

Singular Values and Maximum Rank Minors of Generalized Inverses

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Abstract

Singular values and maximum rank minors of generalized inverses are studied. Proportionality of maximum rank minors is explained in terms of space equivalence. The Moore–Penrose inverse A^\dagger is characterized as the $\{1\}$ -inverse of A with minimal volume.

Key words: Singular values. Volume. Generalized Inverses. The Moore–Penrose Inverse. Compound Matrices. Space Equivalent Matrices.

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1 Introduction

Throughout this paper A is an $m \times n$ real matrix of rank r , a fact denoted by $A \in \mathbf{R}_r^{m \times n}$. The singular values of A are denoted $\{\sigma_i(A) : i = 1, \dots, r\}$. The vector in \mathbf{R}^{mn} obtained by reading the columns of A one by one is denoted $\text{vec } A$.

For $k = 1, \dots, r$, the k -th compound of A , denoted $C_k(A)$, is the $\binom{m}{k} \times \binom{n}{k}$ matrix whose elements are the $k \times k$ minors of A , i.e. the determinants of its $k \times k$ submatrices ordered lexicographically. The $r \times r$ minors of A (i.e. the elements of $C_r(A)$) are called its **maximum rank minors**.

We denote by $Q_{k,n}$ the set of increasing sequences of k elements from $\{1, 2, \dots, n\}$. Given index sets $I \subset \{1, \dots, m\}$ and $J \subset \{1, \dots, n\}$ we denote by A_{IJ} the corresponding submatrix of A . The submatrix of columns in J is denoted A_{*J} .

Definition 1 For $k = 1, \dots, r$, the k -**volume** of A is defined as the Frobenius norm of the k -th compound matrix $C_k(A)$,

$$\text{vol}_k A := \sqrt{\sum_{I \in Q_{k,m}, J \in Q_{k,n}} |\det A_{IJ}|^2} \quad (1.1a)$$

or equivalently,

$$\text{vol}_k A = \sqrt{\sum_{I \in Q_{k,r}} \left(\prod_{i \in I} \sigma_i^2(A) \right)} \quad (1.1b)$$

the square root of the k -th symmetric function¹ of $\{\sigma_1^2(A), \dots, \sigma_r^2(A)\}$.

We use the convention

$$\text{vol}_k A := 0, \quad \text{for } k = 0 \text{ or } k > \text{rank } A. \quad (1.2)$$

It helps to think of the k -volume of A as the (ordinary) Euclidean norm of $\text{vec } C_k(A)$. In particular, for $k = 1$, the 1-**volume** of $A = (a_{ij})$ is its Frobenius norm

$$\text{vol}_1(A) = \sqrt{\sum_{i,j} |a_{ij}|^2} = \sqrt{\text{tr } A^T A} \quad (1.3)$$

and for $r = \text{rank } A$, the r -**volume** of A is

$$\text{vol}_r A := \sqrt{\sum_{I \in Q_{r,m}, J \in Q_{r,n}} |\det A_{IJ}|^2} \quad (1.4a)$$

$$= \prod_{i=1}^r \sigma_i(A). \quad (1.4b)$$

The r -volume $\text{vol}_r A$ is sometimes called just the **volume** of A , as in [3], and denoted by $\text{vol } A$.

It should be noted that the k -volume of A is not the volume of its k -th compound. Indeed, for $k = 1, \dots, r = \text{rank } A$, the rank of $C_k(A)$ is $\binom{r}{k}$. Its volume (i.e. its $\binom{r}{k}$ -volume) is given in terms of the r -volume of A as

$$\text{vol} \binom{r}{k} C_k(A) = (\text{vol}_r A)^{\binom{r-1}{k-1}}, \quad k = 1, \dots, r. \quad (1.5)$$

¹The k -volume was defined in [6] as the product of the k largest singular values of A . Definition (1.1) is more natural.

The left side is a product of the singular values of A , each appearing exactly $\binom{r-1}{k-1}$ times, and the result follows from (1.4b).

The study of generalized inverses reveals instances where corresponding maximum rank minors of two matrices A, B are proportional, i.e.

$$\det A_{IJ} = \alpha \det B_{IJ} \quad (1.6)$$

for some $\alpha \neq 0$. For example, the corresponding maximum rank minors of A^\dagger and A^T satisfy

$$\det (A^\dagger)_{IJ} = \frac{1}{\text{vol}^2 A} \det (A^T)_{IJ} \quad (1.7)$$

see [3, Lemma 3.2]. Proportionality of maximum rank minors is an essential feature in the study of generalized inverses for matrices over integral domains, see [1]. We explain this proportionality in § 2, through the concept of state equivalence. Singular values of generalized inverses are studied in § 3. The Moore–Penrose inverse is characterized as the $\{1\}$ -inverse of minimal volume in § 4.

In § 2 we have occasion to use Plücker coordinates, a concept from multilinear algebra, see e.g. [8], [9]. The **Plücker coordinates** of an r -dimensional subspace $L \subset \mathbf{R}^n$ are the components of the exterior product $\mathbf{x}_1 \wedge \mathbf{x}_2 \wedge \cdots \wedge \mathbf{x}_r$ where $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r\}$ is any basis of L . The Plücker coordinates of

L are determined up to a scalar multiple, i.e. they span a line in $\mathbf{R}^{\binom{n}{r}}$. Thus there is a one-to-one correspondence between r -dimensional subspaces L in \mathbf{R}^n and 1-dimensional subspaces in $\mathbf{R}^{\binom{n}{r}}$, see e.g. [10, Theorem 4.9].

For example, given $A \in \mathbf{R}_r^{m \times n}$, the Plücker coordinates of $R(A)$, the **range** of A , are the components of $\text{vec } C_r(A)$, i.e. the maximum rank minors of A .

2 Space equivalent matrices

The following definition describes matrices representing linear transformations between the same subspaces.

Definition 2 Two $m \times n$ matrices A, B are called **space equivalent** if

$$R(A) = R(B), \quad (2.1a)$$

$$\text{and } R(A^T) = R(B^T). \quad (2.1b)$$

Let L, M be subspaces of \mathbf{R}^n , with dimensions ℓ, m respectively, and let $\ell \leq m$. We denote by $\cos\{L, M\}$ the product of the cosines of the ℓ principal angles between L and M , see e.g. [6]. In particular, $\cos\{L, M\} = 1$ if and only if $L \subset M$. The following version of the Cauchy-Schwarz inequality was proved in [6, Theorem 5], for full column-rank matrices $A, B \in \mathbf{R}_r^{m \times r}$,

$$\text{vol} (B^T A) = \text{vol } A \text{ vol } B \cos\{R(A), R(B)\} \quad (2.2)$$

We extend this result to matrices of arbitrary rank in Theorem 1 below. First we need

Lemma 1 Let $S \in \mathbf{R}^{m \times m}$, $A \in \mathbf{R}_m^{m \times n}$. Then

$$\text{vol}_m (SA) = |\det S| \text{vol } A. \quad (2.3)$$

Proof: If S is singular, then both sides of (2.3) are zero. Let S be nonsingular. Then $\text{rank}(SA) = m$, and

$$\begin{aligned} \text{vol}_m(SA) &= \text{vol}(SA) = \sqrt{\sum_{J \in Q_{m,n}} \det^2(SA)_{*J}} \\ &= \sqrt{\sum_{J \in Q_{m,n}} \det^2 S \det^2 A_{*J}} \\ &= |\det S| \text{vol} A . \end{aligned}$$

□

Theorem 1 Let $A, B \in \mathbf{R}_r^{m \times n}$. Then

$$\text{vol}_r(B^T A) = \text{vol}_r A \text{vol}_r B \cos\{R(A), R(B)\} \quad (2.4a)$$

$$\text{vol}_r(AB^T) = \text{vol}_r A \text{vol}_r B \cos\{R(A^T), R(B^T)\} . \quad (2.4b)$$

Proof of (2.4a): If $\text{rank} B^T A < r$ then there is an $x \in \mathbf{R}^n$ such that $Ax \neq 0$ and $B^T Ax = 0$. Therefore one of the principal angles between $R(A)$ and $R(B)$ is $\frac{\pi}{2}$, and (2.4a) gives $0 = 0$.

Assume $\text{rank} B^T A = r$, and let all volumes below be r -volumes. Let $A = C_A R_A$ and $B = C_B R_B$ be full rank factorizations of A and B . Then

$$\begin{aligned} B^T A &= (C_B R_B)^T (C_A R_A) \\ &= R_B^T (C_B^T C_A R_A) \end{aligned}$$

is a full rank factorization if $\text{rank} B^T A = r$. Its volume is

$$\begin{aligned} \text{vol}(B^T A) &= \text{vol} R_B \text{vol}(C_B^T C_A R_A) , \quad \text{by [3, Lemma 2.2]} , \\ &= \text{vol} R_B \left| \det(C_B^T C_A) \right| \text{vol} R_A , \quad \text{by Lemma 1} \\ &= \text{vol} R_B \text{vol} R_A (\text{vol} C_B \text{vol} C_A \cos\{R(C_A), R(C_B)\}) , \quad \text{by [6, Theorem 5]} \\ &= (\text{vol} C_A \text{vol} R_A) (\text{vol} C_B \text{vol} R_B) \cos\{R(A), R(B)\} , \quad \text{since } R(C_A) = R(A), R(C_B) = R(B) \\ &= \text{vol} A \text{vol} B \cos\{R(A), R(B)\} . \end{aligned}$$

The proof of (2.4b) is similar. □

Example 1 If P is idempotent then its eigenvalues are 1, 0 and its nonzero singular values are all ≥ 1 . Thus $\text{vol} P \geq 1$. More precisely,

$$\text{vol} P = \frac{1}{\cos\{R(P), R(I-P)^\perp\}} ,$$

where $R(P)$ is the range of P , and $R(I-P)$ is its null-space. This follows from (2.4a) with $A = P$, $B = P^T$ so that $B^T A = P^2 = P$.

Therefore $\text{vol} P = 1$ if and only if $P = P^T$, i.e. P is an orthogonal projector. □

The vectors $\text{vec } C_r(A)$ and $\text{vec } C_r(B)$ give the Plücker coordinates of the subspaces $R(A)$ and $R(B)$ respectively. The (ordinary) angle between these vectors, in the space $\mathbb{R}^{\binom{m}{r} \binom{n}{r}}$, has cosine equal to $\cos\{R(A), R(B)\}$. Statements (2.4a) and (2.4b) are Cauchy–Schwarz inequalities for the vectors $\text{vec } C_r(A)$ and $\text{vec } C_r(B)$. As expected, equality holds if their components (i.e. the maximum rank minors of A, B) are proportional, see (2.6) below.

Theorem 2 Let $A, B \in \mathbb{R}_r^{m \times n}$. Then the following are equivalent:

- (a) A and B are space equivalent.
- (b) There are matrices $X, Y \in \mathbb{R}^{n \times m}$ such that

$$A = BXB \tag{2.5a}$$

$$B = AYA \tag{2.5b}$$

(c) $\text{vol}_r(B^T A) = \text{vol}_r(A B^T) = \text{vol } A \text{ vol } B$.

- (d) The r -compounds of A, B satisfy

$$C_r(A) = \alpha C_r(B), \quad \text{for some } \alpha \neq 0. \tag{2.6}$$

Proof: (b) \implies (a) is obvious. To prove (a) \implies (b), we use $R(A) = R(B) \implies A = BB^\dagger A$ and $R(A^T) = R(B^T) \implies A = AB^\dagger B$ to show that $A = BB^\dagger A = BB^\dagger AB^\dagger B$, proving (2.5a) for $X = B^\dagger AB^\dagger$. (2.5b) is similarly proved.

(a) \implies (c) from (2.4a) and (2.4b), and (c) \implies (d) by the Cauchy–Schwarz inequality for $\text{vec } C_r(A)$ and $\text{vec } C_r(B)$. To prove (d) \implies (a) we note that the matrix $C_r(A)$ is of rank 1, and of the form xy^T where x and y are the Plücker coordinates of the subspaces $R(A)$ and $R(A^T)$, respectively. From (d) it follows that $C_r(B) = \alpha xy^T$, proving that $R(A)$ and $R(B)$ have the same Plücker coordinates and therefore $R(A) = R(B)$. Similarly $R(A^T) = R(B^T)$. \square

Example 2 The matrices A^\dagger and A^T are space equivalent. Therefore

$$\det(A^\dagger)_{IJ} = \alpha \det(A^T)_{IJ}$$

for all indices IJ of $r \times r$ submatrices. Adding the squares of these expressions we get

$$\text{vol}^2 A^\dagger = \alpha^2 \text{vol}^2 A^T$$

and

$$\alpha = \frac{1}{\text{vol}^2 A}, \quad \text{since } \text{vol } A^T = \text{vol } A \text{ and } \text{vol } A^\dagger = \frac{1}{\text{vol } A},$$

proving (1.7).

3 Singular values of generalized inverses

Let $A \in \mathbb{R}_r^{m \times n}$ have the singular value decomposition (SVD)

$$A = U \begin{pmatrix} \Sigma & O \\ O & O \end{pmatrix} V^T \tag{3.1}$$

where U, V are orthogonal, and Σ is a diagonal matrix, with the singular values of A

$$\sigma_1(A) \geq \sigma_2(A) \geq \cdots \geq \sigma_r(A) . \quad (3.2)$$

The general $\{1\}$ -inverse of A is

$$G = V \begin{pmatrix} \Sigma^{-1} & X \\ Y & Z \end{pmatrix} U^T \quad (3.3)$$

where X, Y, Z are arbitrary submatrices of appropriate sizes. In particular,

$Z = Y \Sigma X$ gives the general $\{1, 2\}$ inverses, i.e. the solutions of $AXA = A, XAX = X$,
 $X = O$ gives the general $\{1, 3\}$ -inverses (the solutions of $AXA = A, (AX)^T = AX$),
 $Y = O$ gives the general $\{1, 4\}$ -inverses (the solutions of $AXA = A, (XA)^T = XA$),
 finally, the Moore–Penrose inverse is (3.3) with $X = O, Y = O$ and $Z = O$.

We show next that each singular value of the Moore–Penrose inverse A^\dagger is dominated by a corresponding singular value of any $\{1\}$ -inverse of A .

Theorem 3 Let G be a $\{1\}$ -inverse of A with singular values

$$\sigma_1(G) \geq \sigma_2(G) \geq \cdots \geq \sigma_s(G) \quad (3.4)$$

where $s = \text{rank } G (\geq \text{rank } A)$. Then

$$\sigma_i(G) \geq \sigma_i(A^\dagger) , \quad i = 1, \dots, r . \quad (3.5)$$

Proof: Dropping U, V we write

$$\begin{aligned} GG^T &= \begin{pmatrix} \Sigma^{-1} & X \\ Y & Z \end{pmatrix} \begin{pmatrix} \Sigma^{-1} & Y^T \\ X^T & Z^T \end{pmatrix} \\ &= \begin{pmatrix} \Sigma^{-2} + XX^T & ? \\ ? & ? \end{pmatrix} , \end{aligned}$$

where $?$ denotes a submatrix not needed in this proof. Then for $i = 1, \dots, r$,

$$\begin{aligned} \sigma_i^2(G) &:= \lambda_i(GG^T) \\ &\geq \lambda_i(\Sigma^{-2} + XX^T) , \quad (\text{e.g. [5, Chapter 11, Theorem 11]}) \\ &\geq \lambda_i(\Sigma^{-2}) , \quad (\text{e.g. [5, Chapter 11, Theorem 9]}) \\ &= \sigma_i^2(A^\dagger) , \end{aligned}$$

proving the theorem. □

Corollary 1 If G is a $\{2\}$ -inverse of A of rank $q (\leq \text{rank } A)$, then

$$\sigma_i(A) \geq \sigma_i(G^\dagger) , \quad i = 1, \dots, q . \quad (3.6)$$

Proof: The statement that G is a $\{2\}$ -inverse of A is equivalent to the statement that A is a $\{1\}$ -inverse of G . Then (3.6) follows from (3.5) by reversing the roles of A and G . □

Note: For a $\{1, 2\}$ -inverse the inequalities (3.6) are equivalent to (3.5), and give no further information.

If G is a $\{1, 3\}$ -inverse of A , the inequalities (3.5) can be reversed in the following sense.

Theorem 4 Let $A \in \mathbf{R}_r^{m \times n}$ and let G be a $\{1, 3\}$ -inverse of A , with singular values

$$\sigma_1(G) \geq \sigma_2(G) \geq \cdots \geq \sigma_s(A), \quad \text{where } s = \min\{m, n\}.$$

Then

$$\sigma_i(G) \geq \sigma_i(A^\dagger) \geq \sigma_{n-r+i}(G), \quad i = 1, \dots, r. \quad (3.7)$$

In particular, if $m = n$ and $r = n - 1$, then

$$\sigma_i(G) \geq \sigma_i(A^\dagger) \geq \sigma_{i+1}(G), \quad i = 1, \dots, r. \quad (3.8)$$

Proof: With $X = O$ in (3.3), the matrix GG^T becomes

$$GG^T = \begin{pmatrix} \Sigma^{-2} & ? \\ ? & ? \end{pmatrix}$$

and the results follow from Poincaré's Separation Theorem, see [5, Chapter 11, Theorem 12]. \square

4 Minimal volume characterization of the Moore–Penrose inverse

It was shown in [7] that the Moore–Penrose inverse A^\dagger is of minimal r -volume among all $\{1, 2\}$ -inverses of A , and it is the unique minimizer, i.e. this property characterizes the Moore–Penrose inverse. The Moore–Penrose inverse was also shown in [4] to be the unique minimizer among all $\{1, 3\}$ -inverses of a class of functions including the unitarily invariant matrix norms.

From Theorem 3 we conclude that for each $k = 1, \dots, r$, the Moore–Penrose inverse A^\dagger is of minimal k -volume among all $\{1\}$ -inverses G of A ,

$$\text{vol}_k G \geq \text{vol}_k A^\dagger, \quad k = 1, \dots, r. \quad (4.1)$$

Moreover, this property is a characterization of A^\dagger , as indicated in the following results.

Theorem 5 Let $A \in \mathbf{R}_r^{m \times n}$, and let k be any integer in $\{1, \dots, r\}$. Then the Moore–Penrose inverse A^\dagger is the unique $\{1\}$ -inverse of A with minimal k -volume.

Proof: We prove this result directly, by solving the k -volume minimization problem, showing it to have the Moore–Penrose inverse as the unique solution.

The easiest case is $k = 1$. The claim is that A^\dagger is the unique solution $X = (x_{ij})$ of the minimization problem

$$(P.1) \quad \text{minimize } \frac{1}{2} \text{vol}_1^2 X \quad \text{such that } AXA = A,$$

where by (1.3)

$$\text{vol}_1^2(x_{ij}) = \sum_{ij} |x_{ij}|^2 = \text{tr } X^T X.$$

We use the Lagrangian function

$$L(X, \Lambda) := \frac{1}{2} \text{tr } X^T X - \text{tr } \Lambda^T (AXA - A) \quad (4.2)$$

where $\Lambda = (\lambda_{ij})$ is a matrix Lagrange multiplier. The Lagrangian can be written, using the “vec” notation, as

$$L(X, \Lambda) = \frac{1}{2} (\text{vec } X)^T (\text{vec } X) - (\text{vec } \Lambda)^T (A^T \otimes A) \text{vec } X$$

and its derivative with respect to $\text{vec } X$ is

$$(\nabla_X L(X, \Lambda))^T = (\text{vec } X)^T - (\text{vec } \Lambda)^T (A^T \otimes A)$$

see e.g. [5]. The necessary condition for optimality is that the derivative vanishes,

$$\begin{aligned} (\text{vec } X)^T - (\text{vec } \Lambda)^T (A^T \otimes A) &= \text{vec } O \\ \text{or equivalently, } X &= A^T \Lambda A^T. \end{aligned} \quad (4.3)$$

This condition is also sufficient, since (P.1) is a problem of minimizing a convex function subject to linear constraints. Indeed, the Moore–Penrose inverse A^\dagger is the unique $\{1\}$ -inverse of A satisfying (4.3) for some Λ (see e.g. [2]). Therefore A^\dagger is the unique solution of (P.1).

An alternative (simpler) way to show this is by writing (3.3) as

$$G = U \begin{pmatrix} \Sigma^{-1} & X \\ Y & Z \end{pmatrix} V^T = U \begin{pmatrix} \Sigma^{-1} & O \\ O & O \end{pmatrix} V^T + U \begin{pmatrix} O & X \\ Y & Z \end{pmatrix} V^T = A^\dagger + (G - A^\dagger). \quad (4.4)$$

We conclude that

$$\text{vol}_1^2 G = \text{vol}_1^2 A^\dagger + \text{vol}_1^2 (G - A^\dagger), \quad \text{whenever } AGA = A \quad (4.5)$$

proving that A^\dagger is the unique minimal norm $\{1\}$ -inverse of A .

For any $1 \leq k \leq r$ the problem analogous to (P.1) is

$$(P.k) \quad \text{minimize } \frac{1}{2} \text{vol}_k^2 X \quad \text{such that } AXA = A.$$

We note that $AXA = A$ implies

$$C_k(A)C_k(X)C_k(A) = C_k(A). \quad (4.6)$$

Taking (4.6) as the constraint in (P.k), we get the Lagrangian

$$L(X, \Lambda) := \frac{1}{2} \sum_{I \in Q_{k,n}, J \in Q_{k,m}} |\det X_{IJ}|^2 - \text{tr } C_k(\Lambda)^T (C_k(A)C_k(X)C_k(A) - C_k(A)).$$

It follows, in analogy with the case $k = 1$, that a necessary and sufficient condition for optimality of X is

$$C_k(X) = C_k(A^T)C_k(\Lambda)C_k(A^T). \quad (4.7)$$

Moreover, A^\dagger is the unique $\{1\}$ -inverse satisfying (4.7), and is therefore the unique solution of (P.k). \square

Note: The rank s of a $\{1\}$ -inverse G may be greater than r , in which case the volumes

$$\text{vol}_{r+1}(G), \text{vol}_{r+2}(G), \dots, \text{vol}_s(G)$$

are positive. However, the corresponding volumes of A^\dagger are zero, by Definition (1.2), so the inequalities (4.1) still hold.

The optimality characterization (4.1) has an interesting geometric interpretation. Consider first the case $k = 1$. Simplifying the identity (4.5) we get an equivalent condition

$$\text{tr } (A^\dagger)^T (G - A^\dagger) = 0, \quad \text{whenever } AGA = A, \quad (4.8)$$

i.e. A^\dagger is orthogonal to all matrices $G - A^\dagger$, where G ranges over $\{1\}$ -inverses of A , and the inner product $\langle X, Y \rangle := \text{tr } X^T Y$ is used. This makes sense since:

the set $A\{1\} = \{X : AXA = A\}$ of $\{1\}$ -inverses of A is an affine set in $\mathbf{R}^{n \times m}$,

the set $A\{1\} - A^\dagger = \{X : AXA = O\}$ is a subspace in $\mathbf{R}^{n \times m}$, and A^\dagger is the minimal norm element of $A\{1\}$, therefore A^\dagger is orthogonal to the subspace $A\{1\} - A^\dagger$.

For $k \geq 1$, the result analogous to (4.5) is

$$\begin{aligned} \text{vol}_k^2 G &:= \text{vol}_1^2 C_k(G) \\ &= \text{vol}_1^2 C_k(A^\dagger) + \text{vol}_1^2 (G - A^\dagger), \quad \text{from (4.4)} \\ &= \text{vol}_k^2 A^\dagger + \text{vol}_1^2 (G - A^\dagger) \end{aligned} \tag{4.9}$$

and the equivalent orthogonality condition (analogous to (4.8)) is

$$(\text{vec } C_k(A^\dagger))^T (\text{vec } C_k(G) - \text{vec } C_k(A^\dagger)) = 0, \tag{4.10}$$

for all $k = 1, \dots, r$ and $\{1\}$ -inverses G of A . The geometric interpretation is again that the set $C_k(A)\{1\}$ of $\{1\}$ -inverses of $C_k(A)$ is an affine set in $\mathbf{R}^{\binom{n}{k} \times \binom{m}{k}}$, and the vector $\text{vec } C_k(A^\dagger)$ is orthogonal to the subspace $C_k(A)\{1\} - C_k(A^\dagger)$.

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