

A note on subset selection for matrices

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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 $\mathbf{X} \in \mathbf{R}^{m \times n}$ find a permutation matrix $\mathbf{P} \in \mathbf{R}^{m \times m}$ so that

$$\mathbf{PX} = \begin{bmatrix} \mathbf{A} \\ \mathbf{B} \end{bmatrix}, \quad \mathbf{A} \in \mathbf{R}^{k \times n}, \quad (1)$$

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

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

$$\mathbf{y} = \mathbf{A}\boldsymbol{\theta} + \boldsymbol{\delta},$$

where $\mathbf{A} \in \mathbf{R}^{k \times n}$ is a design matrix whose rows are a subset of the rows of $\mathbf{X} \in \mathbf{R}^{m \times n}$, $\boldsymbol{\theta} \in \mathbf{R}^n$ is a vector of unknown parameters that is to be determined and $\boldsymbol{\delta} \in \mathbf{R}^k$ 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 $\hat{\boldsymbol{\theta}} = \mathbf{A}^+ \mathbf{y}$ where \mathbf{A}^+ is the Moore-Penrose inverse. For a given design matrix \mathbf{A} and confidence coefficient, the confidence ellipsoid for $\boldsymbol{\theta}$ is given by $\left\{ \boldsymbol{\theta} \mid (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T \mathbf{A}^T \mathbf{A} (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) \leq \text{constant} \right\}$. The content of

this ellipsoid is proportional to $(\det \mathbf{A}^T \mathbf{A})^{-\frac{1}{2}}$ and it is natural to make this as small as possible. That is, we choose the design matrix \mathbf{A} to maximise $\det \mathbf{A}^T \mathbf{A}$. 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

$\|\mathbf{A}^+\|_F = \sqrt{\text{Trace}(\mathbf{A}^T \mathbf{A})^{-1}}$ ensures that the expected mean squared error of $\boldsymbol{\theta}$ is minimised. E-optimal designs (see Silvey [5]) maximise the smallest singular value of \mathbf{A} (or equivalently, maximise $\|\mathbf{A}^+\|_2 = \|(\mathbf{A}^T \mathbf{A})^{-1}\|_2^{\frac{1}{2}}$). Further applications are described in [2]

Row selection is often implemented using a QR decomposition of \mathbf{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 $\det \mathbf{A}^T \mathbf{A}$.

In [2] the present authors derived upper bound for $\|\mathbf{A}^+\|_F$ and the singular values of \mathbf{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 $\det \mathbf{A}^T \mathbf{A}$. In section 2 we give the main results and in particular a sharper bound for $\|\mathbf{A}^+\|_F$. 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

$$\mathbf{P}\mathbf{X} = \begin{bmatrix} \mathbf{A} \\ \mathbf{B} \end{bmatrix} = \begin{bmatrix} \mathbf{Q} \\ \mathbf{Y} \end{bmatrix} (\mathbf{A}^T \mathbf{A})^{\frac{1}{2}} \quad (2)$$

where

$$\mathbf{Q} := \mathbf{A} (\mathbf{A}^T \mathbf{A})^{-\frac{1}{2}}$$

$$\mathbf{Y} := \mathbf{B} (\mathbf{A}^T \mathbf{A})^{-\frac{1}{2}}$$

It follows that,

$$\mathbf{X}^T \mathbf{X} = (\mathbf{A}^T \mathbf{A})^{\frac{1}{2}} (\mathbf{I} + \mathbf{Y}^T \mathbf{Y}) (\mathbf{A}^T \mathbf{A})^{\frac{1}{2}} \quad (3)$$

Thus

$$\det(\mathbf{X}^T \mathbf{X}) = \det(\mathbf{I} + \mathbf{Y}^T \mathbf{Y}) \det(\mathbf{A}^T \mathbf{A}) \quad (4)$$

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

$$\det(\mathbf{I} + \mathbf{Y}^T \mathbf{Y}) \leq \left(1 + \frac{1}{n} \|\mathbf{Y}\|_F^2\right)^n \quad (5)$$

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

$$\sigma_l^2(\mathbf{A}) \leq \sigma_l^2(\mathbf{X}) \leq \left(1 + \|\mathbf{Y}\|_2^2\right) \sigma_l^2(\mathbf{A}), \quad l = 1, \dots, n \quad (6)$$

where $\sigma_l(\mathbf{A})$ and $\sigma_l(\mathbf{X})$ 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, is 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

$$\mathbf{A}_j := \begin{bmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_{j-1}^T \\ \mathbf{a}_{j+1}^T \\ \vdots \\ \mathbf{a}_k^T \end{bmatrix}, \quad \mathbf{B}_j := \begin{bmatrix} \mathbf{a}_j^T \\ \mathbf{B} \end{bmatrix},$$

and can then write for some permutation matrix $\tilde{\mathbf{P}}_j$

$$\tilde{\mathbf{P}}_j \mathbf{X} = \begin{bmatrix} \mathbf{A}_j \\ \mathbf{B}_j \end{bmatrix}, \quad \mathbf{A}_j \in \mathbf{R}^{(k-1) \times n}, \quad \mathbf{B}_j \in \mathbf{R}^{(m-k+1) \times n}.$$

From this it follows that

$$\tilde{\mathbf{P}}_j \mathbf{X} = \begin{bmatrix} \mathbf{A}_j \\ \mathbf{B}_j \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_j \\ \mathbf{Y}_j \end{bmatrix} (\mathbf{A}_j^T \mathbf{A}_j)^{\frac{1}{2}},$$

where

$$\mathbf{Q}_j = \mathbf{A}_j (\mathbf{A}_j^T \mathbf{A}_j)^{-\frac{1}{2}}, \quad \mathbf{Y}_j = \mathbf{B}_j (\mathbf{A}_j^T \mathbf{A}_j)^{-\frac{1}{2}}.$$

We have

$$\begin{aligned} \|\mathbf{Y}_j\|_F^2 &= \text{Trace} \left((\mathbf{A}_j^T \mathbf{A}_j)^{-\frac{1}{2}} \mathbf{B}_j^T \mathbf{B}_j (\mathbf{A}_j^T \mathbf{A}_j)^{-\frac{1}{2}} \right) \\ &= \text{Trace} \left(\mathbf{B}_j^T \mathbf{B}_j (\mathbf{A}_j^T \mathbf{A}_j)^{-1} \right) \\ &= \text{Trace} \left((\mathbf{B}^T \mathbf{B} + \mathbf{a}_j \mathbf{a}_j^T) (\mathbf{A}^T \mathbf{A} - \mathbf{a}_j \mathbf{a}_j^T)^{-1} \right) \\ &= \text{Trace} \left((\mathbf{Y}^T \mathbf{Y} + \mathbf{q}_j \mathbf{q}_j^T) (\mathbf{I} - \mathbf{q}_j \mathbf{q}_j^T)^{-1} \right) \\ &= \|\mathbf{Y}\|_F^2 + \frac{1}{1 - \|\mathbf{q}_j\|_2^2} \left(\|\mathbf{Y} \mathbf{q}_j\|_2^2 + \|\mathbf{q}_j\|_2^2 \right) \end{aligned}$$

Now let $\|\mathbf{Y}_j\|_F$ be minimized when $p = j$. Then,

$$(1 - \|\mathbf{q}_j\|_2^2) \|\mathbf{Y}_p\|_F^2 \leq (1 - \|\mathbf{q}_j\|_2^2) \|\mathbf{Y}\|_F^2 + \left(\|\mathbf{Y} \mathbf{q}_j\|_2^2 + \|\mathbf{q}_j\|_2^2 \right).$$

On summing over j and noting that

$$\sum_{j=1}^k \|\mathbf{q}_j\|_2^2 = n,$$

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

we obtain

$$(k-n)\|\mathbf{Y}_p\|_F^2 \leq (k-n+1)\|\mathbf{Y}\|_F^2 + n. \quad (7)$$

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

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

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

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

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

Corollary 1 There is a permutation matrix \mathbf{P} so that

$$\det(\mathbf{A}^T \mathbf{A}) \geq \det(\mathbf{X}^T \mathbf{X}) \left(\frac{k-n+1}{m-n+1} \right)^n. \quad (8)$$

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

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

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

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 $\mathbf{X}(\mathbf{X}^T \mathbf{X})^{-\frac{1}{2}}$, there is a permutation matrix \mathbf{P} such that

$$\mathbf{P}\mathbf{X}(\mathbf{X}^T \mathbf{X})^{-\frac{1}{2}} = \begin{bmatrix} \mathbf{W} \\ \mathbf{Z} \end{bmatrix}, \quad \mathbf{W} \in \mathbf{R}^{k \times n},$$

with

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

Moreover,

$$\mathbf{P}\mathbf{X} = \begin{bmatrix} \mathbf{W} \\ \mathbf{Z} \end{bmatrix} (\mathbf{X}^T \mathbf{X})^{\frac{1}{2}} = \begin{bmatrix} \mathbf{A} \\ \mathbf{B} \end{bmatrix},$$

and hence

$$\det(\mathbf{A}^T \mathbf{A}) = \det(\mathbf{W}^T \mathbf{W}) \det(\mathbf{X}^T \mathbf{X}). \quad (9).$$

From the geometric-arithmetic mean inequality, we have

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

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

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

Theorem 3 There is a permutation matrix $\mathbf{P} \in \mathbf{R}^{m \times m}$ such that (1) holds with

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

Proof: As in theorem 1, we have

$$\mathbf{P}\mathbf{X} = \begin{bmatrix} \mathbf{A} \\ \mathbf{B} \end{bmatrix} = \begin{bmatrix} \mathbf{Q} \\ \mathbf{Y} \end{bmatrix} (\mathbf{A}^T \mathbf{A})^{\frac{1}{2}},$$

where

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

and the columns of \mathbf{Q} are orthogonal.

Suppose $k > n$ and that we wish to delete a row of \mathbf{A} . We define

$$\mathbf{A}_j = \begin{bmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_{j-1}^T \\ \mathbf{a}_{j+1}^T \\ \vdots \\ \mathbf{a}_k^T \end{bmatrix}, \quad \mathbf{B}_j = \begin{bmatrix} \mathbf{a}_j^T \\ \mathbf{B} \end{bmatrix},$$

and can then write

$$\tilde{\mathbf{P}}_j \mathbf{X} = \begin{bmatrix} \mathbf{A}_j \\ \mathbf{B}_j \end{bmatrix}, \quad \mathbf{A}_j \in \mathbf{R}^{(k-1) \times n}, \quad \mathbf{B}_j \in \mathbf{R}^{(m-k+1) \times n}.$$

from which it follows that

$$\tilde{\mathbf{P}}_j \mathbf{X} = \begin{bmatrix} \mathbf{A}_j \\ \mathbf{B}_j \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_j \\ \mathbf{Y}_j \end{bmatrix} (\mathbf{A}_j^T \mathbf{A}_j)^{\frac{1}{2}},$$

$$\mathbf{Q}_j = \mathbf{A}_j (\mathbf{A}_j^T \mathbf{A}_j)^{-\frac{1}{2}}, \quad \mathbf{Y}_j = \mathbf{B}_j (\mathbf{A}_j^T \mathbf{A}_j)^{-\frac{1}{2}}.$$

Note that,

$$\det(\mathbf{A}_j^T \mathbf{A}_j) = \det(\mathbf{A}^T \mathbf{A} - \mathbf{a}_j \mathbf{a}_j^T) = (1 - \|\mathbf{q}_j\|_2^2) \det(\mathbf{A}^T \mathbf{A}).$$

Now let $\det(\mathbf{A}_j^T \mathbf{A}_j)$ be maximised when $p = j$. Then,

$$\det(\mathbf{A}_p^T \mathbf{A}_p) \geq (1 - \|\mathbf{q}_j\|_2^2) \det(\mathbf{A}^T \mathbf{A}),$$

and, on summing over j we find that

$$k \det(\mathbf{A}_p^T \mathbf{A}_p) \geq (k-n) \det(\mathbf{A}^T \mathbf{A}). \quad (11)$$

We can use this construction, starting with \mathbf{X} and then deleting a row at the time whilst insuring that $\det(\mathbf{A}^T \mathbf{A})$ is minimised at each step to construct

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

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

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

3 Discussion

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

$$\begin{aligned} \log \prod_{j=k+1}^m \left(\frac{j-n}{j} \right) &= \log \left(\frac{k+1-n}{k+1} \right) - \log \left(\frac{m+1-n}{m+1} \right) + \sum_{j=k+2}^{m+1} \log \left(\frac{j-n}{j} \right) \\ &\geq \log \left(\frac{k+1-n}{k+1} \right) - \log \left(\frac{m+1-n}{m+1} \right) + \int_{k+1}^{m+1} \log \left(\frac{x-n}{x} \right) dx \\ &= \log \frac{(m+1)(k+1-n)}{(k+1)(m+1-n)} + n \log \left(\frac{k+1-n}{m+1-n} \right) + (m+1) \log \left(1 - \frac{n}{m+1} \right) - (k+1) \log \left(1 - \frac{n}{k+1} \right) \\ &= n \log \left(\frac{k+1-n}{m+1-n} \right) + m \log \left(1 - \frac{n}{m+1} \right) - k \log \left(1 - \frac{n}{k+1} \right). \end{aligned}$$

Thus, for $n \geq 2$

$$\begin{aligned} \log \prod_{j=k+1}^m \left(\frac{j-n}{j} \right) - n \log \left(\frac{k+1-n}{m+1-n} \right) &\geq m \log \left(1 - \frac{n}{m+1} \right) - k \log \left(1 - \frac{n}{k+1} \right) \\ &\geq 0 \end{aligned}$$

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

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

$$\approx \left(\frac{n+1}{e} \right)^n.$$

In order to compare the bounds on the singular values given by (6), it makes sense to consider the n th root of $\det \mathbf{A}^T \mathbf{A}$ as this is the square of the geometric mean of the singular values of \mathbf{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.

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