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Matrix rank/inertia formulas for least-squares solutions with statistical applications

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Abstract: Least-Squares Solution (LSS) of a linear matrix equation and Ordinary Least-Squares Estimator (OLSE) of unknown parameters in a general linear model are two standard algebraical methods in computational mathematics and regression analysis. Assume that a symmetric quadratic matrix-valued function $\phi(Z) = Q - ZPZ'$ is given, where Z is taken as the LSS of the linear matrix equation $AZ = B$. In this paper, we establish a group of formulas for calculating maximum and minimum ranks and inertias of $\phi(Z)$ subject to the LSS of $AZ = B$, and derive many quadratic matrix equalities and inequalities for LSSs from the rank and inertia formulas. This work is motivated by some inference problems on OLSEs under general linear models, while the results obtained can be applied to characterize many algebraical and statistical properties of the OLSEs.

Keywords: Linear model, matrix equation, LSS, OLSE, quadratic matrix-valued function, rank, inertia

Dedicated to Professor Simo Puntanen on the occasion of his 70th birthday

1 Introduction

Throughout this paper, $\mathbb{R}^{m\times n}$ stands for the set of all $m \times n$ real matrices. A', $r(A)$ and $\mathscr{R}(A)$ stand for the transpose, rank, and range (column space) of a matrix $A \in \mathbb{R}^{m\times n}$, respectively. I_m denotes the identity matrix of order m. $[\,A,\ B\,]$ denotes a row block matrix consisting of A and B. The Moore–Penrose inverse of $A \in \mathbb{R}^{m\times n}$, denoted by $A^{\dagger}$, is defined to be the unique solution X satisfying the four matrix equations $AXA = A$, $XAX = X$, $(AX)' = AX$ and $(XA)' = XA$. E_A and F_A stand for $E_A = I_m - AA^{\dagger}$ and $F_A = I_n - A^{\dagger}A$ with $r(E_A) = m - r(A)$ and $r(F_A) = n - r(A)$. The Frobenius norm of a matrix $A \in \mathbb{R}^{m\times n}$ is defined to be $\|A\|_F = \sqrt{\mathrm{trace}(AA')}$. The symbols $i_+(A)$ and $i_-(A)$ for $A = A' \in \mathbb{R}^{m\times m}$, called the partial inertia of A, denote the number of the positive and negative eigenvalues of A counted with multiplicities, respectively, both of which satisfy $r(A) = i_+(A) + i_-(A)$. For brief, we use $i_{\pm}(A)$ to denote the both numbers. For a symmetric matrix $A = A' \in \mathbb{R}^{m\times m}$, the notations $A \succ 0$, $A \succcurlyeq 0$, $A \prec 0$ and $A \preccurlyeq 0$ mean that A is positive definite, positive semi-definite, negative definite, and negative semi-definite, respectively. Two symmetric matrices A and B of the same size are said to satisfy the inequalities $A \succ B$, $A \succcurlyeq B$, $A \prec B$ and $A \preccurlyeq B$ in the Löwner partial ordering if $A - B$ is positive definite, positive semi-definite, negative definite, and negative semi-definite respectively. It is well known that the Löwner partial ordering is a surprisingly strong and useful relation between two complex Hermitian (real symmetric) matrices. For more issues about connections between the inertias and the Löwner partial ordering of complex Hermitian (real symmetric) matrices, as well as applications of the matrix inertia and the Löwner partial ordering in statistic analysis, see, e.g., [18, 20, 30, 31].

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Consider a general linear model defined by

$$y = X\beta + e, \quad E(e) = 0, \quad Cov(e) = \sigma^2\Sigma, \tag{1.1}$$

where y is an $n \times 1$ observable random vector, X is an $n \times p$ known matrix of arbitrary rank, β is a $p \times 1$ fixed but unknown parameter vector, e is a random error vector, σ^2 is an unknown positive number, and Σ is an $n \times n$ known positive semi-definite matrix of arbitrary rank.

Recall that the well-known Ordinary Least Squares Estimator (OLSE for short) of the unknown parameter vector β in (1.1) is defined to be

$$\widehat{\beta} = \arg\min_{\beta \in \mathbb{R}^{p\times 1}} (y - X\beta)'(y - X\beta), \tag{1.2}$$

while the OLSE of the parametric vector $K\beta$ under (1.1) is defined to be $K\widehat{\beta}$. A direct decomposition of the norm $(y - X\beta)'(y - X\beta)$ in (1.2) is

$$\begin{aligned}(y - X\beta)'(y - X\beta) &= (y - XX^{\dagger}y)'(y - XX^{\dagger}y) + (XX^{\dagger}y - X\beta)'(XX^{\dagger}y - X\beta)\\ &= y'E_Xy + (P_Xy - X\beta)'(P_Xy - X\beta),\end{aligned}$$

where the two terms on the right-hand side satisfy $y'E_Xy \geqslant 0$ and $(P_Xy - X\beta)'(P_Xy - X\beta) \geqslant 0$. Hence,

$$\min_{\beta \in \mathbb{R}^{p\times 1}} (y - X\beta)'(y - X\beta) = y'E_Xy + \min_{\beta \in \mathbb{R}^{p\times 1}} (P_Xy - X\beta)'(P_Xy - X\beta) = y'E_Xy,$$

where the equation $X\beta = P_Xy$, which is equivalent to the so-called normal equation $X'X\beta = X'y$ by pre-multiplying X', is always consistent; see, e.g., [6, p. 114] and [19, pp. 164–165]. An alternative definition of the OLSE of β in (1.1) is given by

$$\widehat{\beta} = \widehat{L}y \quad \text{and} \quad \widehat{L} = \operatorname{argmin}_{L \in \mathbb{R}^{p\times n}} (y - XLy)'(y - XLy). \tag{1.3}$$

Also notice that $(y - XLy)'(y - XLy)$ in (1.3) can be decomposed as

$$(y - XLy)'(y - XLy) = y'E_Xy + y'(P_X - XL)'(P_X - XL)y,$$

where $y'E_Xy \geqslant 0$ and $y'(P_X - XL)'(P_X - XL)y \geqslant 0$. Hence,

$$\min_{L \in \mathbb{R}^{p\times n}} (y - XLy)'(y - XLy) = y'E_Xy + \min_{L \in \mathbb{R}^{p\times n}} y'(P_X - XL)'(P_X - XL)y = y'E_Xy,$$

where the matrix equation $XL = P_X$ is always solvable for L, say, $L = X^{\dagger}$. Solving the equation $X\beta = P_Xy$ by Lemma 1.5 below yields the following well-known results.

Lemma 1.1. *Assume that $P_Xy \neq 0$. Then, the OLSEs of β and $K\beta$ under* (1.1) *can be written as*

$$\begin{aligned}\widehat{\beta} &= \left(X^{\dagger} + F_XU\right)P_Xy = \left(X^{\dagger} + F_XUP_X\right)y,\\ K\widehat{\beta} &= \left(KX^{\dagger} + KF_XU\right)P_Xy = \left(KX^{\dagger} + KF_XUP_X\right)y,\end{aligned}$$

where $U \in \mathbb{R}^{p\times n}$ is arbitrary. In this setting, the following results hold.

(a) *The expectations of $\widehat{\beta}$ and $K\widehat{\beta}$ are*

$$E(\widehat{\beta}) = \left(X^{\dagger}X + F_XUX\right)\beta, \quad E(K\widehat{\beta}) = \left(KX^{\dagger}X + KF_XUX\right)\beta.$$

(b) *The covariance matrices of $\widehat{\beta}$ and $K\widehat{\beta}$ are*

$$\begin{aligned}Cov(\widehat{\beta}) &= \sigma^2\left(X^{\dagger} + F_XU\right)P_X\Sigma P_X\left(X^{\dagger} + F_XU\right)',\\ Cov(K\widehat{\beta}) &= \sigma^2\left(KX^{\dagger} + KF_XU\right)P_X\Sigma P_X\left(KX^{\dagger} + KF_XU\right)'.\end{aligned}$$

(c) *The matrix mean square errors (MMSEs) of* $\widehat{\beta}$ *and* $K\widehat{\beta}$ *are*

$$\mathrm{MMSE}(\widehat{\beta}) = E\left[(\widehat{\beta}-\beta)(\widehat{\beta}-\beta)'\right] = Cov(\widehat{\beta}) + \mathrm{Bias}(\widehat{\beta})\mathrm{Bias}(\widehat{\beta})',$$

$$\mathrm{MMSE}(K\widehat{\beta}) = E\left[(K\widehat{\beta}-K\beta)(K\widehat{\beta}-K\beta)'\right] = Cov(K\widehat{\beta}) + \mathrm{Bias}(K\widehat{\beta})\mathrm{Bias}(K\widehat{\beta})'.$$

(d) *There exists* $U \in \mathbb{R}^{p\times n}$ *such that*

$$E(K\widehat{\beta}) = (KX^{\dagger}X + KF_XUX)\beta = K\beta$$

holds for all β *if and only if* $\mathscr{R}(K') \subseteq \mathscr{R}(X')$, *namely*, $K\beta$ *is estimable. In this case*,

$$K\widehat{\beta} = KX^{\dagger}y, \;\; E(K\widehat{\beta}) = K\beta, \;\; \mathrm{MMSE}(K\widehat{\beta}) = Cov(K\widehat{\beta}) = \sigma^2 KX^{\dagger}\Sigma(KX^{\dagger})';$$

in particular,

$$X\widehat{\beta} = P_Xy, \;\; E(X\widehat{\beta}) = X\beta, \;\; \mathrm{MMSE}(X\widehat{\beta}) = Cov(X\widehat{\beta}) = \sigma^2 P_X\Sigma P_X.$$

In the inference theory of linear models, there has been considerable interest in establishing estimators of the unknown parameters by certain linear functions of the observed response vectors in the models. The OLSE of unknown parameters in a linear model, as described above, is a simplest linear estimator with extensive applications in regression analysis, while many results on computational and algebraic properties of OLSEs were established in the statistical literature. Once an estimator is defined and derived, it is always desirable to know more behaviors of the estimators under the models. In particular, equalities and inequalities for the covariance matrices of given estimators and the corresponding matrix risk functions, such as

$$Cov(K\widehat{\beta}) = Q \;\; (\succ Q \; \succcurlyeq Q, \; \prec Q, \; \preccurlyeq Q), \;\; \mathrm{MMSE}(K\widehat{\beta}) = Q \;\; (\succ Q \; \succcurlyeq Q, \; \prec Q, \; \preccurlyeq Q)$$

for a given symmetric matrix Q, as well as the matrix minimization problems

$$Cov(K\widehat{\beta}) \overset{\mathrm{L}}{=} \min, \;\; \mathrm{MMSE}(K\widehat{\beta}) \overset{\mathrm{L}}{=} \min$$

in the Löwner partial ordering, can be used to characterize mathematical and statistical properties of the estimators. Note from Lemma 1.1 that $Cov(K\widehat{\beta})$ and $\mathrm{MMSE}(K\widehat{\beta})$ are in fact symmetric quadratic matrix-valued functions with arbitrary matrix U. Hence, equalities and inequalities for $Cov(K\widehat{\beta})$ and $\mathrm{MMSE}(K\widehat{\beta})$ depend on the choices of U.

Motivated by the above considerations in statistical analysis , we propose some general problems on establishing equalities and inequalities for a symmetric quadratic matrix-valued function subject to the Least-Squares Solution (LSS) of a linear matrix equation as follows.

Problem 1.2. Let

$$AZ = B \tag{1.4}$$

be a linear matrix equation, where $A \in \mathbb{R}^{p\times n}$ and $B \in \mathbb{R}^{p\times m}$ are two given matrices. Then, the LSS of (1.4) is defined to be the matrix

$$Z_0 = \underset{Z\in\mathbb{R}^{n\times m}}{\mathrm{argmin}} \parallel AZ - B \parallel_F^2 = \underset{Z\in\mathbb{R}^{n\times m}}{\mathrm{argmin}}\ \mathrm{tr}\left[(AZ-B)'(AZ-B)\right].$$

The solution is not necessarily unique, and let $\mathcal{S}$ be the collection of all LSSs of (1.4):

$$\mathcal{S} = \left\{Z \in \mathbb{R}^{n\times m} \mid \mathrm{tr}[(AZ-B)'(AZ-B)] = \min\right\}.$$

Further, let $\phi(Z) = Q - ZPZ'$ be a quadratic matrix-valued function, where $P = P' \in \mathbb{R}^{m\times m}$ and $Q = Q' \in \mathbb{R}^{n\times n}$ are given matrices. In this setting, establish exact algebraic formulas for calculating the following six maximum and minimum ranks and inertias

$$\max_{Z\in\mathcal{S}} r(Q - ZPZ'), \quad \min_{Z\in\mathcal{S}} r(Q - ZPZ'),$$

$$\max_{Z\in\mathcal{S}} i_{\pm}(Q - ZPZ'), \quad \min_{Z\in\mathcal{S}} i_{\pm}(Q - ZPZ').$$

Problem 1.3. Under the assumptions in Problem 1.2, establish necessary and sufficient conditions for the following two partial ordering optimization problems

$$\left\{Q - ZPZ^{'} \mid Z \in \mathcal{S}\right\} \stackrel{\mathrm{L}}{=} \max, \quad \left\{Q - ZPZ^{'} \mid Z \in \mathcal{S}\right\} \stackrel{\mathrm{L}}{=} \min$$

to have solutions, respectively, and give exact algebraic expressions of the solutions.

Problem 1.4. Under the assumptions in Problem 1.2, establish necessary and sufficient conditions for the following constrained quadratic matrix equation

$$ZPZ^{'} = Q \quad \text{s.t. } Z \in \mathcal{S}$$

to have a solution, as well as necessary and sufficient conditions for the following four constrained quadratic matrix inequalities

$$ZPZ^{'} \succ Q\,(\succcurlyeq Q, \prec Q, \preccurlyeq Q)$$

to hold for a $Z \in \mathcal{S}$ (for all matrices $Z \in \mathcal{S}$), respectively.

Concerning the LSS of (1.4), we have the following direct derivation. Decompose $(B - AZ)^{'}(B - AZ)$ as

$$\begin{aligned}(B - AZ)^{'}(B - AZ) &= (B - AA^{\dagger}B)^{'}(B - AA^{\dagger}B) + (AA^{\dagger}B - AZ)^{'}(AA^{\dagger}B - AZ)\\ &= B^{'}E_AB + (P_AB - AZ)^{'}(P_AB - AZ).\end{aligned}$$

Hence,

$$\begin{aligned}\mathrm{tr}\left[(B - AZ)^{'}(B - AZ)\right] &= \mathrm{tr}(B^{'}E_AB) + \mathrm{tr}\left[(P_AB - AZ)^{'}(P_AB - AZ)\right],\\ \min_{Z\in\mathbb{R}^{n\times m}} \mathrm{tr}\left[(B - AZ)^{'}(B - AZ)\right] &= \mathrm{tr}(B^{'}E_AB) + \min_{Z\in\mathbb{R}^{n\times m}} \mathrm{tr}\left[(P_AB - AZ)^{'}(P_AB - AZ)\right]\\ &= \mathrm{tr}(B^{'}E_AB),\end{aligned}$$

where the equation $AZ = P_AB$, which is equivalent to $A^{'}AZ = A^{'}B$, is always consistent. A seminal result due to [17] on (1.4) is given below.

Lemma 1.5. *The matrix equation in* (1.4) *has a solution if and only if $AA^{\dagger}B = B$. In this case, the general solution can be written in the following parametric form $Z = A^{\dagger}B + F_AV$, where $V \in \mathbb{R}^{n\times m}$ is arbitrary. The solution of* (1.4) *is unique if and only if $r(A) = n$. If* (1.4) *is inconsistent, then the normal equation of* (1.4) *is $A^{'}AZ = A^{'}B$, and the general expression of the LSSs of* (1.4) *can be written as $Z = A^{\dagger}B + F_AV$, where $V \in \mathbb{R}^{n\times m}$ is arbitrary. The LSSs of* (1.4) *is unique if and only if $r(A) = n$.*

Lemma 1.6 ([16]). *The pair of matrix equations $AZ = B$ and $ZC = D$ have a common solution if and only if $AA^{\dagger}B = B$, $DC^{\dagger}C = D$ and $AD = BC$. In this case, the general common solution can be written in the following parametric form $Z = A^{\dagger}B + DC^{\dagger} - A^{\dagger}ADC^{\dagger} + F_AVE_C$, where V is arbitrary.*

Lemma 1.7 ([20]). *Let $\mathcal{S}$ be a set consisting of matrices over $\mathbb{R}^{m\times n}$, and let $\mathcal{H}$ be a set consisting of symmetric matrices over $\mathbb{R}^{m\times m}$. Then, the following assertions hold.*

(a) *Under $m = n$, there exists a nonsingular matrix $Z \in \mathcal{S}$ if and only if $\max_{Z\in\mathcal{S}} r(Z) = m$.*
(b) *Under $m = n$, all $Z \in \mathcal{S}$ are nonsingular if and only if $\min_{Z\in\mathcal{S}} r(Z) = m$.*
(c) *$0 \in \mathcal{S}$ if and only if $\min_{Z\in\mathcal{S}} r(Z) = 0$.*
(d) *$\mathcal{S} = \{0\}$ if and only if $\max_{Z\in\mathcal{S}} r(Z) = 0$.*
(e) *All $Z \in \mathcal{S}$ have the same rank if and only if $\max_{Z\in\mathcal{S}} r(Z) = \min_{Z\in\mathcal{S}} r(Z)$.*
(f) *$\mathcal{H}$ has a matrix $Z \succ 0$ ($Z \prec 0$) if and only if $\max_{Z\in\mathcal{H}} i_{+}(Z) = m$ $\left(\max_{Z\in\mathcal{H}} i_{-}(Z) = m\right)$.*
(g) *All $Z \in \mathcal{H}$ satisfy $Z \succ 0$ ($Z \prec 0$) if and only if $\min_{Z\in\mathcal{H}} i_{+}(Z) = m$ $\left(\min_{Z\in\mathcal{H}} i_{-}(Z) = m\right)$.*
(h) *$\mathcal{H}$ has a matrix $Z \succcurlyeq 0$ ($Z \preccurlyeq 0$) if and only if $\min_{Z\in\mathcal{H}} i_{-}(Z) = 0$ $\left(\min_{Z\in\mathcal{H}} i_{+}(Z) = 0\right)$.*
(i) *All $Z \in \mathcal{H}$ satisfy $Z \succcurlyeq 0$ ($Z \preccurlyeq 0$) if and only if $\max_{Z\in\mathcal{H}} i_{-}(Z) = 0$ $\left(\max_{Z\in\mathcal{H}} i_{+}(Z) = 0\right)$.*

(j) *All* $Z \in \mathcal{H}$ *have the same positive index of inertia if and only if* $\max_{Z\in\mathcal{H}} i_{+}(Z) = \min_{Z\in\mathcal{H}} i_{+}(Z)$.
(k) *All* $Z \in \mathcal{H}$ *have the same negative index of inertia if and only if* $\max_{Z\in\mathcal{H}} i_{-}(Z) = \min_{Z\in\mathcal{H}} i_{-}(Z)$.

The assertions in Lemma 1.7 directly follow from the definitions of rank/inertia, definiteness, and semi-definiteness of (symmetric) matrices. These assertions show that if certain expansion formulas for calculating ranks/inertias of differences of (symmetric) matrices are established, we can use them to characterize the corresponding matrix equalities and inequalities. This fact reflects without doubt the most exciting and intriguing values of matrix ranks/inertias in matrix theory and applications, and thus prompt people to produce a huge amount of matrix rank/inertia formulas from the theoretical and applied points of view in the past 40 years. It has long history to establish rank formulas for block matrices and use the formulas in statistical inferences, and a pioneer work in this aspect can be found in [7]. The intriguing connections between generalized inverses of matrices and rank formulas of matrices were recognized in 1970s, and a seminal work on rank formulas for matrices and their generalized inverses was presented in [15]. Over the last 40 years, the theory of matrix ranks/inertias has grown into an active area of research in its own right, and now becomes a magic weapon of simplifying various matrix expressions and establishing various matrix equalities and inequalities according to the assertions in Lemma 1.7.

It should be pointed out that matrix rank and inertia optimization problems are a class of discontinuous optimization problems on finding the global maximum and minimum ranks and inertias of matrix-valued functions, in which the variable matrices are running over certain feasible matrix sets. Concerning the analytical formulas for calculating the global maximum and minimum ranks and inertias of $Q - ZPZ'$ subject to $AZ = B$, we have the following known results.

Lemma 1.8 ([22]). *Let* $\phi(Z)$ *be as given in Problem* 1.2, *and assume that* (1.4) *is consistent*. *Then*, *the following six formulas hold*

$$\begin{aligned}
&\max_{AZ=B} r(\,Q - ZPZ'\,)\\
&= \min\left\{2n + r(\,AQA' - BPB'\,) - 2r(A),\ n + r[\,AQ,\ BP\,] - r(A),\ r(Q) + r(P)\right\},\\
&\min_{AZ=B} r(\,Q - ZPZ'\,) = \max\{\,s_1,\ s_2,\ s_3,\ s_4\,\},\\
&\max_{AZ=B} i_{\pm}(\,Q - ZPZ'\,) = \min\left\{n + i_{\pm}(\,AQA' - BPB'\,) - r(A),\ \ i_{\pm}(Q) + i_{\mp}(P)\right\},\\
&\min_{AZ=B} i_{\pm}(\,Q - ZPZ'\,) = \max\{\,u_{\pm},\ v_{\pm}\,\},
\end{aligned}$$

where

$$\begin{aligned}
s_1 &= r(\,AQA' - BPB'\,) + 2r[\,AQ,\ BP\,] - 2r[\,AQA',\ BP\,],\\
s_2 &= 2r[\,AQ,\ BP\,] + r(Q) - r(P) - 2r(AQ),\\
s_3 &= 2r[\,AQ,\ BP\,] + i_{+}(\,AQA' - BPB'\,) - r[\,AQA',\ BP\,] + i_{-}(Q) - i_{-}(P) - r(AQ),\\
s_4 &= 2r[\,AQ,\ BP\,] + i_{-}(\,AQA' - BPB'\,) - r[\,AQA',\ BP\,] + i_{+}(Q) - i_{+}(P) - r(AQ),\\
u_{\pm} &= i_{\pm}(\,AQA' - BPB'\,) + r[\,AQ,\ BP\,] - r[\,AQA',\ BP\,],\\
v_{\pm} &= r[\,AQ,\ BP\,] + i_{\pm}(Q) - i_{\pm}(P) - r(AQ).
\end{aligned}$$

2 Main results

Theorem 2.1. *Let* $\phi(Z)$ *and* $\mathcal{S}$ *be as given in Problem* 1.2. *Then*, *the following results hold*.

(a) *The maximum rank of $\phi(Z)$ subject to $Z \in \mathcal{S}$ is*

$$\max_{Z\in\mathcal{S}} r(\,Q - ZPZ'\,) = \min\Big\{2n + r(\,A'AQA'A - A'BPB'A\,) - 2r(A),\\ n + r[\,A'AQ,\ A'BP\,] - r(A),\ r(Q) + r(P)\Big\}.$$

(b) *The minimum rank of $\phi(Z)$ subject to $Z \in \mathcal{S}$ is*

$$\min_{Z\in\mathcal{S}} r(\,Q - ZPZ'\,) = \max\{\,s_1,\ s_2,\ s_3,\ s_4\,\},$$

where

$$\begin{aligned} s_1 &= r(\,A'AQA'A - A'BPB'A\,) + 2r[\,A'AQ,\ A'BP\,] - 2r[\,A'AQA',\ A'BP\,],\\ s_2 &= 2r[\,A'AQ,\ A'BP\,] + r(Q) - r(P) - 2r(AQ),\\ s_3 &= 2r[\,A'AQ,\ A'BP\,] + i_+(\,A'AQA'A - A'BPB'A\,) - r[\,A'AQA',\ A'BP\,]\\ &\quad + i_-(Q) - i_-(P) - r(AQ),\\ s_4 &= 2r[\,A'AQ,\ A'BP\,] + i_-(\,A'AQA'A - A'BPB'A\,) - r[\,A'AQA',\ A'BP\,]\\ &\quad + i_+(Q) - i_+(P) - r(AQ). \end{aligned}$$

(c) *The maximum partial inertia of $\phi(Z)$ subject to $Z \in \mathcal{S}$ are*

$$\max_{Z\in\mathcal{S}} i_\pm(\,Q - ZPZ'\,) = \min\Big\{n + i_\pm(\,A'AQA'A - A'BPB'A\,) - r(A),\ \ i_\pm(Q) + i_\mp(P)\Big\}.$$

(d) *The minimum partial inertia of $\phi(Z)$ subject to $Z \in \mathcal{S}$ are*

$$\min_{Z\in\mathcal{S}} i_\pm(\,Q - ZPZ'\,) = \max\{u_\pm,\ v_\pm\},$$

where

$$\begin{aligned} u_\pm &= i_\pm(\,A'AQA'A - A'BPB'A\,) + r[\,A'AQ,\ A'BP\,] - r[\,A'AQA',\ A'BP\,],\\ v_\pm &= r[\,A'AQ,\ A'BP\,] + i_\pm(Q) - i_\pm(P) - r(AQ). \end{aligned}$$

Proof. It can be seen from Lemma 1.5 that

$$\begin{aligned} &\max_{Z\in\mathcal{S}} r(\,Q - ZPZ'\,) = \max_{A'AZ=A'B} r(\,Q - ZPZ'\,), \quad \min_{Z\in\mathcal{S}} r(\,Q - ZPZ'\,) = \min_{A'AZ=A'B} r(\,Q - ZPZ'\,),\\ &\max_{Z\in\mathcal{S}} i_\pm(\,Q - ZPZ'\,) = \max_{A'AZ=A'B} i_\pm(\,Q - ZPZ'\,), \quad \min_{Z\in\mathcal{S}} i_\pm(\,Q - ZPZ'\,) = \min_{A'AZ=A'B} i_\pm(\,Q - ZPZ'\,). \end{aligned}$$

In these cases, replacing A with $A'A$ and B with $A'B$ in Lemma 1.8 and simplifying, we obtain the formulas in (a)–(d). □

Applying Lemma 1.7 to Theorem 2.1, we obtain the following consequences. Their proofs are omitted.

Corollary 2.2. *Let $\phi(Z)$ and $\mathcal{S}$ be as given in Problem 1.2, $s_1, \ldots, s_4$ be as given in Theorem 2.1. Then, the following results hold.*

(a) *$AZ = B$ has an LSS such that $Q - ZPZ'$ is nonsingular if and only if*

$$r(\,A'AQA'A - A'BPB'A\,) \geqslant 2r(A) - n,\ \ r[\,A'AQ,\ A'BP\,] = r(A),\ \ r(Q) + r(P) \geqslant n.$$

(b) *$Q - ZPZ'$ is nonsingular for all LSSs of $AZ = B$ if and only if one of $s_i = n$, $i = 1, \ldots, 4$ holds.*

(c) *$AZ = B$ has an LSS such that $ZPZ' = Q$ if and only if*

$$A'AQA'A = A'BPB'A,\ \ \mathscr{R}(A'AQ) \subseteq \mathscr{R}(A'BP), \quad r(A'BP) + i_\pm(Q) \leqslant i_\pm(P) + r(AQ).$$

(d) *All LSSs of $AZ = B$ satisfy $ZPZ' = Q$ if and only if $r(A) = n$ and $A'AQA'A = A'BPB'A$, or $Q = 0$ and $P = 0$.*

(e) *$AZ = B$ has an LSS such that $Q - ZPZ^{'} \succ 0$ if and only if*

$$i_{+}(A^{'}AQA^{'}A - A^{'}BPB^{'}A) = r(A) \text{ and } i_{+}(Q) + i_{-}(P) \geqslant n.$$

(f) *All LSSs of $AZ = B$ satisfy $Q - ZPZ^{'} \succ 0$ if and only if*

$$i_{+}(A^{'}AQA^{'}A - A^{'}BPB^{'}A) + r[A^{'}AQ,\ A^{'}BP] = n + r[A^{'}AQA^{'},\ A^{'}BP]$$

or

$$r[A^{'}AQ,\ A^{'}BP] + i_{+}(Q) = n + i_{+}(P) + r(AQ).$$

(g) *$AZ = B$ has an LSS such that $Q - ZPZ^{'} \prec 0$ if and only if*

$$i_{-}(A^{'}AQA^{'}A - A^{'}BPB^{'}A) = r(A) \text{ and } i_{-}(Q) + i_{+}(P) \geqslant n.$$

(h) *All LSSs of $AZ = B$ satisfy $Q - ZPZ^{'} \prec 0$ if and only if*

$$i_{-}(A^{'}AQA^{'}A - A^{'}BPB^{'}A) + r[A^{'}AQ,\ A^{'}BP] = n + r[A^{'}AQA^{'},\ A^{'}BP]$$

or

$$r[A^{'}AQ,\ A^{'}BP] + i_{-}(Q) = n + i_{-}(P) + r(AQ).$$

(i) *$AZ = B$ has an LSS such that $Q - ZPZ^{'} \succcurlyeq 0$ if and only if*

$$A^{'}AQA^{'}A \succcurlyeq A^{'}BPB^{'}A,\ \ r[A^{'}AQA^{'},\ A^{'}BP] = r[A^{'}AQ,\ A^{'}BP] \leqslant i_{-}(P) - i_{-}(Q) + r(AQ).$$

(j) *All LSSs of $AZ = B$ satisfy $Q - ZPZ^{'} \succcurlyeq 0$ if and only if $r(A) = n$ and $A^{'}AQA^{'}A \succcurlyeq A^{'}BPB^{'}A$, or $Q \succcurlyeq 0$ and $P \preccurlyeq 0$;*

(k) *$AZ = B$ has an LSS such that $Q - ZPZ^{'} \preccurlyeq 0$ if and only if*

$$A^{'}AQA^{'}A \preccurlyeq A^{'}BPB^{'}A,\ \ r[A^{'}AQA^{'},\ A^{'}BP] = r[A^{'}AQ,\ A^{'}BP] \leqslant i_{+}(P) - i_{+}(Q) + r(AQ).$$

(l) *All LSSs of $AZ = B$ satisfy $Q - ZPZ^{'} \preccurlyeq 0$ if and only if $r(A) = n$ and $A^{'}AQA^{'}A \preccurlyeq A^{'}BPB^{'}A$, or $Q \preccurlyeq 0$ and $P \succcurlyeq 0$.*

The following two corollaries follow directly from Theorem 2.1.

Corollary 2.3. *Let $\phi(Z)$ and $\mathcal{S}$ be as given in Problem 1.2 with $P \succ 0$ and $Q \succ 0$. Then,*

$$\max_{Z \in \mathcal{S}} r(Q - ZPZ^{'}) = \min \left\{ n,\ \ 2n + r(A^{'}AQA^{'}A - A^{'}BPB^{'}A) - 2r(A) \right\},$$

$$\min_{Z \in \mathcal{S}} r(Q - ZPZ^{'}) = \max \left\{ r(A^{'}AQA^{'}A - A^{'}BPB^{'}A),\ \ i_{-}(A^{'}AQA^{'}A - A^{'}BPB^{'}A) + n - m \right\},$$

$$\max_{Z \in \mathcal{S}} i_{\pm}(Q - ZPZ^{'}) = \min \left\{ n + i_{\pm}(A^{'}AQA^{'}A - A^{'}BPB^{'}A) - r(A),\ \ i_{\pm}(I_n) + i_{\mp}(I_m) \right\},$$

$$\min_{Z \in \mathcal{S}} i_{\pm}(Q - ZPZ^{'}) = \max \left\{ i_{\pm}(A^{'}AQA^{'}A - A^{'}BPB^{'}A),\ \ i_{\pm}(I_n) - i_{\pm}(I_m) \right\}.$$

In consequence, the following results hold.

(a) *$AZ = B$ has an LSS such that $Q - ZPZ^{'}$ is nonsingular if and only if*

$$r(A^{'}AQA^{'}A - A^{'}BPB^{'}A) \geqslant 2r(A) - n.$$

(b) *$Q - ZPZ^{'}$ is nonsingular for all LSSs of $AZ = B$ if and only if*

$$r(A^{'}AQA^{'}A - A^{'}BPB^{'}A) = n \ \text{ or } \ i_{-}(A^{'}AQA^{'}A - A^{'}BPB^{'}A) = m.$$

(c) *$AZ = B$ has a least-squares solution such that $ZPZ^{'} = Q$ if and only if $A^{'}AQA^{'}A = A^{'}BPB^{'}A$ and $m \geqslant n$.*

(d) *All LSSs of $AZ = B$ satisfy $ZPZ^{'} = Q$ if and only if $A^{'}AQA^{'}A = A^{'}BPB^{'}A$ and $r(A) = n$.*

(e) *$AZ = B$ has an LSS such that $Q \succ ZPZ'$ if and only if $i_+(A'AQA'A - A'BPB'A) = r(A)$.*
(f) *All LSSs of $AZ = B$ satisfy $Q \succ ZPZ'$ if and only if $i_+(A'AQA'A - A'BPB'A) = n$.*
(g) *$AZ = B$ has an LSS such that $Q \prec ZPZ'$ if and only if $i_-(A'AQA'A - A'BPB'A) = r(A)$ and $m \geqslant n$.*
(h) *All LSSs of $AZ = B$ satisfy $Q \prec ZPZ'$ if and only if $i_-(A'AQA'A - A'BPB'A) = n$.*
(i) *$AZ = B$ has an LSS such that $Q \succcurlyeq ZPZ'$ if and only if $A'AQA'A \succcurlyeq A'BPB'A$.*
(j) *All LSSs of $AZ = B$ satisfy $Q \succcurlyeq ZPZ'$ if and only if $A'AQA'A \succcurlyeq A'BPB'A$ and $r(A) = n$.*
(k) *$AZ = B$ has an LSS such that $Q \preccurlyeq ZPZ'$ if and only if $A'AQA'A \preccurlyeq A'BPB'A$ and $n \leqslant m$.*
(l) *All LSSs of $AZ = B$ satisfy $Q \preccurlyeq ZPZ'$ if and only if $A'AQA'A \preccurlyeq A'BPB'A$ and $r(A) = n$.*

Corollary 2.4. *Let $\mathcal{S}$ be as given in Problem 1.2. Then,*

$$\max_{Z\in\mathcal{S}} r(I_n - ZZ') = \min\left\{n,\ \ 2n + r(A'AA'A - A'BB'A) - 2r(A)\right\},$$

$$\min_{Z\in\mathcal{S}} r(I_n - ZZ') = \max\left\{r(A'AA'A - A'BB'A),\ \ i_-(A'AA'A - A'BB'A) + n - m\right\},$$

$$\max_{Z\in\mathcal{S}} i_\pm(I_n - ZZ') = \min\left\{n + i_\pm(A'AA'A - A'BB'A) - r(A),\ \ i_\pm(I_n) + i_\mp(I_m)\right\},$$

$$\min_{Z\in\mathcal{S}} i_\pm(I_n - ZZ') = \max\left\{i_\pm(A'AA'A - A'BB'A),\ \ i_\pm(I_n) - i_\pm(I_m)\right\}.$$

In consequence, the following results hold.
(a) *$AZ = B$ has an LSS such that $I_n - ZZ'$ is nonsingular if and only if $r(A'AA'A - A'BB'A) \geqslant 2r(A) - n$.*
(b) *$I_n - ZZ'$ is nonsingular for all LSSs of $AZ = B$ if and only if $r(A'AA'A - A'BB'A) = n$ or $i_-(A'AA'A - A'BB'A) = m$.*
(c) *$AZ = B$ has an LSS such that $ZZ' = I_n$, i.e., the rows of a solution of $AZ = B$ are orthogonal, if and only if $A'AA'A = A'BB'A$ and $m \geqslant n$.*
(d) *All LSSs of $AZ = B$ satisfy $ZZ' = I_n$ if and only if $A'AA'A = A'BB'A$ and $r(A) = n$.*
(e) *$AZ = B$ has an LSS such that $ZZ' \prec I_n$ if and only if $i_+(A'AA'A - A'BB'A) = r(A)$.*
(f) *All LSSs of $AZ = B$ satisfy $ZZ' \prec I_n$ if and only if $i_+(A'AA'A - A'BB'A) = n$.*
(g) *$AZ = B$ has an LSS such that $ZZ' \succ I_n$ if and only if $i_-(A'AA'A - A'BB'A) = r(A)$ and $m \geqslant n$.*
(h) *All LSSs of $AZ = B$ satisfy $ZZ' \succ I_n$ if and only if $i_-(A'AA'A - A'BB'A) = n$.*
(i) *$AZ = B$ has an LSS such that $ZZ' \preccurlyeq I_n$ if and only if $A'AA'A \succcurlyeq A'BB'A$.*
(j) *All LSSs of $AZ = B$ satisfy $ZZ' \preccurlyeq I_n$ if and only if $A'AA'A \succcurlyeq A'BB'A$ and $r(A) = n$.*
(k) *$AZ = B$ has an LSS such that $ZZ' \succcurlyeq I_n$ if and only if $A'AA'A \preccurlyeq A'BB'A$ and $m \geqslant n$.*
(l) *All LSSs of $AZ = B$ satisfy $ZZ' \succcurlyeq I_n$ if and only if $A'AA'A \preccurlyeq A'BB'A$ and $r(A) = n$.*

In mathematics, the collection of all matrices Z that satisfy $ZZ' = I_n$ is called a complex Stiefel manifold; see, e.g., [8, 11], while the collections of all matrices Z that satisfy $ZZ' \succ I_n$ ($\succcurlyeq I_n$, $\prec I_n$, $\preccurlyeq I_n$) are called generalized complex Stiefel manifolds. The results in Corollary 2.4 characterize some basic relations between the manifold $\mathcal{S}$ and these Stiefel manifolds.

In the remaining part of this section, we solve Problem 1.3, i.e., to find $\widehat{Z}$, $\widetilde{Z} \in \mathcal{S}$ such that

$$\phi(Z) \preccurlyeq \phi(\widehat{Z}) \ \text{ for all } \ Z \in \mathcal{S}, \tag{2.1}$$

$$\phi(Z) \succcurlyeq \phi(\widetilde{Z}) \ \text{ for all } \ Z \in \mathcal{S} \tag{2.2}$$

hold, respectively.

Theorem 2.5. *Let $\phi(Z)$ and $\mathcal{S}$ be as given in Problem 1.2 with $r(A) < n$. Then, the following results hold.*
(a) *There exists a $\widehat{Z} \in \mathcal{S}$ such that (2.1) holds if and only if $P \succcurlyeq 0$ and $A'BP = 0$. In this case, the maximizer and the corresponding maximum matrix are given by*

$$\operatorname*{argmax}_{\succcurlyeq}\left\{\phi(Z)\,|\,Z \in \mathcal{S}\right\} = A^{\dagger}B + F_AUF_P, \quad \max_{\succcurlyeq}\left\{\phi(Z)\,|\,Z \in \mathcal{S}\right\} = Q,$$

where $U \in \mathbb{R}^{n\times m}$ is arbitrary.

(b) *There exists a* $\widetilde{Z} \in \mathcal{S}$ *such that* (2.2) *holds if and only if* $P \preccurlyeq 0$ *and* $A^{'}BP = 0$. *In this case, the minimizer and the corresponding minimum matrix are given by*

$$\underset{\succcurlyeq}{\operatorname{argmin}} \left\{ \phi(Z) \,|\, Z \in \mathcal{S} \right\} = A^{\dagger}B + F_A U F_P, \quad \underset{\succcurlyeq}{\min} \left\{ \phi(Z) \,|\, Z \in \mathcal{S} \right\} = Q,$$

where $U \in \mathbb{R}^{n\times m}$ *is arbitrary.*

Proof. Under $r(A) = n$, the LSS of $AZ = B$ is unique, so that (2.1) and (2.2) become trivial. Let

$$\phi_M(Z) = \phi(Z) - \phi(\widehat{Z}) = \widehat{Z}P\widehat{Z}^{'} - ZPZ^{'}, \quad \phi_m(Z) = \phi(Z) - \phi(\widetilde{Z}) = \widetilde{Z}P\widetilde{Z}^{'} - ZPZ^{'}.$$

Then, (2.1) and (2.2) are equivalent to

$$\phi_M(Z) \preccurlyeq 0, \;\; Z, \; \widehat{Z} \in \mathcal{S},$$
$$\phi_m(Z) \succcurlyeq 0, \;\; Z, \; \widetilde{Z} \in \mathcal{S},$$

respectively. It can be seen from Corollary 2.2(j) and (l) that they are further equivalent to

$$\widehat{Z}P\widehat{Z}^{'} \preccurlyeq 0, \;\; A^{'}A\widehat{Z} = A^{'}B, \;\; P \succcurlyeq 0,$$
$$\widetilde{Z}P\widetilde{Z}^{'} \succcurlyeq 0, \;\; A^{'}A\widetilde{Z} = A^{'}B, \;\; P \preccurlyeq 0,$$

respectively. The two inequalities $\widehat{Z}P\widehat{Z}^{'} \preccurlyeq 0$ and $\widetilde{Z}P\widetilde{Z}^{'} \succcurlyeq 0$ are equivalent to $\widehat{Z}P = 0$ and $\widetilde{Z}P = 0$ when P is definite. Hence, the above two groups of equality and inequality reduce to

$$\widehat{Z}P = 0, \;\; A^{'}A\widehat{Z} = A^{'}B, \;\; P \succcurlyeq 0,$$
$$\widetilde{Z}P = 0, \;\; A^{'}A\widetilde{Z} = A^{'}B, \;\; P \preccurlyeq 0,$$

respectively. From Lemma 1.6, the above two equations for $\widehat{Z}$ have a common solution if and only if $A^{'}BP = 0$. In this case, the general common solution $\widehat{Z}$ is $\widehat{Z} = A^{\dagger}B + F_A U F_P$. Substituting this solution into $\phi(Z)$ gives $\phi(\widehat{Z}) = Q$, establishing (a). Result (b) can be shown similarly. □

The results and techniques in this section can be applied to establish many rank/inertia formulas, equalities, and inequalities for the covariance matrices and MMSEs in Lemma 1.1. For instance, let $X \in \mathbb{R}^{n\times p}$ and denote

$$\mathcal{S} = \left\{ Z \,|\, \operatorname{tr}\left[(XZ - I_n)^{'}(XZ - I_n) \right] = \min \right\} = \left\{ Z \,|\, X^{'}XZ = X^{'} \right\}.$$

Then, we obtain from Lemma 1.1(b) and (c) that

$$\begin{aligned} Q - \operatorname{MMSE}(\widehat{\beta}) &= Q - \sigma^2 (X^{\dagger} + F_X U)P_X \Sigma P_X (X^{\dagger} + F_X U)^{'} - \operatorname{Bias}(\widehat{\beta})\operatorname{Bias}(\widehat{\beta})^{'} \\ &= Q - \operatorname{Bias}(\widehat{\beta})\operatorname{Bias}(\widehat{\beta})^{'} - \sigma^2 Z P_X \Sigma P_X Z^{'}, \;\; Z \in \mathcal{S}, \end{aligned}$$

which are special forms of $\mathcal{S}$ and $\phi(Z)$ in Problem 1.2. Hence, many new and valuable features of the MMSE, as exercises in linear algebra, can be derived from the previous algebraic methods.

Statistical methods in many areas of application require mathematical computations with vectors and matrices, while various formulas and algebraic tricks for handling matrices in linear algebra and matrix theory play important roles in the derivations and characterizations of estimators and their properties under linear regression models. Recall that ranks and inertias of real symmetric (complex Hermitian) matrices are conceptual foundation in elementary linear algebra, which are the most significant finite integers in reflecting intrinsic properties of matrices. Dislike the quantities with continuous properties of determinants, norms, traces of matrices, rank/inertia are unique quantities to demonstrate finite-dimensional properties of matrix algebra, and are unreplaceable in role and cannot directly be extended to infinite-dimensional matrices and operators. There were many classic approaches on rank/inertia theory of real symmetric (complex Hermitian) matrices and their applications in the mathematical literature; see, e.g., [1–5, 9, 10, 12], while a variety of new formulas for calculating maximum/minimum ranks/inertias of linear/nonlinear real symmetric (complex Hermitian) matrix-valued functions were established, e.g., in [13, 14, 20–29]. It has been realized that matrix rank/inertia formulas can be utilized to characterize many features and performances of real symmetric (complex Hermitian) matrix-valued functions, such as, establishing and simplifying various complicated matrix expressions, deriving matrix equalities/inequalities that involve generalized inverses of matrices, characterizing definiteness/semi-definiteness of real symmetric (complex Hermitian) matrix-valued functions, and deriving exact algebraic solutions to the corresponding real symmetric (complex Hermitian) matrix-valued function optimization problems in the Löwner partial ordering.

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