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REMARKS ON THE ROWS AND COLUMNS OF P IN THE MATRIX EQUATION $A = PP^*$

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If A is a positive semi-definite hermitian matrix then $A = PP^*$ for some matrix P. There is, of course, some choice is selecting such a P. In fact, it is known that P can be chosen to be lower triangular. The objective of this paper is to describe the vectors available in determining either the rows or the columns of P. Some applications of the results obtained will also be given.

Our method of presentation is to first consider the results which describe the column vectors available in determining P, and then the results which describe the row vectors available in determining P.

Our column vector result requires the following lemma.

Lemma 1. *Suppose A is an $n \times n$ positive semi-definite hermitian matrix. Then $[x, y] = y^*Ax$ is an inner product on $R(A)$, the range of A.*

Proof. We need only show that $[x, x] = 0$ for $x \in R(A)$ implies that $x = 0$. Write $A = P^*P$ for some $n \times n$ matrix P. Then $0 = x^*Ax = x^*P^*Px$ so that $Px = 0$ and hence $Ax = 0$. Since $x \in R(A)$, there is a $y \in C^n$ so that $x = Ay$. Hence $A^2y = Ax = 0$. Now, as the null spaces of A and A^2 are identical, $0 = Ay = x$ from which the lemma follows.

Our column vector result now follows.

Theorem 1. *Suppose A is an $n \times n$ positive semi-definite hermitian matrix and* rank $A = r$. *Then there is an $n \times r$ matrix P so that $A = PP^*$ where p^k, the k-th column of P, can be arbitrarily chosen, within a scalar multiple from some subspace of $R(A)$ of dimension k.*

Proof. Let A^+ denote the pseudoinverse of A. As A is positive semi-definite hermitian, so is A^+. Consider the inner product $[x, y] = y^*A^+x$ on $R(A^+) = R(A^*) = R(A)$. We now inductively construct the columns p^k of P.

If $k = r$, pick any nonzero vector $x \in R(A)$. Set $p^r = x/[x, x]^{1/2}$. Now suppose $p^{k+1}, \ldots, p^r$ in $R(A)$ have been chosen so that $[p^i, p^j] = \delta_{ij}$, the Kronecker δ, for $i, j = k + 1, \ldots, r$. Consider $V_k = \{x \in R(A) \mid [x, p^{k+1}] = \ldots = [x, p^r] = 0\}$. Then $\dim V_k = k$. Pick any $x \in V_k$ so that $x \neq 0$. Set $p^k = x/[x, x]^{1/2}$.

Hence, we determine a sequence $p^1, p^2, \ldots, p^r$ in $R(A)$ so that $[p^i, p^j] = \delta_{ij}$ for $i, j = 1, 2, \ldots, r$. Set $p = (p^1 p^2 \ldots p^r)$. Then $P^* A^+ P = I$. Hence $(P^*)^+ P^* A^+ P P^+ = (P^*)^+ P^+$ as $(P^*)^+ P^* A^+ = A^+$ and $A^+ P P^+ = A^+$ it follows that $A^+ = (P^*)^+ P^+$. Finally, as $r = \operatorname{rank} P = \operatorname{rank} P^*$, $A = PP^*$ and the theorem follows.

We now apply this result to determine a P, with specified zero positions, so that $A = PP^*$. To develop this work, for any $x \in C^n$, let $\mathscr{P}(x) = y$ denote the $(0, 1)$-vector so that $y_i = 1$ if and only if $x_i \neq 0$. We call $\mathscr{P}(x)$ the pattern of x. Further, for any two patterns z and w, we write $z' \leqq w$ if and only if $z_i = 1$ implies $w_i = 1$. Using this notation we have the following.

Theorem 2. *Suppose A is an $n \times n$ positive semi-definite hermitian matrix where* rank $A = r$. *Suppose $p^{k+1}, \ldots, p^r$ in $R(A)$ have been chosen so that $[p^i, p^j] = \delta_{ij}$ for $i, j = k + 1, \ldots, r$. Pick any $(0, 1)$-vector $p \in C^n$ having precisely $n - k + 1$ components equal to one. Then there is an $n \times r$ matrix P with $A = PP^*$ where $\mathscr{P}(p^k) \leqq p$.*

Proof. Consider $V_k = \{x \in R(A) \mid [x, p^{k+1}] = \ldots = [x, p^r] = 0\}$ and $S = \{x \in C^n \mid \mathscr{P}(x) \leqq p\}$. Then as $\dim V_k = k$ and $\dim S = n - k + 1$ there is a nonzero $x \in V_k \cap S$. Set $p^k = x/[x, x]^{1/2}$. Now extend $p^k, p^{k+1}, \ldots, p^r$ to $p^1, p^2, \ldots \ldots, p^r$ by applying the technique used in Theorem 1. Set $P = (p^1 p^2 \ldots p^r)$ and the result follows.

As a consequence of this theorem we have the following.

Corollary 1. *If A is an $n \times n$ positive semi-definite hermitian matrix then there is an $n \times n$ lower triangular matrix T so that $A = TT^*$.*

Proof. Suppose rank $A = r$. Construct P, an $n \times r$ matrix, by using the theorem, so that $p_{ij} = 0$ for $i < j$. Now set $T = (PO)$ an $n \times n$ matrix. Then $A = TT^*$ and the result follows.

As an application of Theorems 1 and 2 where $A = PP^*$, consider the positive definite hermitian form $q = x^* A x$. Then, for $P^* x = y$, $q = y^* y$. In the analysis of variance in statistics it is important to specify the components of one of the columns of P to be the desired weights for the sample means. Then the components of the other columns are specified using certain zero patterns so that they represent the desired comparison sbetween the weighted means. For example, in [1] it is required that

$$\bar{y}_n = \sum_{i=1}^{n} \frac{\sum_{j=1}^{n} a_{ij} \bar{x}_i}{(\sum_{i,j} a_{ij})^{1/2}} \cdot$$

It is easily seen that this requirement can be achieved by setting

$$p^n = \left(\frac{\sum_{j=1}^{n} a_{ij}}{(\sum_{i,j} a_{ij})^{1/2}} \right).$$

Lemma 2. *If*

$$p^n = \left(\frac{\sum_{j=1}^{n} a_{ij}}{(\sum_{i,j} a_{ij})^{1/2}} \right)$$

then $[p^n, p^n] = 1$.

Proof. Let e be the column vector all of whose components are one. Let $R_i = \sum_{j=1}^{n} a_{ij}$ for $i = 1, 2, \ldots, n$. Then $Ax = R$ has solution e so that $e = A^{-1}R$. Now

$$[p^n, p^n] = (p^n) A^{-1} p^{n*} = (\sum_{i,j} a_{ij})^{-1} R^* A^{-1} R = (\sum_{i,j} a_{ij})^{-1} R^* e = 1\,.$$

By prudent choices of the columns of P other variants of the above problem can also be achieved.

Our presentation now concerns the row vectors available in forming P. We begin this work with the following example.

Example. Let $A = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$. Then $A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$. Set $T = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$. Now

$$T \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{2}{\sqrt{2}} & 0 \end{pmatrix}$$

and

$$T \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & -\frac{2}{\sqrt{2}} \end{pmatrix}.$$

Hence, if p_1, the first row of P, is specified as $(1/\sqrt{2}, -1/\sqrt{2})$ then the second row of P, p_2, can be $(0, -2/\sqrt{2})$ or $(2/\sqrt{2}, 0)$. Note however that the only subspace which contains both of these vectors is C^2 yet the choice of p_2 can not come from this vector space.

The description of the row vectors available in forming P is now given.

Theorem 3. *Suppose A is an $n \times n$ positive definite hermitian matrix. Then there is an $n \times n$ matrix P so that $A = PP^*$ where, on some specified sphere of some hyperplane of dimension k, p_k may be arbitrarily chosen.*

Proof. Write $A = TT^*$ foı some upper triangular matrix T. Then $\{n \times n$ matrices $R | \; A = RR^*\} = \{TQ | \; Q$ is unitary$\}$. Now pick any p_n of length t_{nn}. Set $q_n = (1/t_{nn})\, p_n$.

Suppose now that $p_n, p_{n-1}, \ldots, p_{k+1}$ have been chosen and $q_n, q_{n-1}, \ldots, q_{k+1}$ determined so that $q_n, q_{n-1}, \ldots, q_{k+1}$ is an orthonormal set and $t_{rr}q_r + t_{rr+1}q_{r+1} + \ldots$ $\ldots + t_{rn}q_n = p_r$ for $r = k + 1, \ldots, n$. Now consider the hyperplane

$$H_k = \{x | \; (x, q_n) = t_{kn}, \ldots, (x, q_{k+1}) = t_{kk+1}\}$$

which is of dimension k. Pick any $p_k \in H_k$ so that $|p_k| = (|t_{kk}|^2 + \ldots + |t_{kn}|^2)^{1/2}$. The set of all such p_k is a sphere in H_k as can be seen by noting that if $\{q, q_n, \ldots, q_{k+1}\}$ is any orthonormal set then

$$t_{kk}q + t_{kk+1}q_{k+1} + \ldots + t_{kn}q_n = p_k$$

provides such a p_k. Set $q = p_k - t_{kk+1}q_{k+1} - \ldots - t_{kn}q_n$. Then $(q, q_r) = (p_k, q_n) =$ $= t_{kn} = 0$ for $r = k + 1, \ldots, n$. Set $q_k = (1/t_{kk})\, q$. Then $t_{kk}q_k + t_{kk+1}q_{k+1} + \ldots$ $\ldots + t_{kn}q_n = p_k$.

Hence, by induction, we can construct a unitary Q os that $TQ = P$ where p_k is on some specified sphere of some hyperplane of dimension k for $k = 1, 2, \ldots, n$.

This result may be generalized as follows.

Corollary 2. *Suppose A is an $n \times n$ positive semi-definite hermitian matrix and that* rank $A = r$. *Suppose further that the submatrix A_r in the rows and columns labeled 1 through r of A is nonsingular. Then there is an $n \times r$ matrix P so that $A = PP^*$ where, on some specified sphere of dimension k, p_k may be arbitrarily chosen for $k = 1, 2, \ldots, r$.*

Proof. By Theorem 3, there is an $r \times r$ matrix P_1 so that $A_r = P_1P_1^*$ where the k-th row of P_1 may be arbitrarily chosen from some specified sphere of some dimension k. Partition

$$A = \begin{pmatrix} A_r & A_{12} \\ A_{21} & A_2 \end{pmatrix}.$$

Set $P_2 = A_{21}(P_1^*)^{-1}$ and

$$P = \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}.$$

Then $A = PP^*$ and the result follows.

As some application of these results we have the following.

Corollary 3. *Suppose A is an $n \times n$ positive definite hermitian matrix. Then $A = PP^*$ where p_k is any vector in*

$$H_k = \{x| \, (x, p_1) = a_{k1}, \, (x, p_2) = a_{k2}, \ldots, (x, x) = a_{kk}\}$$

for $k = 1, 2, \ldots, n$.

Proof. First note that if Q is an $n \times n$ permutation matrix then Q^*AQ is a positive definite hermitian matrix. Thus $Q^*AQ = RR^*$ for some $n \times n$ matrix R where, on some specified sphere of some hyperplane of dimension k, r_k may be arbitrarily chosen for $k = 1, 2, \ldots, n$. Thus, $A = (QR)(QR)^*$. Hence, by prudent choices of Q, it is seen that for any ordering of row indices, say $i_1, i_2, \ldots, i_n$, $A = PP^*$ where, on some specified sphere of some hyperplane of dimension k, p_{i_k} may be arbitrarily chosen. Hence, we may choose $p_1 \in H_1$, $p_2 \in H_2, \ldots, p_n \in H_n$ and $A = PP^*$.

As a consequence of this corollary it is seen that if A is positive semi-definite, then a P, such that $A = PP^*$, can be computed by solving $(p_1, p_1) = a_{11}$ for p_1, then $(p_2, p_2) = a_{22}$ and $(p_2, p_1) = a_{12}$ for p_2 etc.

Concerning the possibility of zero pattern results for Theorem 3 we include the following example.

Example. Let

$$A = \begin{pmatrix} \frac{1}{2} & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 2 \end{pmatrix}.$$

Then A is positive definite hermitian. Consider

$$A = \begin{pmatrix} a & b & c \\ 0 & d & e \\ \sqrt{2} & 0 & 0 \end{pmatrix} \begin{pmatrix} \bar{a} & 0 & \sqrt{2} \\ \bar{b} & \bar{d} & 0 \\ \bar{c} & \bar{e} & 0 \end{pmatrix}.$$

Then $1 = a_{32} = 0 \, . \sqrt{2} + 0 \, . \, \bar{d} + 0 \, . \, \bar{e}$ has no solution and so the second row of P can not be chosen so that $P(p_2) \leqq (0, 1, 1)$.

Thus, this example shows that a zero pattern result, of the type in Theorem2, is notpossible.

Reference

[1] *Harold Hotelling:* "The selection of variates for use in prediction with comments on the general problem of nuisance parameters," Annals of Mathematical Statistics II, (1940), 271—283.

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