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SUFFICIENT CONDITIONS FOR COMPLETE POSITIVITY

ROBERT REAMS

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Abstract. Marcus and Minc gave sufficient conditions on the diagonal entries of a doubly nonnegative doubly stochastic $n \times n$ matrix A, that there is a doubly nonnegative doubly stochastic matrix C with $A = C^2$. In this event, A is completely positive. We shall assume that A is doubly nonnegative and irreducible and provide slightly more general sufficent conditions on the diagonal entries of A for the existence of C. Our main result provides sufficient conditions on the principal 2×2 minors of a doubly nonnegative doubly stochastic irreducible matrix A for the existence of C.

1. Introduction

Let $A = (a_{ij}) \in \mathbf{R}^{n \times n}$. We will say A is *nonnegative* when $a_{ij} \geqslant 0$, for $1 \leqslant i, j \leqslant n$, and in the same way for $x = (x_1, \ldots, x_n)^T \in \mathbf{R}^n$ we will call the vector x *nonnegative* when $x_i \geqslant 0$ for $1 \leqslant i \leqslant n$. As usual e_i will denote the ith standard basis vector. If A is nonnegative and has row and column sums 1 then A is called *doubly stochastic*. For $x = (x_1, \ldots, x_n)^T \in \mathbf{R}^n$, we will write $x \geqslant 0$ to mean x is nonnegative, and $x > 0$ to mean x is *positive*, which is to say $x_i > 0$ for all $1 \leqslant i \leqslant n$. A is said to be *positive semidefinite* if A is symmetric and $x^T A x \geqslant 0$, for all $x \in \mathbf{R}^n$. A is said to be *doubly nonnegative* if it is both nonnegative and positive semidefinite. A is said to be *completely positive* if $A = B^T B$, where $B \in \mathbf{R}^{m \times n}$ is nonnegative. A is said to be *irreducible* if there is no permutation matrix $P \in \mathbf{R}^{n \times n}$ such that $P^T A P$ can be written in block form as $P^T A P = \begin{pmatrix} A_{11} & O \\ A_{21} & A_{22} \end{pmatrix}$, where O is a zero block matrix (which is not $n \times n$). The Perron-Fröbenius Theorem [5] states that an $n \times n$ irreducible nonnegative matrix A has a real eigenvalue $r > |\lambda_i|$, where λ_i, for $2 \leqslant i \leqslant n$, are the other eigenvalues of A. Additionally, this theorem states that A has a positive eigenvector v corresponding to r. The eigenvalue r is often called the *Perron root* and v the *Perron vector*. With the eigenvalues ordered as $r \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, we will denote the eigenvector corresponding to λ_2 by $w = (w_1, \ldots, w_n)^T$. Let $A \in \mathbf{R}^{m \times n}$ and k be such that $1 \leqslant k \leqslant \min\{m, n\}$, then $A^{(k)}$ will denote the kth compound matrix [3]. That is to say $A^{(k)}$ is the $\binom{m}{k} \times \binom{n}{k}$ matrix whose entries are the $k \times k$ minors of A listed in $A^{(k)}$ in lexicographic order. We will say $C \in \mathbf{R}^{n \times n}$ is a *square root* of $A \in \mathbf{R}^{n \times n}$, if $A = C^2$.

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In Section 2, we extend a result due to Marcus and Minc [8] (also in [2] and [10]). Their result gives sufficient conditions on the diagonal entries of $A \in \mathbf{R}^{n\times n}$, for the existence of a positive semidefinite doubly stochastic square root C if A is positive semidefinite and doubly stochastic. Theorem 1 is similarly concerned with the existence of a positive semidefinite square root which is nonnegative, but only requires A to be doubly nonnegative and irreducible. In Section 3, Theorem 3 gives sufficient conditions on the 2×2 principal minors of doubly nonnegative, doubly stochastic and irreducible A for the existence of a nonnegative positive semidefinite square root C.

2. Conditions on diagonal entries

Marcus and Minc's result [8] is a corollary of Theorem 1.

THEOREM 1. *Let $A = (a_{ij}) \in \mathbf{R}^{n\times n}$ be doubly nonnegative and irreducible. Then $A = C^2$, for positive semidefinite $C = (c_{ij}) \in \mathbf{R}^{n\times n}$. Let r be the Perron root of A, and $v = (v_1,\ldots,v_n)^T$ its Perron vector. If $a_{ii} \leqslant \dfrac{rv_i^2}{\sum_{j\neq p} v_j^2}$, for all i, $1 \leqslant i \leqslant n$, for all p, $1 \leqslant p \leqslant n$, then C is nonnegative.*

Proof. Write $A = U^T\Lambda U$, where U is orthogonal and $\Lambda = \mathrm{diag}(r,\lambda_2,\ldots,\lambda_n)$, then $C = U^T\Lambda^{\frac{1}{2}}U$ is positive semidefinite (and unique [5]). A irreducible implies $r > 0$ and $v > 0$.

If $c_{i_0j_0} < 0$, for some i_0, j_0, $i_0 \neq j_0$, then

$$a_{i_0i_0} = e_{i_0}^T C^2 e_{i_0} = c_{1i_0}^2 + \cdots + c_{ni_0}^2 > \sum_{j\neq j_0} c_{ji_0}^2 \geqslant \frac{(\sum_{j\neq j_0} c_{ji_0}v_j)^2}{\sum_{j\neq j_0} v_j^2} > \frac{(\sqrt{r}v_{i_0})^2}{\sum_{j\neq j_0} v_j^2} = \frac{rv_{i_0}^2}{\sum_{j\neq j_0} v_j^2},$$

where the second inequality is from Cauchy-Schwartz and the third from $c_{i_0j_0} < 0$. $\square$

Since C is symmetric we remark that if $c_{i_0j_0} < 0$ we also have $a_{j_0j_0} > \frac{rv_{j_0}^2}{\sum_{i\neq i_0} v_i^2}$. Marcus and Minc's result has $r = 1$ and $v = (1,1,\ldots,1)^T$ in Theorem 1.

COROLLARY 2. (Marcus and Minc) *Let $A = (a_{ij}) \in \mathbf{R}^{n\times n}$ be positive semidefinite and doubly stochastic, and $A = C^2$, where $C \in \mathbf{R}^{n\times n}$ is positive semidefinite. Then $a_{ii} \leqslant \dfrac{1}{n-1}$, for all i, $1 \leqslant i \leqslant n$, implies C is nonnegative.*

For $n \leqslant 4$, Maxfield and Minc [9] proved that if an $n\times n$ matrix is doubly nonnegative then it is completely positive. Hall [7], and later Gray and Wilson [4], gave examples to show that a 5×5 doubly nonnegative matrix need not be completely positive. Kaykobad [6] proved that a diagonally dominant symmetric nonnegative matrix is completely positive, and there are other results known that relate a completely positive matrix to its graph (see [1], [2]).

It is possible for A to be completely positive but not writeable in the form $A = C^2$, where C is nonnegative and positive semidefinite. There is no example to illustrate this fact by using 2×2 matrices. However, there are examples with 3×3 matrices, for instance $A = \begin{pmatrix} \frac{81}{64} & 0 & \frac{15}{16} \\ 0 & \frac{81}{64} & \frac{15}{16} \\ \frac{15}{16} & \frac{15}{16} & \frac{3}{2} \end{pmatrix}$, for which $A = C^2$, when $C = \begin{pmatrix} 1 & -\frac{1}{8} & \frac{1}{2} \\ -\frac{1}{8} & 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 1 \end{pmatrix}$. C is the unique positive semidefinite square root of A, but A is doubly nonnegative and therefore completely positive from Maxfield and Minc's result [9]. In fact, $A = B^T B$, where $B = \begin{pmatrix} \frac{9}{8} & 0 & \frac{5}{6} \\ 0 & \frac{9}{8} & \frac{5}{6} \\ 0 & 0 & \frac{1}{3} \end{pmatrix}$.

3. Conditions on principal 2×2 minors

Finally we come to our main result, Theorem 3, which extends Theorem 1 when $v = e$.

THEOREM 3. *For $n \geqslant 3$ let $A = (a_{ij}) \in \mathbf{R}^{n\times n}$ be positive semidefinite, doubly stochastic, irreducible, and $A = C^2$, where $C \in \mathbf{R}^{n\times n}$ is positive semidefinite. Let w be an eigenvector corresponding to λ_2, where λ_2 is the second largest eigenvalue of A, and P a permutation matrix so that Pw has its components in increasing order. Let $B = PAP^T = (b_{ij})$. If $\begin{vmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{vmatrix} \leqslant \dfrac{\lambda_2 (w_j - w_i)^2}{\sum_{1\leqslant k<l\leqslant n,(k,l)\neq(p,q)} (w_l - w_k)^2}$, for all (i,j), $1 \leqslant i,j \leqslant n$, for all (p,q), $1 \leqslant p < q \leqslant n$, and either $b_{11} \leqslant \frac{1}{n-1}$ or $b_{nn} \leqslant \frac{1}{n-1}$ then C is nonnegative.*

Proof. The denominator $\sum_{1\leqslant k<l\leqslant n,(k,l)\neq(p,q)} (w_l - w_k)^2$ in the inequality of the theorem cannot be zero for any (p,q), since if it were then w would be a multiple of e which is not possible.

Note that we must have $c_{ii} > 0$ for all i, $1 \leqslant i \leqslant n$, since for any positive semidefinite matrix $C = (c_{ij})$ if the diagonal entry $c_{ii} = 0$, then the ith row and ith column of C would be all zeros, which would make C and therefore A reducible. Now to prove our theorem suppose, for the sake of obtaining a contradiction, that C has a negative entry. Since $A = C^2$ if and only if $B = (PCP^T)^2$, without loss of generality we may replace C by PCP^T, where P is as stated in the theorem. With $i_0 \neq j_0$ we'll say that $c_{i_0 j_0} < 0$.

If $(i_0, j_0) = (1,n)$ then $b_{11} > \frac{1}{n-1}$ and $b_{nn} > \frac{1}{n-1}$ from the proof of Theorem 1 when $v = e$ and the remark after Theorem 1, which would contradict $b_{11} \leqslant \frac{1}{n-1}$ or $b_{nn} \leqslant \frac{1}{n-1}$ in the statement of the theorem. Thus $(i_0, j_0) \neq (1,n)$. We claim we can argue that $C^{(2)}$ has a negative entry. Fix (i_0, j_0) for the remainder of the proof. For any m, $1 \leqslant m \leqslant n$, if $m > i_0$ and $m > j_0$ (assuming there is such an m) consider the pair of 2×2 minors $\begin{vmatrix} c_{i_0 i_0} & c_{i_0 m} \\ c_{j_0 i_0} & c_{j_0 m} \end{vmatrix}$ and $\begin{vmatrix} c_{i_0 j_0} & c_{i_0 m} \\ c_{j_0 j_0} & c_{j_0 m} \end{vmatrix}$. We will see that for some m satisfying $m > i_0$ and $m > j_0$, at least one of these 2×2 minors is negative. If $m < i_0$ and $m < j_0$ (assuming there is such an m) consider $\begin{vmatrix} c_{i_0 m} & c_{i_0 j_0} \\ c_{j_0 m} & c_{j_0 j_0} \end{vmatrix}$ and $\begin{vmatrix} c_{i_0 m} & c_{i_0 i_0} \\ c_{j_0 m} & c_{i_0 j_0} \end{vmatrix}$.

Suppose to the contrary that for all m satisfying $m > i_0$ and $m > j_0$ we have both

$$c_{i_0i_0}c_{j_0m} \geqslant c_{i_0m}c_{i_0j_0}, \tag{1}$$

and

$$c_{i_0j_0}c_{j_0m} \geqslant c_{i_0m}c_{j_0j_0}, \tag{2}$$

and for all m satisfying $m < i_0$ and $m < j_0$ we have both

$$c_{i_0m}c_{j_0j_0} \geqslant c_{i_0j_0}c_{j_0m}, \tag{3}$$

and

$$c_{i_0m}c_{i_0j_0} \geqslant c_{i_0i_0}c_{j_0m}. \tag{4}$$

If for $m > i_0$ and $m > j_0$ we have $c_{i_0m} \geqslant 0$, then inequality (2) implies $c_{j_0m} \leqslant 0$, whereas if $c_{i_0m} \leqslant 0$ then inequality (1) implies $c_{j_0m} \geqslant 0$. So far we have only argued that c_{i_0m} and c_{j_0m} are oppositely signed or one of them (at least) is zero. For $m < i_0$ and $m < j_0$ a similar argument shows c_{i_0m} and c_{j_0m} are oppositely signed or one of them (at least) is zero.

Suppose now that $c_{i_0j_0}$ is on the superdiagonal, and consider row i_0 and row j_0 of C. With $c_{i_0j_0}$ on the superdiagonal this means that for all $m \neq i_0$ and $m \neq j_0$ we have $m > i_0$ and $m > j_0$, or we have $m < i_0$ and $m < j_0$. Then the dot product of row i_0 and row j_0, thought of as vectors, which equals $(\sum_{m\neq i_0, m\neq j_0} c_{i_0m}c_{j_0m}) + c_{i_0i_0}c_{j_0i_0} + c_{i_0j_0}c_{j_0j_0}$, must be negative. But this would imply the (i_0, j_0) entry of A is negative, which is not the case.

We next argue that with C having a negative off-diagonal entry, not in the upper right (or lower left) corner and not on the superdiagonal, then if $C^{(2)}$ has all nonnegative entries this would contradict C being irreducible, which is not possible.

Suppose that $i_0 = 1$ and $3 \leqslant j_0 \leqslant n-1$. Suppose that c_{1j_0} is the leftmost negative entry in the first row, so that $c_{1l} \geqslant 0$ for all l, $3 \leqslant l < j_0$. We must have $c_{1l}c_{j_0l} > 0$ for at least one l, $2 \leqslant l < j_0$, since otherwise $a_{1j_0} = c_{11}c_{1j_0} + \sum_{1<l<j_0} c_{1l}c_{j_0l} + c_{1j_0}c_{j_0j_0} + \sum_{j_0<l\leqslant n} c_{1l}c_{j_0l}$ would be negative since $c_{1l}c_{j_0l} \leqslant 0$ for all $l > j_0$, from inequalities (1)–(2) and the reasoning of the paragraph immediately after them. Fix l, $2 \leqslant l < j_0$, for which $c_{1l}c_{j_0l} > 0$. Since $c_{1l} \geqslant 0$ this implies $c_{1l} > 0$ and $c_{j_0l} > 0$. If now $\begin{vmatrix} c_{1l} & c_{1n} \\ c_{j_0l} & c_{j_0n} \end{vmatrix} \geqslant 0$, this implies $c_{1n} = 0$ and $c_{j_0n} = 0$, since $c_{j_0n} \leqslant 0$. Then letting $k \in \{2, \ldots, n-1\}$, if we have $\begin{vmatrix} c_{1l} & c_{1n} \\ c_{kl} & c_{kn} \end{vmatrix} \geqslant 0$, this implies $c_{kn} \geqslant 0$, and then $\begin{vmatrix} c_{1j_0} & c_{1n} \\ c_{kj_0} & c_{kn} \end{vmatrix} \geqslant 0$ implies $c_{kn} = 0$. But now we have that all entries of the nth column of C, except c_{nn}, are zeroes, implying C, and therefore A, is reducible, contrary to our assumption.

Finally, suppose $c_{i_0j_0} < 0$, where $i_0 > 1$ and $j_0 > i_0$, and furthermore $c_{1l} \geqslant 0$ for all l, $1 \leqslant l \leqslant n$. Then $\begin{vmatrix} c_{1i_0} & c_{1j_0} \\ c_{i_0i_0} & c_{i_0j_0} \end{vmatrix} \geqslant 0$ implies $c_{1i_0} = 0$ and $c_{1j_0} = 0$. But then $\begin{vmatrix} c_{11} & c_{1j_0} \\ c_{i_01} & c_{i_0j_0} \end{vmatrix} \geqslant 0$ is not possible.

Now $Ae = re$ and $Aw = \lambda_2 w$ implies $AX = X\,\mathrm{diag}(r,\lambda_2)$, where X is the $n\times 2$ matrix with 1st column e and 2nd column w, and $\mathrm{diag}(r,\lambda_2)$ is 2×2. Taking the 2nd compound of both sides, and with $x = X^{(2)}$, we can say $A^{(2)}x = r\lambda_2 x$, where x is the vector with its components written in lexicographic order, so that here $x = (w_2 - w_1, w_3 - w_1, \dots)^T$. Then $(C^{(2)})^2 x = r\lambda_2 x$, where $r = 1$. Since by replacing A with PAP^T and the components of Pw are increasing we may assume (after making the replacement) that the components of x are nonnegative. Then $C^{(2)}$, being the unique positive semidefinite square root of $A^{(2)}$, has eigenvector x, and corresponding eigenvalue $\sqrt{\lambda_2}$. Labeling the negative entry in $C^{(2)}$ (or one of the negative entries if there is more than one) as $\begin{vmatrix} c_{i_0p} & c_{i_0q} \\ c_{j_0p} & c_{j_0q}\end{vmatrix}$, a similar argument to that given in the proof Theorem 1 is all that remains.

$$\begin{vmatrix} a_{i_0i_0} & a_{i_0j_0} \\ a_{i_0j_0} & a_{j_0j_0}\end{vmatrix} = \sum_{1\leqslant k<l\leqslant n} \begin{vmatrix} c_{i_0k} & c_{i_0l} \\ c_{j_0k} & c_{j_0l}\end{vmatrix}^2, \tag{5}$$

$$> \sum_{1\leqslant k<l\leqslant n,(k,l)\neq(p,q)} \begin{vmatrix} c_{i_0k} & c_{i_0l} \\ c_{j_0k} & c_{j_0l}\end{vmatrix}^2, \tag{6}$$

$$\geqslant \frac{\left(\sum_{(k,l)\neq(p,q)} \begin{vmatrix} c_{i_0k} & c_{i_0l} \\ c_{j_0k} & c_{j_0l}\end{vmatrix} x_{kl}\right)^2}{\sum_{(k,l)\neq(p,q)} x_{kl}^2}, \tag{7}$$

$$\geqslant \frac{(\sqrt{\lambda_2}x_{i_0j_0})^2}{\sum_{(k,l)\neq(p,q)} x_{kl}^2}, \tag{8}$$

$$= \frac{\lambda_2 x_{i_0j_0}^2}{\sum_{(k,l)\neq(p,q)} x_{kl}^2}, \tag{9}$$

where equality (5) follows from $A^{(2)} = (C^{(2)})^2$, inequality (7) from Cauchy-Schwartz, and inequality (8) from $C^{(2)}x = \sqrt{r\lambda_2}x$, where $r = 1$ here. Note that the vector x is nonnegative, unlike the vector v in Theorem 1 which is necessarily a positive vector. $\square$

4. An example

When $n = 2$ the sufficient conditions of Corollary 2 that $a_{ii} \leqslant 1$, for each i, $1 \leqslant i \leqslant 2$, are redundant since they are a consequence of A being doubly stochastic. We saw in the paragraph after Corollary 2 that in any case we can write $A = C^2$. Consider Corollary 2 and Theorem 3 with the following 3×3 example when $e = (1,1,1)^T$, $w = (-2,1,1)^T$ and

$$C = \beta ee^T + \gamma ww^T = \begin{pmatrix} \beta+4\gamma & \beta-2\gamma & \beta-2\gamma \\ \beta-2\gamma & \beta+\gamma & \beta+\gamma \\ \beta-2\gamma & \beta+\gamma & \beta+\gamma \end{pmatrix}.$$

Then since $e^T w = 0$, $||e||^2 = 4$, and $||w||^2 = 6$, we have that

$$A = C^2 = 3\beta^2 ee^T + 6\gamma^2 ww^T = \begin{pmatrix} 3\beta^2 + 24\gamma^2 & 3\beta^2 - 12\gamma^2 & 3\beta^2 - 12\gamma^2 \\ 3\beta^2 - 12\gamma^2 & 3\beta^2 + 6\gamma^2 & 3\beta^2 + 6\gamma^2 \\ 3\beta^2 - 12\gamma^2 & 3\beta^2 + 6\gamma^2 & 3\beta^2 + 6\gamma^2 \end{pmatrix}.$$

Taking $3\beta^2 = \frac{1}{3}$ and $\frac{1}{6} \geqslant \gamma \geqslant 0$ the matrix A is doubly stochastic and positive semidefinite with second largest eigenvalue $36\gamma^2$, and C is positive semidefinite. Then since $\frac{1}{6} \geqslant \gamma$ the diagonal entry $\frac{1}{3} + 6\gamma^2 \leqslant \frac{1}{2}$, but if we also take $\gamma > \frac{1}{12}$ the diagonal entry $\frac{1}{3} + 24\gamma^2 > \frac{1}{2}$ so the sufficient conditions of Corollary 2 do not hold. However, the 2×2 minors $\begin{vmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{vmatrix}$ in lexicographic order are $18\gamma^2, 18\gamma^2, 0$ respectively. The $r\lambda_2 = \lambda_2$ eigenvector of $A^{(2)}$ being $x = (w_j - w_i) = (3,3,0)$ means that the denominator on the right hand side of the inequalities of Theorem 3 is largest when it is 18. Then in lexicographic order the right hand sides of these inequalities are $36\gamma^2 \frac{9}{18}, 36\gamma^2 \frac{9}{18}, 0$, respectively, at their smallest. Thus, the inequalities of Theorem 3 are satisfied but those of Corollary 2 are not.

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Robert Reams
Department of Mathematics
SUNY Plattsburgh
101 Broad Street
NY 12901
e-mail: robert.reams@plattsburgh.edu