ON THE MATRIX EQUATION $X'X = A$

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1. Introduction

If X is a matrix with non-negative entries then $X'X$ is positive semi-definite with non-negative entries. Conversely, if A is positive semi-definite then there exist matrices Y, not necessarily with non-negative entries, such that $Y'Y = A$. In the present paper we investigate whether, given a positive semi-definite matrix A with non-negative entries, the equation $X'X = A$ has a solution X with non-negative entries. An equivalent statement of the problem is: Can a positive semi-definite matrix with non-negative entries be expressed as a sum of rank 1 positive semi-definite matrices with non-negative entries? We answer the question in the affirmative for $n \leqq 4$ and quote the following example due to M. Hall (**1**) to show that the answer is in the negative for $n \geqq 5$:

The matrix
$$A = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 1 & \frac{3}{4} & 0 & \frac{1}{2} \\ 0 & \frac{3}{4} & 1 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 1 \end{pmatrix}$$
is positive semi-definite, yet there exists no matrix X with non-negative entries such that $X'X = A$.

There is a rather surprising geometrical consequence of this answer: In an n-dimensional space ($n \geqq 5$) not every pencil of n vectors such that the angle between any two vectors does not exceed $\pi/2$ can be placed in the non-negative orthant of coordinates by a rotation or by a rotation followed by a reflection.

We are indebted to Marvin Marcus and Morris Newman for drawing our attention to the problem.

2. Results

Lemma 1. *Let* $A = (a_{ij})$ *be a positive semi-definite matrix,* $a_{ij} \geqq 0$. *Then for any* i, j, k *at most one of* $a_{ij}a_{kk} - a_{ik}a_{jk}$, $a_{ik}a_{jj} - a_{ij}a_{jk}$, $a_{jk}a_{ii} - a_{ij}a_{ik}$ *can be negative.*

Proof. Suppose that $a_{ij}a_{kk} < a_{ik}a_{jk}$ and $a_{ik}a_{jj} < a_{ij}a_{jk}$. Then $a_{ij}a_{kk}a_{ik}a_{jj} < a_{ik}a_{jk}a_{ij}a_{jk}$, i.e. $a_{jj}a_{kk} < a_{jk}^2$ which is impossible since $a_{jj}a_{kk} - a_{jk}^2$ is a principal minor of the positive semi-definite matrix A.

Lemma 2. *Let* A *be a 4-square positive semi-definite matrix,* $a_{ij} \geqq 0$. *Then there exists a permutation matrix* P *such that all the entries in the leading 3-square* *principal submatrix of $C_2(PAP')$, the second compound matrix of PAP', are non-negative unless $a_{ij}a_{kk}<a_{ik}a_{jk}$, $a_{ij}a_{mm}<a_{im}a_{jm}$, $a_{km}a_{ii}<a_{ik}a_{im}$, $a_{km}a_{jj}<a_{jk}a_{jm}$ for $(i, j, k, m) = (1, 2, 3, 4)$ or $(1, 3, 2, 4)$ or $(1, 4, 2, 3)$.*

Proof. The diagonal entries in $C_2(PAP')$ being principal minors of a positive semi-definite matrix are non-negative. The remaining entries are equal to $a_{ij}a_{kk}-a_{ik}a_{jk}$, $a_{im}a_{kk}-a_{ik}a_{km}$, $a_{jm}a_{kk}-a_{jk}a_{km}$. Hence the upper 3-square principal submatrix of $C_2(PAP')$ has non-negative entries if and only if a row in

$$\begin{pmatrix} |231| & |241| & |341| \\ |132| & |142| & |342| \\ |123| & |143| & |243| \\ |124| & |134| & |234| \end{pmatrix},$$

where $|ijk| = a_{kk}a_{ij}-a_{ik}a_{jk}$, has non-negative entries. Suppose that all rows have at least one negative entry. Let $|ijk|<0$. Then, by Lemma 1, $|jki|\geqq 0$ and $|ikj|\geqq 0$. If there is a negative entry in the jth row it must be either $|imj|$ or $|kmj|$.

(i) If $|imj|<0$, then $|jmi|\geqq 0$ and $|ijm|\geqq 0$. Thus if the ith row contains a negative entry it must be $|kmi|$. Hence $|ikm|\geqq 0$ and all the entries in the mth row are non-negative. For if $|jkm|<0$ we have:

$$\begin{aligned} a_{kk}a_{ij} &< a_{ik}a_{jk}, \\ a_{mm}a_{jk} &< a_{jm}a_{km}, \\ a_{ii}a_{km} &< a_{ik}a_{im}, \\ a_{jj}a_{im} &< a_{ij}a_{jm} \end{aligned}$$

and therefore $a_{ii}a_{jj}a_{kk}a_{mm}<a_{ik}^2a_{jm}^2$. But $a_{ii}a_{kk}-a_{ik}^2$ and $a_{jj}a_{mm}-a_{jm}^2$ are principal minors of positive semi-definite matrix A and thus are non-negative. Contradiction.

(ii) If $|kmj|<0$ it is easy to see that all entries in the ith or in the mth row are non-negative unless $|kmi|<0$ and $|ijm|<0$, as stated in the lemma.

The last proviso in Lemma 2 cannot be omitted. For example,

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

is positive semi-definite but there exists no permutation matrix P for which the leading 3-square principal submatrix of $C_2(PAP')$ has non-negative entries.

Theorem. *Let $A = (a_{ij})$ be a positive semi-definite n-square matrix $(n\leqq 4)$ with non-negative entries. Then there exists an n-square matrix X with non-negative entries such that $X'X = A$.*

Proof. The theorem is trivial for $n = 1$. We prove it for $n = 2$, 3 and 4. We can assume therefore, without loss of generality, that no main diagonal element of A is 0, for if an n-square positive semi-definite matrix has a diagonal element 0 then every element in the same row and column must vanish and we are essentially dealing with an $(n-1)$-square matrix.

(i) $n=2$.

$$X = \begin{bmatrix} a_{11} & \dfrac{a_{12}}{\sqrt{a_{11}}} \\ 0 & \dfrac{\sqrt{|A|}}{\sqrt{a_{11}}} \end{bmatrix}.$$

(ii) $n = 3$. Let $Q = \mathrm{diag}\{\sqrt{a_{11}}, \sqrt{a_{22}}, \sqrt{a_{33}}\}$ and let $B = (b_{ij}) = Q^{-1}AQ^{-1}$. Then it is easy to see that unless all $b_{ij} = 1$, in which case we choose $X = BQ/\sqrt{3}$, at least one principal minor of order 2 of B is strictly positive. Let $1-b_{ij}^2>0$. Then $1>b_{ij}$ and either $b_{jk}-b_{ij}b_{ik}\geqq 0$ or $b_{ik}-b_{ij}b_{jk}\geqq 0$. In either case there exists a permutation matrix P such that $PBP' = C = (c_{ij})$ where $1-c_{12}^2>0$ and $c_{23}-c_{12}c_{13}\geqq 0$. Then $X = YPQ$ where

$$Y = \begin{bmatrix} 1 & c_{12} & c_{13} \\ 0 & \sqrt{1-c_{12}^2} & \dfrac{c_{23}-c_{12}c_{13}}{\sqrt{1-c_{12}^2}} \\ 0 & 0 & \dfrac{\sqrt{|C|}}{\sqrt{1-c_{12}^2}} \end{bmatrix}.$$

(iii) $n = 4$. Let $Q = \mathrm{diag}\{\sqrt{a_{11}}, \sqrt{a_{22}}, \sqrt{a_{33}}, \sqrt{a_{44}}\}$ and let $B = (b_{ij}) = Q^{-1}AQ^{-1}$.

(a) First suppose that the conditions of Lemma 2 are satisfied and that there exists a permutation matrix P such that all the entries in the leading 3-square submatrix of $C_2(PBP')$ are non-negative.

Let $PBP' = C = \left(\begin{array}{c|ccc} 1 & c_{12} & c_{13} & c_{14} \\ \hline c_{12} & & & \\ c_{13} & & C_{11} & \\ c_{14} & & & \end{array}\right)$ and let $Z = \left(\begin{array}{c|ccc} 1 & c_{12} & c_{13} & c_{14} \\ \hline 0 & & & \\ 0 & & Y & \\ 0 & & & \end{array}\right)$.

Then $Z'Z = \left(\begin{array}{c|ccc} 1 & c_{12} & c_{13} & c_{14} \\ \hline c_{12} & & & \\ c_{13} & & V'V+Y'Y & \\ c_{14} & & & \end{array}\right)$ where $V = (c_{12}\, c_{13}\, c_{14})$.

Thus we can find a matrix Z with non-negative entries such that $Z'Z = C$ if a 3-square matrix Y with non-negative entries can be found such that $Y'Y = C_{11}-V'V$. Now, $C_{11}-V'V$ is precisely the leading 3-square submatrix of $C_2(PBP')$ all of whose entries are non-negative. Hence, by part (ii), the required Y can be be found.

(b) Suppose now that $b_{ij}-b_{ik}b_{jk}$, $b_{ij}-b_{im}b_{jm}$, $b_{km}-b_{ik}b_{im}$ and $b_{km}-b_{jk}b_{jm}$ are all negative. Without loss of generality we can assume that $(i, j, k, m) = (1, 2, 3, 4)$. We first show that there exists a matrix R with non-negative entries such that $(R^{-1})'BR^{-1} = C = (c_{ij})$ has at least 4 entries equal to 0.

Let
$$R^{-1}=\begin{pmatrix} 1 & -b_{12} & -x_1 & -x_2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where x_1, x_2 are non-negative numbers to be determined. We have $c_{12}=0$, $c_{13}=b_{13}-x_1$, $c_{14}=b_{14}-x_2$, $c_{23}=b_{23}-b_{12}b_{13}$, $c_{24}=b_{24}-b_{12}b_{14}$, $c_{34}=f(x_1, x_2)=b_{34}-b_{14}x_1-b_{13}x_2+x_1x_2$. Since $b_{12}-b_{13}b_{23}<0$ and $b_{12}-b_{14}b_{24}<0$ both c_{23} and c_{24} are, by Lemma 1, non-negative. Choose x_1, x_2 so that $x_1 \leqq b_{13}$, $x_2 \leqq b_{14}$ and $f(x_1, x_2)=0$. This can always be done since $f(0, 0)=b_{34} \geqq 0$ while $f(b_{13}, b_{14})<0$. Then C, which is positive semi-definite, has 0 in the (1, 2), (2, 1), (3, 4) and (4, 3) positions and non-negative entries elsewhere.

Let $Z=(z_{ij})$ be a 4-square matrix with

$$z_{12}=z_{14}=z_{21}=z_{24}=z_{32}=z_{33}=z_{41}=z_{43}=0.$$

We show that we can determine the other z_{ij} in such a way that $z_{ij} \geqq 0$ and $Z'Z=C$, i.e.

$$z_{11}^2+z_{31}^2=z_{22}^2+z_{42}^2=z_{13}^2+z_{23}^2=z_{34}^2+z_{44}^2=1$$

and

$$z_{11}z_{13}=c_{13}, \quad z_{31}z_{34}=c_{14}, \quad z_{22}z_{23}=c_{23}, \quad z_{42}z_{44}=c_{24}.$$

It will follow that all entries in ZRQ are non-negative and $(ZRQ)'ZRQ=A$.

A straightforward computation gives

$$z_{11}^4(1-c_{23}^2-c_{24}^2)-z_{11}^2(1+c_{13}^2-c_{14}^2-c_{23}^2-c_{24}^2-c_{13}^2c_{24}^2+c_{14}^2c_{23}^2)$$
$$+c_{13}^2(1-c_{14}^2-c_{24}^2)=0.$$

Denote z_{11}^2 by z and the minor of c_{ij} by $|C_{ij}|$. The equation becomes

$$z^2|C_{11}|-z(|C|-2c_{13}|C_{13}|)+c_{13}^2|C_{33}|=0. \tag{1}$$

We prove first that the roots of (1) are real. The discriminant of (1) is

$$D=(|C|-2c_{13}|C_{13}|)^2-4c_{13}^2|C_{11}||C_{33}|.$$

But, by the classical theorem of Jacobi on the minors of $adj(C)$,

$$|C_{11}||C_{33}|-|C_{13}|^2=|C|(1-c_{24}^2).$$

Therefore
$$\begin{aligned} D &= |C|^2-4c_{13}|C||C_{13}|+4c_{13}^2|C_{13}|^2 \\ &\quad -4c_{13}^2|C|+4c_{13}^2c_{24}^2|C|-4c_{13}^2|C_{13}|^2 \\ &= |C|\{|C|-4c_{13}(|C_{13}|+c_{13}-c_{13}c_{24}^2)\} \\ &= |C|(|C|+4c_{13}c_{14}c_{23}c_{24}) \end{aligned}$$

which is non-negative. Therefore the roots of (1) are real. The coefficient of z in (1) is

$$-|C|+2c_{13}|C_{13}| = -|C|-2c_{13}\{c_{13}(1-c_{24}^2)+c_{12}c_{24}c_{34}\}$$

which is non-positive and, since $c_{13}^2 \mid C_{33} \mid \geqq 0$, both roots are non-negative. Hence there is a real non-negative root for z_{11}.

The corresponding equations for z_{22}, z_{33} and z_{44} yield similar results.

REFERENCE

(1) Marshall Hall, Jr., *A Survey of Combinatorial Analysis*, Surveys in Applied Mathematics IV (Wiley, 1958), 35-104.

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