$\leq \rho \sqrt{(m - k + 1)(n - k + 1)} |A_{11}/B|$$

$$\leq \rho \sqrt{(m - k + 1)(n - k + 1)} k \sigma_k(A_{11}),$$

where the first inequality is from [6, Theorem 2.7] and the last inequality from Lemma 4.2 and the fact that $B$ has maximum volume in $A_{11}$.

\[ \square \]

**Corollary 4.5.** Let $A \in \mathbb{R}^{m \times n}$ and $A_{11}$ be a nonsingular $k \times k$ submatrix of local $\rho$-maximum volume. Then

$$\sigma_k(A) \geq \sigma_{\min}(A_{11}) \geq \frac{1}{\rho k \sqrt{(m - k + 1)(n - k + 1)}} \sigma_k(A).$$

\[ \text{Proof.} \] The first inequality comes from the interlacing property of singular values [3, Corollary 8.6.3]. The second inequality follows from Lemma 4.4 \[ \square \]

Theorem 4.1 follows from Corollaries 4.5 and 4.3.

**5 Comparison to Pan’s Method**

Pan [6] uses the maximum volume concept in a rank revealing factorization algorithm based on Gaussian elimination, which yields a submatrix $A_{11}$ that has very similar properties to the submatrix obtained from Algorithm 1. This section compares the two methods regarding their use of the maximum volume property and possible implementations.

Given $A \in \mathbb{R}^{m \times n}$, $\rho \geq 1$ and $k \leq \text{rank}(A)$, Pan’s method first chooses an $m \times k$ submatrix $A_{J\gamma}$ of local $\rho$-maximum volume in $A$, and then a $k \times k$ submatrix $A_{11}$ of local $\rho$-maximum volume in $A_{J\gamma}$. We say that $A_{11}$ has *normal $\rho$-maximum volume* in $A$ to distinguish it from
our definition of local maximum volume. Theorem 3.8 in [6] proves the following bounds on
the singular values for $m = n$, which are almost identical to those in Theorem 4.1:

$$
\sigma_k(A) \geq \sigma_{\min}(A_{11}) \geq \frac{1}{k(n-k)\rho^2 + 1}\sigma_k(A),
$$

$$
\sigma_{k+1}(A) \leq \|A/A_{11}\|_2 \leq (k(n-k)\rho^2 + 1)\sigma_{k+1}(A).
$$

Pan’s method uses the normal matrix $A^TA$ to find a column subset of local $\rho$-maximum
volume in $A$. The algorithm applies symmetric row and column interchanges to $A^TA$ until
the volume of the leading $k \times k$ block cannot be increased by more than a factor $\rho$ when
interchanging one row and column. The second step of Pan’s method, finding a $k \times k$
submatrix of local $\rho$-maximum volume in $A_J$, is the same task as finding the submatrix $A_B$
in our method. The setting in [6] assumes the dimension of $A_{11}$ to be given. However, choosing
it dynamically by means of a tolerance $\beta$ as in Algorithm 1 can be easily incorporated into
the algorithm for finding the column subset $J$. Therefore Pan’s method and our method
provide the same functionality.

We consider it an advantage of our method not to use the normal matrix, but instead
to work with the augmented matrix $A$. For sparse matrices forming and factorizing $A_J^TA_J$
usually leads to more fill-in and can be much more expensive than factorizing $A_B$.

It will be shown by two examples that normal maximum volume and local maximum
volume are different properties and neither implies the other. First, consider

$$
A = \begin{bmatrix}
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & 1
\end{bmatrix}
$$

and let $A_{11}$ be the leading $3 \times 3$ block. It can be computed analytically that the singular
values of any three columns of $A$ are $(\sqrt{5}, \sqrt{2}, \sqrt{2})$, so that the first three columns have local
maximum volume in $A$. From Lemma 2.3 it is obvious that $A_{11}$ has local maximum volume
within the first three columns. Hence it has normal maximum volume in $A$. However, it can
be verified from Lemma 2.5 that $A_{11}$ does not have maximum volume in the leading $4 \times 4$
block and therefore does not have local maximum volume in $A$.

For the opposite part consider

$$
A = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
d & -1 & -d \\
-1 & d & -d
\end{bmatrix}
$$

with $d = 0.99$ and let $A_{11}$ be the leading $2 \times 2$ block. It can be verified from Lemma 2.5 that
$A_{11}$ has local maximum volume in $A$. By computing singular values we obtain the volume
of the matrix composed of columns 1 and 2 to be 2.2272 and the volume of the matrix
composed of columns 1 and 3 to be 2.4169. Hence the first two columns do not have local
maximum volume in $A$, and $A_{11}$ does not have normal maximum volume in $A$.

More insight into the difference between normal and local maximum volume is obtained
from the characterization [1, Example 2.1] of the volume of a rectangular matrix. Let
$A_{\mathcal{J}} \in \mathbb{R}^{m \times k}$ have rank $k$. Then

$$\text{vol}(A_{\mathcal{J}}) = \left( \sum_B \text{vol}(B)^2 \right)^{1/2},$$

where the sum runs over all nonsingular $k \times k$ submatrices of $A_{\mathcal{J}}$. Hence a subset of $k$ columns has local maximum volume in $A \in \mathbb{R}^{m \times n}$ if exchanging a column does not increase the “Euclidean mean” volume of its $k \times k$ submatrices. In contrast, let $A_{11}$ have local maximum volume in $A$ and $A_{\mathcal{J}}$ be the column subset that contains $A_{11}$. Then exchanging a column of $A_{\mathcal{J}}$ does not increase $\text{vol}(A_{11})$ or $\text{vol}(B)$ for any $B$ that is neighbour to $A_{11}$ (i.e. $B$ is obtained by replacing one row of $A_{11}$ by a row of $A_{\mathcal{J}}$ not in $A_{11}$). This property is an immediate consequence of the definition of local maximum volume.

Let $A_{21}$ denote the lower left $2 \times 2$ block in (13), which is not neighbour to $A_{11}$. Exchanging columns 2 and 3 in $A$ changes the volume of $A_{21}$ by a factor

$$\frac{\text{vol}\left(\begin{bmatrix} d & -d \\ -1 & -d \end{bmatrix}\right)}{\text{vol}\left(\begin{bmatrix} d & -1 \\ -1 & d \end{bmatrix}\right)} = 99$$

and also increases the Euclidean mean volume of the $2 \times 2$ submatrix of $A_{\mathcal{J}}$. Therefore the first two columns do not have local maximum volume in $A$.

### 6 Implementation and Results

We have implemented a simplicial version of Algorithm 1 in C code\(^1\). By “simplicial” we mean that the implementation does not work on block submatrices and makes no use of optimized BLAS. It therefore is slower than an optimized singular value decomposition. Our interest is to examine the number of pivot operations required and to verify the reliability of the method. Discussing an optimized implementation is beyond the scope of the paper.

Initially the matrix $W = [A \mid I_m]$ is stored. The logical columns are not explicitly scaled by $\beta$ to avoid values with very different order of magnitude in the computation. Instead multiplications with $\beta$ and $\beta^{-1}$ are applied on the fly when logical columns are involved.

In each iteration the algorithm chooses a pivot element in the following order:

(i) If $|W|$ has entries corresponding to block $A_{11}^{-1}$ in (9) that are larger than $\rho \beta^{-1}$, then the maximum such entry is chosen as pivot.

(ii) If $|W|$ has entries corresponding to block $A_{11}^{-1}A_{12}$ or $-A_{21}A_{11}^{-1}$ in (9) that are larger than $\rho$, then the maximum such entry is chosen as pivot.

(iii) If $|W|$ has entries corresponding to block $A/A_{11}$ in (9) that are larger than $\rho \beta$, then the maximum such entry is chosen as pivot.

The reason behind the order of choosing a pivot element is to prefer having logical columns in the basis for numerical stability. If a pivot is found, then its column is transformed into a unit column by applying row operations to $W$. If none of the cases (i)–(iii) yields a pivot element, the algorithm terminates.

The new rank revealing Gaussian elimination algorithm (RRGE) is evaluated on matrices from the San Jose State University Singular Matrix Database \(^2\). We use the 327 matrices (as of January 2018) for which $\min(m, n) \leq 1000$. The matrices are transposed if necessary so that $m \leq n$. The parameters used are $\rho = 2.0$ and $\beta$ as in (14). For comparison a singular

\(^1\)http://www.maths.ed.ac.uk/ERGO/LURank

\(^2\)http://www.maths.ed.ac.uk/ERGO/SingularMatrixDatabase
56 matrices with ill-defined rank

Figure 1: Ratios $\sigma_r(A)/\sigma_s(A)$ ("+"") and $\sigma_{r+1}(A)/\sigma_{s+1}(A)$ ("o") for matrices with $r \neq s$. The "o" marker is missing when $r = m$ (7 matrices).

value decomposition (SVD) of $A$ is computed and the numerical rank of $A$ is determined as the largest index $s$ such that

$$\sigma_s(A) \geq \max(m, n) \varepsilon_{\text{mach}} \sigma_1(A).$$

(14)

All matrices in the test set are rank deficient by means of (14).

For 56 matrices the numerical ranks determined by SVD and RRGE differ. This is legitimate if there is no large gap between any two consecutive singular values. To verify that the rank $r$ determined by RRGE is acceptable with respect to the singular values of $A$, Figure 1 shows the ratios $\sigma_r(A)/\sigma_s(A)$ and $\sigma_{r+1}(A)/\sigma_{s+1}(A)$ for those matrices where $r \neq s$. Since the ratios are not too far away from 1.0, it can be concluded that $\sigma_{r+1}(A) = \mathcal{O}(\sigma_{s+1}(A))$ and $\sigma_r(A) = \Omega(\sigma_s(A))$ and therefore the rank determined by RRGE is "correct" for all matrices in the test set.

Table 1 categorizes the 327 matrices into buckets by means of $\sigma_r(A_{11})/\sigma_r(A)$ and by the number of pivot operations required by RRGE. In most cases $\sigma_r(A_{11})$ is much closer to $\sigma_r(A)$ than Corollary 4.5 guarantees. Because our implementation starts from the all logical basis, a minimum of $r$ pivots is required. For $\rho = 2.0$ the number of pivots is almost always within 5% of the optimum. The computational cost for RRGE is roughly twice the cost of an LU factorization of $A$ with complete pivoting. For $\rho = 1.1$ the number of pivots significantly increases on many matrices, but the ratios $\sigma_r(A_{11})/\sigma_r(A)$ do not improve relevantly.

7 Conclusions

We have presented an algorithm for revealing the numerical rank of $A$ by Gaussian elimination on the matrix $[A \ \beta l_m]$. The bounds on the revealed singular values are very similar
\[ \frac{\sigma_r(A_{11})}{\sigma_r(A)} \]

| \(\rho = 2.0\) | \(\rho = 1.1\) | \(\text{pivots/r}\) |
|-----------------|-----------------|-----------------|
| \(10^{-1}, 10^0\) | 252              | 255             | [1.00, 1.05] | 325 | 159 |
| \(10^{-2}, 10^{-1}\) | 60              | 69             | [1.05, 1.50] | 2  | 124 |
| \(10^{-3}, 10^{-2}\) | 15              | 3               | [1.5, 4.0] | 0  | 37  |
|                  |                 |                 | [4.0, 5.0] | 0  | 7   |

Table 1: Matrices categorized by \(\sigma_r(A_{11})/\sigma_r(A)\) and by number of pivot operations.

to those given in [6], but our algorithm does not make use of the normal matrix. A prototype implementation has shown that the number of pivot operations required in practice is only slightly larger than the rank of \(A\). Because the algorithm allows some flexibility in choosing pivot elements, it can be implemented with blocked memory access to achieve high floating point performance. An advantage over the singular value decomposition is to obtain a square nonsingular submatrix and thereby a maximum set of linearly independent rows and columns. A rank revealing factorization for sparse matrices based on the results from this paper is a topic for further research.

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