ON THE MAXIMAL ANGLE BETWEEN COPOSITIVE MATRICES

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Abstract. Hiriart-Urruty and Seeger have posed the problem of finding the maximal possible angle $\theta_{\text{max}}(C_n)$ between two copositive matrices of order $n$. They have proved that $\theta_{\text{max}}(C_2) = \frac{3\pi}{4}$ and conjectured that $\theta_{\text{max}}(C_n)$ is equal to $\frac{3\pi}{4}$ for all $n \geq 2$. In this note we disprove their conjecture by showing that $\lim_{n \to \infty} \theta_{\text{max}}(C_n) = \pi$. Our proof uses a construction from algebraic graph theory. We also consider the related problem of finding the maximal angle between a nonnegative matrix and a positive semidefinite matrix of the same order.

Key words. copositive matrix, convex cone, critical angle, strongly regular graph, symmetric nonnegative inverse eigenvalue problem

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1. Introduction. A matrix $A$ is called copositive if $x^T A x \geq 0$ for every vector $x \geq 0$. The set of $n \times n$ copositive matrices $C_n$ is a closed convex cone in the space $S_n$ of $n \times n$ symmetric matrices. By the definition, the cone $C_n$ includes as subsets the cone $P_n$ of positive semidefinite matrices and the cone $N_n$ of symmetric nonnegative matrices of order $n$. Therefore, it is easy to see that $P_n + N_n \subseteq C_n$.

In [7] Diananda proved that for $n \leq 4$ this set inclusion is in fact an equality, and also cited an example due to A. Horn that shows that for $n \geq 5$ there are copositive matrices which cannot be decomposed as a sum of a positive semidefinite and a nonnegative matrix (see also [12, p. 597]). In a remarkable recent paper [11] Hildebrand has described all extreme rays of $C_5$, but very little is known about the structure of $C_n$ for $n \geq 6$.

Understanding the structure of this cone is important, among other reasons, since many combinatorial and nonconvex quadratic optimization problems can be equivalently reformulated as linear problems over the cone $C_n$ or its dual, the cone $C_n^\ast$ of $n \times n$ completely positive matrices (i.e., matrices $A$ that possess a factorization $A = B B^T$, where $B \geq 0$). For more information about copositive matrices and copositive optimization we refer the reader to the recent surveys [12, 8, 4] and the references therein.

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This paper is dedicated to the solution of a problem posed by Hiriart-Urruty and Seeger in their survey \[12\]:

*What is the greatest possible angle between two matrices in \( C_n \) ?*

The angle between vectors \( u, v \) in an inner product space \( V \) is:

\[
\angle(u, v) = \arccos \frac{\langle u, v \rangle}{||u|| \cdot ||v||}.
\]

Given a convex cone \( K \subseteq V \), the maximal angle attained between two vectors in the cone \( K \) is denoted \( \theta_{\text{max}}(K) \), and a pair of vectors attaining this angle is called *antipodal*. For the study of maximal angles of cones we refer to \[13, 14\].

Here we consider \( V = S_n \), with the standard inner product

\[
\langle A, B \rangle = \text{Tr} AB
\]

and the norm associated with it, that is the Frobenius norm \( ||A|| = \sqrt{\sum_{i,j=1}^{n} |a_{ij}|^2} \).

In \[12\] it was shown that \( \theta_{\text{max}}(C_2) = \frac{3}{4}\pi \) and the unique pair of \( 2 \times 2 \) matrices (up to multiplication by a positive scalar) that attains this angle was found. Furthermore, in \[12\] Remark 6.18 a somewhat hesitant conjecture was made to the effect that \( \theta_{\text{max}}(C_n) = \frac{3}{4}\pi \) for all \( n \geq 2 \).

We show in this note that the authors of \[12\] were rightly apprehensive about the said conjecture, and that the correct asymptotic answer to their problem is:

\[
\lim_{n \to \infty} \theta_{\text{max}}(C_n) = \pi.
\]

Note that the cone \( C_n \) is *pointed*, i.e., \( C_n \cap (-C_n) = \{0\} \) \[12\] Proposition 1.2], and thus clearly \( \theta_{\text{max}}(C_n) < \pi \) for every \( n \).

For the proof, we consider the maximal angle between a positive semidefinite matrix and a nonnegative matrix of the same order \( n \). Let us denote this maximal angle by \( \gamma_n \), i.e.,

\[
\gamma_n = \max_{0 \neq X \in \mathcal{P}_n} \max_{0 \neq Y \in \mathcal{N}_n} \angle(X, Y) = \max_{0 \neq X \in \mathcal{P}_n, 0 \neq Y \in \mathcal{N}_n} \arccos(X, Y).
\]

This maximum exists, since both \( \mathcal{N}_n \) and \( \mathcal{P}_n \) are closed and their intersection with the unit sphere is compact. Then by the inclusion \( \mathcal{P}_n + \mathcal{N}_n \subseteq \mathcal{C}_n \) we have

\[
\gamma_n \leq \theta_{\text{max}}(\mathcal{P}_n + \mathcal{N}_n) \leq \theta_{\text{max}}(\mathcal{C}_n).
\]

We prove our result on \( \theta_{\text{max}}(\mathcal{C}_n) \) by establishing
Theorem 1.

$$\lim_{n \to \infty} \gamma_n = \lim_{n \to \infty} \theta_{\text{max}}(C_n) = \pi.$$ 

This is achieved by constructing a sequence of pairs $(P_k, N_k)$, $P_k \in \mathcal{P}_{n_k}$ and $N_k \in \mathcal{N}_{n_k}$, where the orders $n_k$ tend to infinity and such that $\angle(P_k, N_k) \to \pi$. Note that $\{\gamma_n\}$ is a non-decreasing sequence, since the angle between $N \in \mathcal{N}_n$ and $P \in \mathcal{P}_n$ is equal to the angle between $N \oplus 0 \in \mathcal{N}_{n+1}$ and $P \oplus 0 \in \mathcal{P}_{n+1}$.

As the problem of calculating or estimating $\gamma_n$ is interesting in its own right, we start in Section 2 with some initial results on this problem, finding $\gamma_3$ and $\gamma_4$. Though the geometry of the cones $\mathcal{P}_n$ and $\mathcal{N}_n$ is much better understood that that of $C_n$, calculating $\gamma_n$ is a very difficult task for $n \geq 5$. We will offer an explanation for this phenomenon by showing that the determination of $\gamma_n$ is closely related to the symmetric nonnegative inverse eigenvalue problem (SNIIEP). Details on SNIIEP and related problems can be found in [2] and the references of [17].

The main result is stated and proved in Section 5 by a construction based on algebraic graph theory. The interceding Sections 3-4 are devoted to the introduction of the relevant tools from this theory, in order to keep this note self-contained, albeit tersely so. We conclude in Section 6 with some remarks.

2. The maximal angle between a positive semidefinite matrix and a nonnegative matrix. In this section we consider the problem of determining maximal angle between a positive semidefinite matrix and a nonnegative matrix of the same order for its own sake. However, the observations made in this section will also be instrumental in establishing the main result.

Every $n \times n$ symmetric matrix $A$ has a unique decomposition as a difference of two positive semidefinite matrices that are orthogonal to each other:

$$A = Q - P, \text{ with } Q, P \in \mathcal{P}_n \text{ and } QP = 0.$$ 

In fact, $Q$ is the projection of $A$ on $\mathcal{P}_n$ and $P$ is the projection of $-A$ on the same cone.

More explicitly, let $\Lambda$ be the multiset of eigenvalues of $A$, and for every $\lambda \in \Lambda$ denote by $E_\lambda$ the orthogonal projection on the eigenspace of $\lambda$. Then

$$A = \sum_{\lambda \in \Lambda} \lambda E_\lambda$$

is the spectral decomposition of $A$.

Denote by $\Lambda_+$ and $\Lambda_-$ the multisets of positive and negative eigenvalues of $A$, respectively. Then $Q = \sum_{\lambda \in \Lambda_+} \lambda E_\lambda$ and $P = -\sum_{\lambda \in \Lambda_-} \lambda E_\lambda$. In particular, the
spectrum of $Q$ consists of the elements of $\Lambda_+$ together with $n - |\Lambda_+|$ zeros and the spectrum of $P$ consists of the absolute values of the elements in $\Lambda_-$ together with $n - |\Lambda_-|$ zeros. We refer to $Q$ and $P$ as the positive definite part and the negative definite part of $A$, respectively.

If $A$ is not positive semidefinite, then obviously $A \neq 0$ and $P \neq 0$, and the cosine of the angle between $A$ and $P$ is

$$
\frac{\langle A, P \rangle}{\|A\| \cdot \|P\|} = \frac{-\langle P, P \rangle}{\|A\| \cdot \|P\|} = \frac{\sqrt{\sum_{\lambda \in \Lambda_-} \lambda^2}}{\sqrt{\sum_{\lambda \in \Lambda_+} \lambda^2}},
$$

(2.1)

For every nonzero symmetric $n \times n$ matrix $A$, let us denote by $\angle(A, P_n)$ the maximal angle between $A$ and a matrix in $P_n$. The following holds:

**Proposition 2.** For every $A \in S_n \setminus P_n$, let $P \in P_n$ be the negative definite part of $A$. Then

$$
\angle(A, P_n) = \angle(A, P) = \arccos \left(\frac{-\sqrt{\sum_{\lambda \in \Lambda_-} \lambda^2}}{\sqrt{\sum_{\lambda \in \Lambda_+} \lambda^2}}\right),
$$

(2.2)

where $\Lambda$ and $\Lambda_-$ are as described above. Moreover, $P$ is the unique matrix in $P_n$, up to multiplication by a positive scalar, which forms this maximal angle with $A$.

**Proof.** For every $0 \neq X \in P_n$ we have

$$
\frac{\langle A, X \rangle}{\|A\| \cdot \|X\|} \geq -\frac{\langle P, X \rangle}{\|A\| \cdot \|X\|} \geq -\frac{\|P\|}{\|A\|} = \frac{\langle A, P \rangle}{\|A\| \cdot \|P\|},
$$

(2.3)

where the first inequality follows from the fact that $Q$, the positive definite part of $A$, satisfies $\langle Q, X \rangle \geq 0$, and the second inequality from the Cauchy-Schwarz inequality. This shows that $\angle(A, X) \leq \angle(A, P)$ for every $X \in P_n$. By the condition for equality in the Cauchy-Schwarz inequality, we get that $\angle(A, X) = \angle(A, P)$ if and only if $X$ is a positive scalar multiple of $P$. \qed

Similarly, every $A \in S_n$ has a unique decomposition as a difference of two non-negative matrices that are orthogonal to each other:

$$
A = M - N, \text{ with } M, N \in N_n \text{ and } M \circ N = 0,
$$

where $\circ$ denotes the entrywise product of matrices (also often called the Hadamard product).

In fact, $M = \max(A, 0)$, with the maximum defined entrywise, is the projection of $A$ on $N_n$, and $N = \max(-A, 0)$ is the projection of $-A$ on that cone. We refer to
$M$ and $N$ as the *positive part* and the *negative part* of $A$, respectively. If $A \notin \mathcal{N}_n$, then $A, N \neq 0$, and the cosine of the angle between $A$ and $N$ is

$$\frac{\langle A, N \rangle}{\|A\| \cdot \|N\|} = -\frac{\langle N, N \rangle}{\|A\| \cdot \|N\|} = -\frac{\sqrt{\sum_{a_{ij} < 0} a_{ij}^2}}{\sqrt{\sum a_{ij}^2}}. \quad (2.4)$$

We denote by $\angle(A, \mathcal{N}_n)$ the maximal angle between $A$ and a matrix in $\mathcal{N}_n$. Then the following holds:

**Proposition 3.** For every $A \in \mathcal{S}_n \setminus \mathcal{N}_n$, let $N \in \mathcal{P}_n$ be the negative part of $A$. Then

$$\angle(A, \mathcal{N}_n) = \angle(A, N) = \arccos \left( -\frac{\sqrt{\sum_{a_{ij} < 0} a_{ij}^2}}{\sqrt{\sum a_{ij}^2}} \right). \quad (2.5)$$

Moreover, $N$ is the unique matrix in $\mathcal{N}_n$, up to multiplication by a positive scalar, which forms this maximal angle with $A$.

The proof is completely parallel to the proof of Proposition 2.2 and is therefore omitted. The next proposition demonstrates the computation of $\angle(P, \mathcal{N}_n)$ in a special case.

**Proposition 4.** Let $P \in \mathcal{P}_n \setminus \mathcal{N}_n$ have rank 1. Then $\angle(P, \mathcal{N}_n) \leq \frac{3}{4}\pi$. Furthermore, there exists a rank 1 positive semidefinite matrix $P \in \mathcal{P}_n \setminus \mathcal{N}_n$ such that $\angle(P, \mathcal{N}_n) = \frac{3}{4}\pi$.

**Proof.** By the assumptions, $P = uu^T$, where $u$ has both positive and negative entries. By a suitable permutation of rows and columns of $P$ we may assume that

$$u = \begin{bmatrix} v \\ -w \end{bmatrix}, \quad v, w \geq 0, \quad v, w \neq 0.$$

Then

$$P = \begin{bmatrix} vv^T & -vw^T \\ -ww^T & ww^T \end{bmatrix},$$

and the negative part of $P$ is

$$N = \begin{bmatrix} 0 & vv^T \\ ww^T & 0 \end{bmatrix}.$$

For any two vectors $x$ and $y$,

$$\|xy^T\| = \sqrt{\text{Tr}(xy^Tyx^T)} = \|x\|\|y\|.$$
Thus
\[ ||P|| = ||u||^2 = ||v||^2 + ||w||^2, \quad ||N|| = \sqrt{2} ||v|| \cdot ||w||, \]
and
\[ \langle P, N \rangle = -2 ||vw||^2 = -2 ||v||^2 ||w||. \]

Thus
\[ \frac{\langle P, N \rangle}{||P|| \cdot ||N||} = -\frac{\sqrt{2} ||v|| \cdot ||w||}{||v||^2 + ||w||^2} \geq -\frac{\sqrt{2}}{2}. \]

Equality holds in the last inequality if and only if \( ||v|| = ||w|| \). Thus \( \angle(P, N) \leq \frac{3}{4} \pi \), with equality if and only if \( ||v|| = ||w|| \). \( \square \)

In particular, the last proposition implies the following known result (known by the proof of Proposition 6.15 in [12], and the monotonicity of \( \{\gamma_n\} \)).

**Corollary 5.** For every \( n \geq 2 \), \( \gamma_n \geq \frac{3}{4} \pi \).

We can now prove

**Proposition 6.** Let \( n \geq 2 \), and let \( P \in \mathcal{P}_n \) and \( N \in \mathcal{N}_n \) be any two matrices such that \( \angle(P, N) = \gamma_n \). Then \( \langle P, N \rangle < 0 \), \( \text{diag} N = 0 \), and \( 1 \leq \text{rank} P \leq n - 1 \).

**Proof.** By Corollary \( \square \) \( \gamma_n \geq \frac{3}{4} \pi \), and thus \( \langle P, N \rangle < 0 \). This implies that \( P \notin \mathcal{N}_n \) and \( N \notin \mathcal{P}_n \). Since \( \angle(P, N) \) is the maximal possible angle between a positive semidefinite and a nonnegative matrix of the same order, \( N \) has to be the nonnegative matrix forming the maximal possible angle with \( P \), and \( P \) has to be the nonnegative matrix forming the maximal possible angle with \( N \).

By the uniqueness parts in Propositions \( \square \) and \( \square \) \( N \) is a positive scalar multiple of the negative part of \( P \), and \( P \) is a positive scalar multiple of the negative definite part of \( N \). Since \( \text{diag} P \geq 0 \) and \( N \) is the negative part of \( P \), we get that \( \text{diag} N = 0 \). By the Perron-Frobenius Theorem the nonzero \( N \) has at least one positive eigenvalue, so its negative definite part \( P \) satisfies \( \text{rank} P \leq n - 1 \). \( \square \)

**Proposition 7.** Let \( n \geq 2 \), let \( N \in \mathcal{N}_n \) have \( \text{diag} N = 0 \) and let \( P \) be its negative definite part. If \( \text{rank} P = n - 1 \), then \( \angle(N, \mathcal{P}_n) < \frac{3}{4} \pi \).

**Proof.** By the assumptions on \( N \), its eigenvalues are \( \rho = \lambda_1 > 0 \), and \( n - 1 \) negative eigenvalues \( \lambda_2, \ldots, \lambda_n \) with \( \sum_{i=2}^{n} \lambda_i = -\rho \). By Proposition \( \square \)
\[ \cos \angle(N, \mathcal{P}_n) = -\frac{\sqrt{\sum_{i=2}^{n} \lambda_i^2}}{\sqrt{\rho^2 + \sum_{i=2}^{n} \lambda_i^2}}. \]
The function \( g(x_2, \ldots, x_n) = \sum_{i=2}^{n} x_i^2 \) is convex, and thus attains its maximum on the compact convex set
\[
\Delta = \left\{ (x_2, \ldots, x_n) \in \mathbb{R}^{n-1} : x_i \leq 0, \ i = 2, \ldots, n-1, \ \text{and} \ \sum_{i=2}^{n} x_i = -\rho \right\}
\]
at an extreme point of this set, i.e., at a point \( x \) such that \( x_i = -\rho \) for some \( i \) and \( x_j = 0 \) for \( j \neq i \). That is,
\[
\max_{x \in \Delta} g(x) = \rho^2.
\]

The function \( f(t) = -\sqrt{\frac{t}{\rho^2 + t}} \) is decreasing on \([0, \infty)\), and thus \( f(g(x_2, \ldots, x_2)) \) attains a minimum on \( \Delta \) where \( g \) attains its maximum, and \( \min_{x \in \Delta} f(g(x)) = -\sqrt{\frac{\rho^2}{2}} \). Since \( \cos \angle(N, P_n) = f(g(\lambda_2, \ldots, \lambda_n)) \), and \( (\lambda_2, \ldots, \lambda_n) \in \Delta \), we get that \( \angle(N, P_n) \leq \cos(\min_{x \in \Delta} f(g(x))) = \frac{3}{4} \pi \).

By the assumption that \( \text{rank } P = n - 1 \) we see that \( (\lambda_2, \ldots, \lambda_n) \) is not an extreme point of \( \Delta \), and since \( g(x) \) is strictly convex on \( \Delta \), it does not attain its maximum on \( (\lambda_2, \ldots, \lambda_n) \), and neither does \( \arccos(f(g(x))) \). Hence the strict inequality.

In other words, Proposition 7 tells us that if \((N, P)\) is a pair attaining \( \gamma_n \), then we must have \( \text{rank } P \leq n - 2 \).

We can now show:

**Theorem 8.** For \( n \leq 4 \), \( \gamma_n = \frac{3}{4} \pi \).

**Proof.** Propositions 4, 6 and 7 imply that \( \gamma_n = \frac{3}{4} \pi \) for \( n \leq 3 \). It remains to consider the case of \( n = 4 \). Also, by these propositions it suffices to consider \( \angle(N, P_n) \) for \( N \in \mathcal{N}_4 \) with \( \text{diag } N = 0 \) and a negative definite part \( P \) of rank 2. Such \( N \) has a Perron eigenvalue \( \rho > 0 \), and its complete set of eigenvalues is

\[
\rho \geq \mu \geq 0 > \lambda_3 \geq \lambda_4,
\]
where \( \lambda_3 + \lambda_4 = -\rho - \mu \) and \( \lambda_4 \geq -\rho \). Then
\[
\cos \angle(N, P_n) = -\frac{\sqrt{\lambda_3^2 + \lambda_4^2}}{\sqrt{\rho^2 + \mu^2 + \lambda_3^2 + \lambda_4^2}}.
\]

Similarly to the previous proof, we note that \( g(x, y) = x^2 + y^2 \) is a convex function, and the set
\[
\Delta = \{(x, y) \in \mathbb{R}^2 : 0 \geq x \geq y \geq -\rho \ \text{and} \ x + y = -\rho - \mu \}\]
is a compact convex set. By the assumptions on $\rho$ and $\mu$, $\Delta$ is the line segment
\[ y = -\rho - \mu - x , \quad -\frac{\rho + \mu}{2} \leq x \leq -\mu. \]
Its extreme points are
\[ (-\mu, -\rho) \text{ and } \left( -\frac{\rho + \mu}{2}, -\frac{\rho + \mu}{2} \right), \]
and the maximal of $g$ on $\Delta$ is the greater of
\[ g(-\mu, -\rho) = \mu^2 + \rho^2 \text{ and } g \left( -\frac{\rho + \mu}{2}, -\frac{\rho + \mu}{2} \right) = \frac{(\rho + \mu)^2}{2}. \]
Thus
\[ \max_{(x,y) \in \Delta} g(x,y) = \mu^2 + \rho^2, \]
and it is attained when $x = -\mu$ and $y = -\rho$. The function $f(t) = -\sqrt{\frac{t}{\rho^2 + \mu^2 + t}}$ is a decreasing function on $[0, \infty)$, and therefore $f(g(x,y))$ attains a minimum on $\Delta$ at $(-\mu, -\rho)$, and $\min_{(x,y) \in \Delta} f(g(x)) = -\sqrt{\frac{\rho^2 + \mu^2}{\rho^2 + \mu^2}} = -\frac{\sqrt{\pi}}{2}$. Since $(\lambda_3, \lambda_4) \in \Delta$, we get that $\angle(N, P_4) \leq \arccos(\min_{(x,y) \in \Delta} f(g(x))) = \frac{3}{4} \pi$. Together with Corollary 5 this completes the proof.

Note that the matrix
\[ N = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 1 & 0
\end{bmatrix} \]
has eigenvalues 1, 1, -1, -1, and thus by the above argument $\gamma_4 = \frac{3}{4} \pi$ is attained also by a pair $(N, P)$, where $P$ is the positive semidefinite part of $N$ and rank $P = 2$.

For $n = 5$ the result of Theorem 8 no longer holds:

**Example 9.** Let
\[ N = \begin{bmatrix}
0 & 1 & 0 & 0 & 1 \\
1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 1 & 0
\end{bmatrix} \]
be the adjacency matrix of the 5-cycle. Its eigenvalues are well known (they are easily computed by the formula for the eigenvalues of a circulant matrix): the simple
eigenvalue $2$, the positive eigenvalue $2 \cos(2\pi/5) = \frac{-1+\sqrt{5}}{2}$ of multiplicity $2$, and the negative eigenvalue $-2 \cos(\pi/5) = \frac{-1+\sqrt{5}}{2}$ of multiplicity $2$. Thus the negative definite part $P$ of $N$ satisfies:

$$\cos \angle(P, N) = -\frac{\sqrt{8 \cos^2(\pi/5)}}{\sqrt{4 + 8 \cos^2(2\pi/5) + 8 \cos^2(\pi/5)}} = -\frac{1+\sqrt{5}}{2} < -\frac{\sqrt{2}}{2},$$

implying that

$$\gamma_5 \geq \arccos \left(-\frac{1+\sqrt{5}}{2}\right) \approx 0.7575 \pi > \frac{3}{4} \pi.$$

The negative definite part of $N$ is a scalar multiple of

$$P = \begin{bmatrix}
1 & -\cos(\pi/5) & \cos(2\pi/5) & \cos(2\pi/5) & -\cos(\pi/5) \\
-\cos(\pi/5) & 1 & -\cos(\pi/5) & \cos(2\pi/5) & \cos(2\pi/5) \\
\cos(2\pi/5) & -\cos(\pi/5) & 1 & -\cos(\pi/5) & \cos(2\pi/5) \\
-\cos(\pi/5) & \cos(2\pi/5) & -\cos(\pi/5) & 1 & -\cos(\pi/5) \\
\end{bmatrix}.$$

Indeed, the kind of argument that we used to prove Theorem 8 is no longer sufficient for the determination of $\gamma_n$ for $n \geq 5$. Here we present some considerations which explain the new difficulties which arise in the case $n \geq 5$.

Our proofs for the case $n \leq 4$ involved optimization of a convex function of the non-positive eigenvalues of a matrix $0 \neq N \in \mathcal{N}_n$ with zero diagonal, over a convex set formed by such eigenvalue-tuples. Continuing this line of proof for $n \geq 5$ would require some information on the possible sets of eigenvalues of a nonnegative $n \times n$ matrix with a zero diagonal. It is known that the eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$$

of a matrix $0 \neq N \in \mathcal{N}_n$ with zero diagonal satisfy

$$\lambda_1 > 0, \quad \lambda_n \geq -\lambda_1 \quad \text{and} \quad \sum_{i=1}^{n} \lambda_i = 0. \quad (2.7)$$

But for $n \geq 5$ not all sequences satisfying (2.6) and (2.7) are eigenvalues of some such $N$. The problem of determining necessary and sufficient conditions for a set of real numbers to be the eigenvalues of some $N \in \mathcal{N}_n$ with a zero diagonal is part of the Symmetric Inverse Eigenvalue Problem (SINEP), which is difficult and generally open. For $n \leq 4$ the conditions (2.6) and (2.7) are also sufficient, by results of [9] and [15]. For $n = 5$ it is shown in [17] that necessary and sufficient conditions for (2.6) to
be eigenvalues of some $N \in \mathcal{N}_n$ are \eqref{2.7} together with
\[ \lambda_2 + \lambda_5 \geq 0 \text{ and } \sum_{i=1}^{5} \lambda_i^3 \geq 0. \] (2.8)

For $n \geq 6$ the SNIEP is still open even for trace zero matrices.

The solution of the trace-zero SNIEP for $n = 5$ demonstrates a second difficulty in applying our approach, even for $n = 5$: The last condition in \eqref{2.8} is not redundant, and the set of all non-increasing 5-tuples that are eigenvalues of a nonnegative trace zero matrix is not convex, complicating the relevant optimization problem. It seems that a new approach is needed for the computation of $\gamma_n$, $n \geq 5$.

For our purpose, of proving that $\lim_{n \to \infty} \gamma_n = \infty$, we will show that a judicious choice of a nonnegative matrix $N$ will allow the pair $(N, P)$, where $P$ is the negative definite part of the nonnegative matrix $N$, to attain ever higher angles. This will be done by taking $N$ as the adjacency matrix of a strongly regular graph.

3. Strongly regular graphs. Recall first the definition of strongly regular graphs, due originally to Bose, and the famous formula for the eigenvalues of such a graph.

**Definition 10** \([5]\). A strongly regular graph with parameters $(n, k, a, c)$ is a $k$-regular graph on $n$ vertices such that any two adjacent vertices have $a$ common neighbours and any two non-adjacent vertices have $c$ common neighbours.

For instance, observe that the pentagon $C_5$ is strongly regular with parameters $(5, 2, 0, 1)$ and that the Petersen graph is strongly regular with parameters $(10, 3, 0, 1)$.

Obviously, not every quadruple of numbers $(a, b, c, d)$ is the parameter vector of a strongly regular graph. A number of necessary conditions are known and may be found in \([10\text{, Chapter 10}])]. We will only mention the simplest one, by way of illustration:
\[ (n - k - 1)c = k(k - a - 1). \] (3.1)

The proof is an easy exercise in double counting.

The crucial fact for us here is that the eigenvalues of the adjacency matrix of a strongly regular graphs and their multiplicities depend only on the parameters (as there may often be many non-isomorphic graphs sharing the same parameters):

**Theorem 11** \([10\text{, Section 10.2}])]. Let $G$ be a connected strongly regular graph with parameters $(n, k, a, c)$ and let $\Delta = (a-c)^2 + 4(k-c)$. The eigenvalues of the adjacency matrix $A(G)$ are:
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- $k$, with multiplicity 1.
- $\theta = \frac{(a-c) + \sqrt{\Delta}}{2}$, with multiplicity $m_\theta = \frac{1}{2} \left( (n - 1) - \frac{2k + (n-1)(a-c)}{\sqrt{\Delta}} \right)$.
- $\tau = \frac{(a-c) - \sqrt{\Delta}}{2}$, with multiplicity $m_\tau = \frac{1}{2} \left( (n - 1) + \frac{2k + (n-1)(a-c)}{\sqrt{\Delta}} \right)$.

Note that $m_\theta$ and $m_\tau$ have to be integers, and this is another necessary condition the parameters $(n, k, a, c)$ have to satisfy.

Let us now take $N$ to be the adjacency matrix of a strongly regular graph, and let be $P$ the negative definite part of $N$. Equation (2.1) takes on the following form then:

$$\langle N, P \rangle = -\sqrt{m_\tau^2 \cdot \frac{nk}{\Delta}}.$$ (3.2)

To complete the proof of Theorem 1 we would now like to exhibit a family of strongly regular graphs $\{G_{nk}\}$ for which the expressions of (3.2) tend to $-1$ as $n_k \to \infty$.

4. Generalized quadrangles.

**Definition 12.** A generalized quadrangle is a finite incidence structure $(\Pi, L)$ with sets $\Pi$ of points and $L$ of lines, such that:

- Two lines meet in at most one point.
- If $u$ is a point not on line $m$, then there is a unique point $v$ on $m$ and a unique line $\ell$ such that $u$ and $v$ are on $\ell$.

For basic facts about generalized quadrangles we refer to [1, Chapter 6]. The advanced theory is laid out in [16]. Our definition here followed [6, p. 129].

If the generalized quadrangle $Q$ has the further property that every line is on $s + 1$ points and every point is on $t + 1$ lines, then we say that $Q$ is of order $(s, t)$ and denote it by $GQ(s, t)$. By [1] Theorem 6.1.1 all generalized quadrangles are either of this form or isomorphic to a grid or to a dual of a grid.

It is not known what are all the pairs $(s, t)$ for which a generalized quadrangle $G(s, t)$ exists. But the so-called “classical” constructions of generalized quadrangles, originally due to Tits, yields specimens of $GQ(s, 1)$, $GQ(s, s)$ and $GQ(s, s^2)$ whenever $s = q$ is a prime power. (cf. [1] p. 118] and [6] pp. 130-131] for descriptions of these constructions.)

We need to introduce one final concept. The collinearity graph $C_Q$ of a generalized quadrangle $Q = (\Pi, L)$ has $\Pi$ for its vertex set and $u, v \in \Pi$ are adjacent in $C_Q$ if and only if $u$ and $v$ lie on a line in $Q$. 
Theorem 13 (\cite{Goldberg2020} Theorem 9.6.2). Let $Q$ be a generalized quadrangle of order $(s, t)$ and let $C_Q$ be its collinearity graph. Then $C_Q$ is strongly regular with parameters $(n, k, a, c) = ((s + 1)(st + 1), s(t + 1), s - 1, t + 1)$ and its spectrum is:

- $k = s(t + 1)$ with multiplicity 1.
- $\theta = s - 1$ with multiplicity $m_\theta = st(s + 1)(t + 1)/(s + t)$.
- $\tau = -(t + 1)$ with multiplicity $m_\tau = s^2(st + 1)/(s + t)$.

5. Piecing everything together.

Proof of Theorem 1. Let $\{n_k\}$ be the sequence of prime powers. For each $q \in \{n_k\}$ there exists a classical generalized quadrangle $Q_k$ of the $GQ(q, q^2)$ type. Let $N_k$ be the adjacency matrix of $C_{Q_k}$ and let $P_k$ be the projection of $(-N_k)$ on $P_n$. Then the angle between $N_k$ and $P_k$ can be calculated with the help of Theorem 13 and (3.2): its cosine is

$$-\sqrt{\frac{m_\tau^2}{nk}} = -\sqrt{\frac{s(t + 1)}{(s + 1)(s + t)}} = -\sqrt{\frac{q^2 + 1}{q + 1}}$$

and this leads to

$$\angle(N_k, P_k) = \arccos\left(-\frac{\sqrt{q^2 + 1}}{q + 1}\right) \quad \xrightarrow{q \to \infty} \arccos(-1) = \pi.$$ 

Since

$$\pi > \theta_{\max}(C_{n_k}) \geq \gamma_{n_k} \geq \angle(N_k, P_k)$$

this implies $\lim_{k \to \infty} \theta_{\max}(C_{n_k}) = \lim_{k \to \infty} \gamma_{n_k} = \pi$, and by the monotonicity of the sequences $\{\theta_{\max}(C_n)\}$ and $\{\gamma_n\}$ the result follows.

Note that we did not actually find the value of $\gamma_n$ for every $n$, which is why we refer to our result as the asymptotic solution of the Hiriart-Urruty and Seeger problem.

To get a feel for the sequence of angles $\{\angle(N_k, P_k)\}$, we list here the first five elements in the sequence. The first five prime powers (our $q$’s) are 2, 3, 4, 5 and 7. The first five orders of the matrix pairs we generate are $n_1 = 27$, $n_2 = 112$, $n_3 = 325$, $n_4 = 756$ and $n_5 = 2752$ ($n = (q + 1)(q^3 + 1)$). Table 1 shows the lower bounds on $\gamma_n$ (and thus on $\theta_{\max}(C_n)$) for these orders, computed using (5.1).

$$\begin{array}{cccc}
n &= 27 & n &= 112 & n &= 325 & n &= 756 & n &= 2752 \\
\arccos\left(-\frac{\sqrt{2}}{2}\right) & \approx 0.7677\pi & \arccos\left(-\frac{\sqrt{3}}{3}\right) & \approx 0.7902\pi & \arccos\left(-\frac{\sqrt{4}}{4}\right) & \approx 0.8086\pi & \arccos\left(-\frac{\sqrt{5}}{5}\right) & \approx 0.8232\pi & \arccos\left(-\frac{\sqrt{7}}{7}\right) & \approx 0.8451\pi \\
\end{array}$$

Table 1: Lower bounds on $\gamma_n$ and $\theta_{\max}(C_n)$.
6. A few remarks.

1. Theorem [1] implies that for large \( n \) there exist a nonnegative matrix and a positive semidefinite matrix that are almost opposite, and the cones \( \mathcal{P}_n + \mathcal{N}_n \) and \( \mathcal{C}_n \) are “barely pointed”.

2. We do not know whether the pair \((N_k, P_k)\) constructed is actually antipodal in either \( \mathcal{C}_{n_k} \) or \( \mathcal{P}_{n_k} + \mathcal{N}_{n_k} \). However, it is not hard to check that this pair satisfies the weaker property of being a critical pair in \( \mathcal{P}_{n_k} + \mathcal{N}_{n_k} \), as defined in [12, Definition 6.11]. Any antipodal pair is critical but not all critical pairs are antipodal. It is not obvious that this pair is a critical pair for \( \mathcal{C}_{n_k} \).

**Question.** Is \( \theta_{\text{max}}(\mathcal{C}_n) = \gamma_n? \) In other words, is the maximal angle in \( \mathcal{C}_n \) always achieved by a nonnegative matrix and a positive semidefinite matrix?

In fact, we do not even know the answer to the following, ostensibly simpler, question:

**Question.** Is \( \theta_{\text{max}}(\mathcal{P}_n + \mathcal{N}_n) = \gamma_n? \)

This is true for \( n = 2 \) by the results of [12].

3. Hiriart-Urruty and Seeger [12, Proposition 6.15] found that the (unique up to multiplication by a positive scalar) pair of antipodal matrices in \( \mathcal{C}_2 \) is:

\[
X = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad Y = \frac{\sqrt{2}}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]

This example is in fact a special case of our construction: \( Y \) can be thought of as the normalized adjacency matrix of the complete graph \( K_2 \) and \( X \) is the negative definite part of \( Y \). The right-hand side of (2.1) equals \(-\frac{\sqrt{2}}{2}\) in this case, as can be easily verified.

We observe that pairs of matrices that yield \(-\frac{\sqrt{2}}{2}\) in (2.1), and thus an angle of \(\frac{3}{4}\pi\), can be easily constructed for every order by taking \( N \) as the adjacency matrix of a bipartite graph, by the Coulson-Rushbrooke Theorem on the symmetry of their spectra (cf. [3, p. 11]).

Another kind of pair which attains the angle \(\frac{3}{4}\pi\) can be constructed for a prime power \( q \) by taking \( n = (q + 1)(q^2 + 1) \) and letting \( N \) be the adjacency matrix of \( C_{GQ(q,q)} \), which is clearly not a bipartite graph.

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