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A Note on Subset Selection for Matrices

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Abstract
In an earlier papers the authors established a result to select subsets of a matrix that are as “non-singular” as possible in a numerical sense. The major result was not constructive. In this note we give a constructive proof and moreover a sharper bound.

1. Introduction

In [2] the problem of selecting $k$ rows from an $m \times n$ matrix such that the resulting matrix was as non-singular as possible was examined. That is, for $X \in \mathbb{R}^{m \times n}$ find a permutation matrix $P \in \mathbb{R}^{m \times m}$ so that

$$PX = \begin{bmatrix} A \\ B \end{bmatrix}, \quad A \in \mathbb{R}^{k \times n},$$

(1)

where $A$ is the matrix in question, $m, k > n$ and $\text{rank}(X) = n$.

To motivate this problem, consider the problem of regression where we have a vector of $n$ observations

$$y = A\theta + \delta,$$

where $A \in \mathbb{R}^{k \times n}$ is a design matrix whose rows are a subset of the rows of $X \in \mathbb{R}^{m \times n}$, $\theta \in \mathbb{R}^n$ is a vector of unknown parameters that is to be determined and $\delta \in \mathbb{R}^k$ is a vector whose components are independent and identically normally distributed. Such problems occur when observations are expensive and only a subset of all possible measurements is feasible. The least squares estimate of the unknown parameters is $\hat{\theta} = A^+y$ where $A^+$ is the Moore-Penrose inverse. For a given design matrix $A$ and confidence coefficient, the confidence ellipsoid for $\theta$ is given by $\left\{ \theta \left| \left( \theta - \hat{\theta} \right)^T A^T A \left( \theta - \hat{\theta} \right) \leq \text{constant} \right\}$. The content of this ellipsoid is proportional to $(\det A^T A)^{-\frac{1}{2}}$ and it is natural to make this as small as possible. That is, we choose the design matrix $A$ to maximise $\det A^T A$. Such designs are called D-optimal designs (see Silvey [5] for a more detailed discussion). However, optimality will depend on the application. For example minimising
\[ \|A^+\|_F = \sqrt{\text{Trace}(A^T A)^{-1}} \] ensures that the expected mean squared error of \( \theta \) is minimised. E-optimal designs (see Silvey [5]) maximise the smallest singular value of \( A \) (or equivalently, maximise \( \|A^+\|_2 = \|A^T A\|_2^{1/2} \)). Further applications are described in [2]

Row selection is often implemented using a QR decomposition of \( X^T \) with column interchange to maximize the size of the pivots (see [1] and also [3], section 12.2). This algorithm usually works well but there are examples [4, p31] where the pivot size does not adequately reflect the size of the singular values. As a consequence bounds from the analysis of such algorithms would lead to poor bounds for the singular values and related quantities such as \( \det A^T A \).

In [2] the present authors derived upper bound for \( \|A^+\|_F \) and the singular values of \( A \). In this note, we extend these results by deriving a constructive derivation for the bounds on the singular values and new lower bounds for \( \det A^T A \).

In section 2 we give the main results and in particular a sharper bound for \( \|A^+\|_F \). In section 3 we show that this bound is sharper than the one obtained earlier, at least asymptotically.

2. Results

We can rewrite (1) as

\[ PX = \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} Q \\ Y \end{bmatrix} (A^T A)^{1/2} \]  \hspace{1cm} (2)

where

\[ Q := A \left( A^T A \right)^{-1/2} \]

\[ Y := B \left( A^T A \right)^{-1/2} \]

It follows that,

\[ X^T X = \left( A^T A \right)^{1/2} \left( I + Y^T Y \right) \left( A^T A \right)^{1/2} \]

Thus

\[ \det(X^T X) = \det(I + Y^T Y) \det(A^T A) \]

(4)
and so maximising \( \det \mathbf{A}^T \mathbf{A} \) is equivalent to minimizing \( \det (\mathbf{I} + \mathbf{Y}^T \mathbf{Y}) \). From the arithmetic-geometric inequality we have

\[
\det (\mathbf{I} + \mathbf{Y}^T \mathbf{Y}) \leq \left( 1 + \frac{1}{n} \|\mathbf{Y}\|_F^2 \right)^n
\]  

(5)

This suggests that when \( \mathbf{P} \) is chosen so that \( \mathbf{Y} \) is not too large, then \( \det \mathbf{A}^T \mathbf{A} \) will not be small. By applying the usual variational formulation for singular values to (3), we obtain

\[
\sigma_i^2(\mathbf{A}) \leq \sigma_i^2(\mathbf{X}) \leq \left( 1 + \|\mathbf{Y}\|_2^2 \right) \sigma_i^2(\mathbf{A}), \quad l = 1, \cdots, n
\]

(6)

where \( \sigma_i(\mathbf{A}) \) and \( \sigma_i(\mathbf{X}) \) are the singular values of \( \mathbf{A} \) and \( \mathbf{X} \) respectively. Thus, the singular values of \( \mathbf{X} \) will not be small if \( \|\mathbf{Y}\|_2 \) is not large.

We now show that a permutation exists so that the matrix \( \mathbf{Y} \) that is not large. This result was established in [2] by assuming that \( \mathbf{P} \) was chosen to maximise \( \det \mathbf{A}^T \mathbf{A} \); the proof, however, as not constructive. In the present note, we give a construction based on a greedy algorithm where rows of \( \mathbf{X} \) are deleted, one at a time, so as to minimise the Frobenius norm of \( \mathbf{Y} \) at each step.

**Theorem 1.** There is a permutation matrix \( \mathbf{P} \) so that (2) holds with

\[
\|\mathbf{Y}\|_F^2 \leq \frac{(m-k)n}{k-n+1}.
\]

**Proof:** Let

\[
\mathbf{A} = \begin{bmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_k^T \end{bmatrix}, \quad \mathbf{Q} = \begin{bmatrix} \mathbf{q}_1^T \\ \vdots \\ \mathbf{q}_k^T \end{bmatrix}, \quad \mathbf{Y} = \begin{bmatrix} \mathbf{y}_1^T \\ \vdots \\ \mathbf{y}_{m-k}^T \end{bmatrix},
\]

and note that the columns of \( \mathbf{Q} \) are orthogonal. Indeed,

\[
\sum_{r=1}^k \mathbf{q}_r \mathbf{q}_r^T = \mathbf{Q}^T \mathbf{Q} = \mathbf{I},
\]

and

\[
\|\mathbf{q}_r\|_2 \leq 1.
\]

Suppose \( k > n \) and that we wish to delete a row of \( \mathbf{A} \). We define
\[
A_j := \begin{bmatrix}
    a_1^T \\
    \vdots \\
    a_{j-1}^T \\
    a_j^T \\
    a_{j+1}^T \\
    \vdots \\
    a_k^T
\end{bmatrix}, \quad B_j := \begin{bmatrix}
    a_j^T \\
    B
\end{bmatrix},
\]

and can then write for some permutation matrix \( \tilde{P}_j \)

\[
\tilde{P}_j X = \begin{bmatrix}
    A_j \\
    B_j
\end{bmatrix}, \quad A_j \in \mathbb{R}^{(k-1)n}, \ B_j \in \mathbb{R}^{(m-k+1)n}.
\]

From this it follows that

\[
\tilde{P}_j X = \begin{bmatrix}
    A_j \\
    B_j
\end{bmatrix}^T = \begin{bmatrix}
    Q_j \\
    Y_j
\end{bmatrix} \left( A_j^T A_j \right)^{-\frac{1}{2}}.
\]

where

\[
Q_j = A_j \left( A_j^T A_j \right)^{-\frac{1}{2}}, \quad Y_j = B_j \left( A_j^T A_j \right)^{-\frac{1}{2}}.
\]

We have

\[
\|Y_j\|_F^2 = \text{Trace} \left( \left( A_j^T A_j \right)^{-\frac{1}{2}} B_j^T B_j \left( A_j^T A_j \right)^{-\frac{1}{2}} \right)
= \text{Trace} \left( B_j^T B_j \left( A_j^T A_j \right)^{-1} \right)
= \text{Trace} \left( (B_j^T B + a_j a_j^T) \left( A_j^T A_j - a_j a_j^T \right)^{-1} \right)
= \text{Trace} \left( (Y_j^T Y + q_j q_j^T) \left( I - q_j q_j^T \right)^{-1} \right)
= \|Y_j\|_F^2 + \frac{1}{1 - \|q_j\|_2^2} \left( \|Y_j q_j\|_2^2 + \|q_j\|_2^2 \right)
\]

Now let \( \|Y_j\|_F \) be minimized when \( p = j \). Then,

\[
\left( 1 - \|q_j\|_2^2 \right) \|Y_p\|_F^2 \leq \left( 1 - \|q_j\|_2^2 \right) \|Y_j\|_F^2 + \left( \|Y_j q_j\|_2^2 + \|q_j\|_2^2 \right).
\]
On summing over $j$ and noting that

$$
\sum_{j=1}^{k} \|q_j\|_2^2 = n,
$$

$$
\sum_{j=1}^{k} \|Yq_j\|_2^2 = \|Y\|_F^2,
$$

we obtain

$$
(k-n)\|Y_r\|_F^2 \leq (k-n+1)\|Y\|_F^2 + n.
$$

(7)

We can use this construction, starting with $X$ and then deleting a row at the time whilst insuring that $\|H\|_F = \|Y\|_F$ is minimised at each step to construct

$$
P X = \begin{bmatrix} A \\ B \end{bmatrix}, \quad A \in \mathbb{R}^{k \times n}, \quad B \in \mathbb{R}^{(m-k) \times n}, \quad k > n.
$$

From (7) it follows by induction that such a construction satisfies

$$
\|Y\|_F^2 \leq \frac{(m-k)n}{k-n+1}.
$$

#

Theorem 1 and (4), (5) imply:

**Corollary 1** There is a permutation matrix $P$ so that

$$
\det(A^T A) \geq \det(X^T X) \left( \frac{k-n+1}{m-n+1} \right)^n.
$$

(8)

In [2, cf Theorem 2], a greedy algorithm was presented where rows of $X$ are deleted, one at a time, so as to minimise the Frobenius norm of $A^+$ at each step was, which read

**Theorem 2** There is a permutation matrix $P \in \mathbb{R}^{m \times m}$ such that (1) holds with

$$
\|A^+\|_F^2 \leq \frac{m-n+1}{k-n+1} \|X^+\|_F^2.
$$

This theorem can also be used to give an alternative proof of Corollary 1 (7)
**Proof** (of Corollary 1, alternative): If we apply Theorem 2 to \(X^T X \frac{1}{2}\), there is a permutation matrix \(P\) such that

\[
PX(X^T X)^{\frac{1}{2}} = \begin{bmatrix} W \\ Z \end{bmatrix}, \quad W \in \mathbb{R}^{k \times n},
\]

with

\[
\text{Trace}(W^T W)^{-\frac{1}{2}} = \|W^+\|_F^2 \leq \frac{m-n+1}{k-n+1} \|X(X^T X)^{-\frac{1}{2}}\|_F^2 = n \left(\frac{m-n+1}{k-n+1}\right).
\]

Moreover,

\[
PX = \begin{bmatrix} W \\ Z \end{bmatrix} (X^T X)^{\frac{1}{2}} = \begin{bmatrix} A \\ B \end{bmatrix},
\]

and hence

\[
\det(A^T A) = \det(W^T W) \det(X^T X). \quad (9)
\]

From the geometric-arithmetic mean inequality, we have

\[
\det(W^T W)^{-\frac{1}{2}} \leq \left(\frac{1}{n} \text{Trace}(W^T W)^{-\frac{1}{2}}\right)^n \leq \left(\frac{m-n+1}{k-n+1}\right)^n,
\]

and the result follows on substitution of this inequality in (9). #

The bound for \(\det A^T A\) in corollary 1 follows from bounds on \(\|Y\|_F\), and proof above on \(\|A^+\|_F\), respectively. A somewhat tighter bound can be obtained by analysing a greedy algorithm where \(\det A^T A\) is maximized at each step.

**Theorem 3** There is a permutation matrix \(P \in \mathbb{R}^{n \times n}\) such that (1) holds with

\[
\det(A^T A) \geq \det(X^T X) \prod_{j=k+1}^m \frac{j-n}{j} = \frac{k!(m-n)!}{m!(k-n)!} \det(X^T X). \quad (10)
\]

**Proof:** As in theorem 1, we have

\[
PX = \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} Q \\ Y \end{bmatrix} (A^T A)^{\frac{1}{2}},
\]

where
\[ A = \begin{bmatrix} a_1^T \\ \vdots \\ a_k^T \end{bmatrix}, \quad Q = \begin{bmatrix} q_1^T \\ \vdots \\ q_k^T \end{bmatrix}, \quad Y = \begin{bmatrix} y_1^T \\ \vdots \\ y_{m-k}^T \end{bmatrix}, \]

and the columns of \( Q \) are orthogonal.

Suppose \( k > n \) and that we wish to delete a row of \( A \). We define

\[ A_j = \begin{bmatrix} a_1^T \\ \vdots \\ a_{j-1}^T \\ a_j^T \\ a_{j+1}^T \\ \vdots \\ a_k^T \end{bmatrix}, \quad B_j = \begin{bmatrix} a_j^T \\ B \end{bmatrix}, \]

and can then write

\[ \tilde{P}_j X = \begin{bmatrix} A_j \\ B_j \end{bmatrix}, \quad A_j \in \mathbb{R}^{(k-1) \times n}, \quad B_j \in \mathbb{R}^{(m-k+1) \times n}. \]

from which it follows that

\[ \tilde{P}_j X = \begin{bmatrix} A_j \\ B_j \end{bmatrix} = \begin{bmatrix} Q_j \\ Y_j \end{bmatrix} (A_j^T A_j)^{-\frac{1}{2}}, \]

\[ Q_j = A_j (A_j^T A_j)^{-\frac{1}{2}}, \quad Y_j = B_j (A_j^T A_j)^{-\frac{1}{2}}. \]

Note that,

\[ \det(A_j^T A_j) = \det(A_j^T A - a_j a_j^T) = \left(1 - \|q_j\|_2^2\right) \det(A_j^T A). \]

Now let \( \det(A_j^T A_j) \) be maximised when \( p = j \). Then,

\[ \det(A_p^T A_p) \geq \left(1 - \|q_j\|_2^2\right) \det(A_j^T A), \]

and, on summing over \( j \) we find that
We can use this construction, starting with $X$ and then deleting a row at the time whilst insuring that $\det(A^T A)$ is minimised at each step to construct

$$PX = \begin{bmatrix} A \\ B \end{bmatrix}, \quad A \in \mathbb{R}^{k \times n}, \quad B \in \mathbb{R}^{(m-k) \times n}, \quad k > n.$$

From (11), it follows by induction that this construction satisfies

$$\det(A^T A) \geq \det(X^T X) \prod_{j=k+1}^{m} \frac{j-n}{j} = \frac{k!(m-n)!}{m!(k-n)!} \det(X^T X).$$

### 3 Discussion

We now compare the bounds given in corollary 1 and Theorem 3 which are the same for $n = 1$. We have

$$\log \prod_{j=k+1}^{m} \frac{j-n}{j} = \log \left( \frac{k+1-n}{k+1} \right) - \log \left( \frac{m+1-n}{m+1} \right) + \sum_{j=k+2}^{m+1} \log \left( \frac{j-n}{j} \right)$$

$$\geq \log \left( \frac{k+1-n}{k+1} \right) - \log \left( \frac{m+1-n}{m+1} \right) + \int_{k+1}^{m+1} \log \left( \frac{x-n}{x} \right) dx$$

$$= \log \left( \frac{m+1}{k+1} \frac{k+1-n}{m+1-n} \right) + n \log \left( \frac{k+1-n}{m+1-n} \right) + m \log \left( 1 - \frac{n}{m+1} \right) - k \log \left( 1 - \frac{n}{k+1} \right)$$

Thus, for $n \geq 2$

$$\log \prod_{j=k+1}^{m} \frac{j-n}{j} - n \log \left( \frac{k+1-n}{m+1-n} \right) \geq m \log \left( 1 - \frac{n}{m+1} \right) - k \log \left( 1 - \frac{n}{k+1} \right).$$

This demonstrates that the bound (10) given in Theorem 3 is superior to the bounds given by (8) in Corollary 1. This difference can be substantial when $k$ is relatively small. For example, if $m$ is large relative to $n$ and $k = n$, then
\[ \prod_{j=1}^{m} \left( \frac{j-n}{j} \right)^{j} \left( \frac{k+1-n}{m+1-n} \right)^{m} \geq \left( 1 - \frac{n}{m+1} \right)^{m} / \left( 1 - \frac{n}{k+1} \right)^{k} \]

\[ = \left( \frac{n+1}{e} \right)^{n}. \]

In order to compare the bounds on the singular values given by (6), it makes sense to consider the \( n \)th root of \( \det A^T A \) as this is the square of the geometric mean of the singular values of \( A \). Given the construction, we find that the bound (8) given in Corollary 1 is similar to that given by (6). However, the bound given by (10) in Theorem 3, provides a substantially sharper estimate.

References


