Algebras, Graphs and Thetas

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Abstract

We extend the clique-coclique inequality, previously known to hold for graphs in association schemes and vertex-transitive graphs, to graphs in homogeneous coherent configurations and 1-walk regular graphs. We further generalize it to a stronger inequality involving the Lovász theta number of such graph, and some theta variants, including characterizations of the equality.

Keywords: clique-coclique inequality, matrix ∗-algebra, Lovász theta function, coherent configuration

1   Introduction

Denote the maximum size of a clique in a graph G by $\omega(G)$ and the maximum size of a coclique by $\alpha(G)$; a coclique is an independent set of vertices, also called a stable set.

Think of a graph with a large clique and a large coclique. In general, there seems to be no (non-obvious) restriction on how large these two substructures can be compared to the size of the graph. However, if the graph displays high regularity or symmetry, then one soon finds out that large cliques cannot appear together with large cocliques, and vice-versa. More specifically, for a graph G on n vertices that is either distance-regular or vertex-transitive, we have $\alpha(G)\omega(G) \leq n$. This is known as the clique-coclique bound; see for instance [8, Chapter 3]. In this paper, we observe that a more general framework in which these graphs and their cliques and cocliques can be cast is sufficient to prove the clique-coclique bound. This appears in Theorems 3.1 and 3.2, and Corollary 4.1.

Our setting also allows for an extension of this inequality to a stronger inequality (which turns out to be an equality) involving the Lovász theta number of a graph and its complement, and another equality for some theta variants. This is found in Corollary 4.2. These results were known for vertex-transitive graphs only, therefore our contribution significantly increases the number of known graphs satisfying the properties displayed.

Some work has been done in the past in topics strongly related to the topic of this paper. Godsil and Meagher [8] present a full account of known bounds for the size of cliques and cocliques in graphs belonging to association schemes. Dukanovic and Rendl [7] proved some equalities involving generalizations of thetas for a vertex-transitive graph and its complement. Roberson [14] pointed that we could somehow relax the requirement of the graph being vertex-transitive. Some of the results in our paper work in the direction of finding exactly which graphs satisfy this relaxed condition. The use of positive semidefiniteness to find bounds in combinatorial structures dates back to Delsarte's thesis [6]. It was revived more recently by Schrijver [16] in the context of coding theory and later applied to some coherent configurations by Hobart [11] and Hobart and Williford [12]. Some surveys can be found in [1]. In all cases, the main tool is the fact that the projection of a positive semidefinite matrix in certain algebras of matrices remains positive semidefinite. We explore this fact in Lemmas 2.5 and 2.6 to build our theoretical framework.

2   Algebras

Equip the complex vector space $\mathrm{M}_n(\mathbb{C})$ of complex $n \times n$ matrices with the trace inner-product $\langle M, N \rangle = \operatorname{tr} MN^*$. We will work on *matrix ∗-algebras*, which means a linear subspace of $\mathbb{C}^{n\times n}$ that is closed under the conventional matrix product and under taking the conjugate transpose. A matrix ∗-algebra is *simple* if it has no non-trivial proper (two-sided) ideal. We start with the following consequence of Wedderburn's Theorem on semisimple algebras ([5, Chapter 5]); see for instance [3,

Theorem 2.7] for a more self-contained version, or [2, Chapter 1].

Theorem 2.1 *If $\mathcal{A}$ is a matrix $*$-algebra, then $\mathcal{A}$ is the direct sum of simple matrix $*$-algebras*

$$\mathcal{A} = \bigoplus_{i=0}^{s} E_i \mathcal{A}, \tag{1}$$

where $\{E_0, \ldots, E_s\}$ is an orthogonal basis of minimal idempotents of the center of $\mathcal{A}$.

Here we rely on the fact [1, Theorem 9.3] that every commutative matrix $*$-algebra $\mathcal{B}$ has an orthogonal basis of matrices $E_0, \ldots, E_s$ such that $E_i^* = E_i$ and $E_i^2 = E_i$ for each i and $E_i E_j = 0$ whenever $i \neq j$; such matrices are called *minimal idempotents* of $\mathcal{B}$.

Given a matrix M, we will use M' to denote the orthogonal projection of M onto $\mathcal{A}$. Because of the decomposition from above, it follows that M' is the sum of the projections of M onto each $E_i \mathcal{A}$. The following fact is also well-known, see for instance [1, Corollary 9.1].

Corollary 2.2 *The projection of a positive semidefinite matrix onto a matrix $*$-algebra is positive semidefinite.*

From here on, we assume all matrices in $\mathcal{A}$ have constant diagonal. This property shall be referred as $\mathcal{A}$ being *homogeneous*.

Lemma 2.3 *If $\mathcal{A}$ is a homogeneous matrix $*$-algebra, then all 01 matrices in $\mathcal{A}$ have constant row sums and constant column sums.*

Moreover, if $\mathcal{A}$ contains an irreducible 01 matrix, then the all 1s matrix J belongs to $\mathcal{A}$.

Finally, if $\mathcal{A}$ contains the all 1s matrix J, then the row sums and the column sums of all matrices in $\mathcal{A}$ are equal, that is, J lies in the center of $\mathcal{A}$.

Proof. Let $A \in \mathcal{A}$ be a 01 matrix. Then $A^* \in \mathcal{A}$, and so $AA^* \in \mathcal{A}$ and $A^*A \in \mathcal{A}$. The diagonal entries of AA^* are the row sums of A, and the diagonal entries of A^*A are the column sums of A. Because $\mathcal{A}$ is homogeneous, all row sums are equal, and the same holds for column sums. Now if A is irreducible, and because its row sums are constant, then by Perron-Frobenius theory the all 1s vector is an eigenvector in a 1-dimensional subspace, and therefore J is a polynomial in A, hence it belongs to $\mathcal{A}$. The result now follows from noting that, for all $M \in \mathcal{A}$, the diagonal entries of MJ and JM are, respectively, the row sums and column sums of M. These are constant diagonals, and because $\operatorname{tr} MJ = \operatorname{tr} JM$, it follows that these diagonal are, in fact, equal. $\square$

As $M \mapsto M'$ is a self-adjoint operator, it follows that

$$\langle M, N' \rangle = \langle M', N \rangle,$$

a fact that we exploit below for two special cases.

Lemma 2.4 *Let M be a matrix, and let $\mathcal{A}$ be a homogeneous matrix $*$-algebra that contains I and J. Then*

$$\operatorname{tr} M' = \operatorname{tr} M,$$

and

$$\operatorname{tr} JM' = \operatorname{tr} JM.$$

Proof. Since I and J belong to $\mathcal{A}$, we have $I' = I$ and $J' = J$. Thus, $\operatorname{tr} M' = \langle M', I \rangle = \langle M, I' \rangle = \operatorname{tr} M$ and $\operatorname{tr} JM' = \operatorname{tr} M'J = \langle M', J \rangle = \langle M, J' \rangle = \operatorname{tr} MJ = \operatorname{tr} JM$. $\qquad\square$

We show below how to obtain a trace inequality in a special but useful case.

Lemma 2.5 *Let $\mathcal{A}$ be a homogeneous matrix $*$-algebra that contains I. Let M and N be positive semidefinite $n \times n$ matrices. Let $I = P_0, P_1, \ldots, P_d$ be an orthogonal basis for the algebra $\mathcal{A}$. Assume that, for all $i \neq 0$, $\langle M, P_i \rangle \langle P_i, N \rangle \leq 0$. Then*

$$\langle M', N' \rangle \leq \frac{(\operatorname{tr} M)(\operatorname{tr} N)}{n}.$$

Moreover, equality holds if and only if, for all $i \neq 0$, $\langle M, P_i \rangle \langle P_i, N \rangle = 0$.

Proof. It is a straightforward computation:

$$\langle M', N' \rangle = \langle M', N \rangle = \operatorname{tr} \left(\sum_{i=0}^{d} \frac{\langle M, P_i \rangle}{\langle P_i, P_i \rangle} P_i \right) N^*$$

$$= \sum_{i=0}^{d} \frac{\langle M, P_i \rangle \langle P_i, N \rangle}{\langle P_i, P_i \rangle}$$

$$\leq \frac{\langle M, I \rangle \langle I, N \rangle}{\langle I, I \rangle}$$

$$= \frac{(\operatorname{tr} M)(\operatorname{tr} N)}{n}.$$

The equality characterization follows immediately. $\qquad\square$

Lemma 2.6 *Let $\mathcal{A}$ be a homogeneous matrix $*$-algebra that contains I and J. Let M and N be positive semidefinite $n \times n$ matrices. Then*

$$\langle M', N' \rangle \geq \frac{(\operatorname{tr} JM)(\operatorname{tr} JN)}{n^2}.$$

Moreover, equality holds if and only if $M'N'$ is a scalar multiple of J.

Proof. By Lemma 2.3 the all 1s vector is an eigenvector of all matrices in $\mathcal{A}$, and J lies in the center of $\mathcal{A}$. Write $\mathcal{A} = \bigoplus_{i=0}^{s} E_i \mathcal{A}$ as in Theorem 2.1. Then $E_i J \neq 0$ for precisely one index i: if $E_i J = \lambda_i J$ and $E_j J = \lambda_j J$ with $\lambda_i \neq 0 \neq \lambda_j$, then $E_i E_j J = \lambda_i \lambda_j J$ which implies $i = j$ since $E_0, \ldots, E_s$ are minimal idempotents. We may assume that $E_0 J \neq 0$. Since $\mathbb{C}J$ is an ideal of the simple matrix $*$-algebra $E_0 \mathcal{A}$, we find that $E_0 \mathcal{A} = \mathbb{C}J$ and so we may assume that $E_0 = J$.

Let M_i denote the projection of M onto each $E_i\mathcal{A}$ from Theorem 2.1, and similarly for N and N_i. Then

$$M' = \sum_{i=0}^{s} M_i \quad \text{and} \quad N' = \sum_{i=0}^{s} N_i,$$

and the matrices M_i and N_i are positive semidefinite by Corollary 2.2. Moreover, the orthogonality of the decomposition implies that

$$M'N' = \sum_{i=0}^{s} M_i N_i.$$

Recall that the trace of the product of positive semidefinite matrices is non-negative. Therefore

$$\operatorname{tr} M'N' = \sum_{i=0}^{s} \operatorname{tr} M_i N_i \geq \operatorname{tr} M_0 N_0 = \frac{(\operatorname{tr} JM)(\operatorname{tr} JN)}{n^2}.$$

Equality holds if and only if $M_i N_i = 0$ for all $i \neq 0$, which is equivalent to $M'N'$ being a scalar multiple of J. $\qquad\Box$

Denote the Schur (componentwise) product of matrices B and C by $B \circ C$. In what follows, we will typically consider positive semidefinite matrices M and N, that with respect to the adjacency matrix A of a graph G and the adjacency matrix $\overline{A} = J - I - A$ of the complement $\overline{G}$, satisfy either of the following two conditions:

$$M \circ A = 0 \text{ and } N \circ \overline{A} = 0, \tag{A}$$
$$M \circ A \leq 0, \ N \circ \overline{A} = 0 \text{ and } N \circ A \geq 0. \tag{B}$$

3 Graphs

We now show two classes of examples of matrix $*$-algebras satisfying the properties of the lemmas above.

3.1 Homogeneous coherent configurations

A *coherent configuration* is a finite set of non-zero 01 matrices $\{A_0, ..., A_d\}$, which satisfies the following properties:

(i) $\sum_{i=0}^{d} A_i = J$.

(ii) For all $i \in \{0, ..., d\}$, if one diagonal entry of A_i is non-zero, then A_i is diagonal.

(iii) The configuration is transpose-closed.

(iv) $A_i A_j$ is a linear combination of the matrices in the configuration, for all i and j.

Coherent configurations appear naturally in connection to design theory, finite geometry, coding theory and representation of finite groups. They were originally

defined by Higman in [10]. When the identity matrix is one of the matrices forming the configuration, we call such configuration *homogeneous*. When the matrices forming the configuration commute, they result in what is known as an association scheme. The theory of association schemes is vast and rich, and the connections to combinatorics are overwhelming; see for instance [4].

From here on, we assume $\{I = A_0, \ldots, A_d\}$ is a homogeneous coherent configuration. These matrices generate a complex algebra, called the *coherent algebra*, which we denote by $\mathcal{A}$. Note that this algebra is a homogeneous matrix $*$-algebra that contains I and J.

A graph belongs to a coherent configuration if its adjacency matrix is a sum of the matrices forming the configuration. The so-called distance-regular graphs are standard examples of graphs found in (and generating) association schemes. Another class of examples comes from vertex-transitive graphs — the permutation matrices corresponding to the automorphisms of the graph form a group, and its commutant in $\mathrm{M}_n(\mathbb{C})$, which contains the adjacency matrix of the graph, is a homogeneous coherent algebra.

If A is the adjacency matrix of a graph and belongs to a homogeneous coherent algebra generated by the configuration $\{I = A_0, \ldots, A_d\}$, it follows that, for some $R \subseteq \{1, \ldots, d\}$, we have

$$A = \sum_{r \in R} A_r.$$

As a consequence,

$$\overline{A} = \sum_{r \in \overline{R}} A_r,$$

where $\overline{R} = \{1, \ldots, d\} \setminus R$. Moreover, if $A_r^* = A_{r^*}$, then $r \in R$ implies $r^* \in R$.

Therefore if M and N are positive semidefinite matrices satisfying either of the conditions (A) and (B), then it follows that $\langle M, A_r \rangle \langle A_r, N \rangle \leq 0$ for all $r \in \{1, \ldots, d\}$, and thus $M, N, \mathcal{A}$ and its basis $\{A_0, \ldots, A_d\}$ satisfy the conditions of Lemma 2.5.

Applying Lemmas 2.3, 2.5 and 2.6, we have the result below.

Theorem 3.1 *Let A be the adjacency matrix of a connected graph that belongs to a homogeneous coherent configuration $\{I = A_0, \ldots, A_d\}$. Let M and N be non-zero positive semidefinite matrices satisfying conditions (A) or (B). Then*

$$n \geq \frac{(\mathrm{tr}\, JM)(\mathrm{tr}\, JN)}{(\mathrm{tr}\, M)(\mathrm{tr}\, N)}.$$

Moreover, equality holds if and only if $M'N'$ is a scalar multiple of J, and either (A) holds or (B) holds in such way that $\langle M, A_r \rangle \langle A_r, N \rangle = 0$ for all $r \neq 0$.

3.2   1-walk regular graphs (and their complements)

A graph G with adjacency matrix A is called 1-walk regular if, for any positive integer k, A^k is constant in the diagonal and in the entries corresponding to the

support of A. That is, for any positive integer k, there are constants a_k and b_k such that

$$A^k \circ I = a_k I \quad \text{and} \quad A^k \circ A = b_k A.$$

Assume G is 1-walk regular, and A is its adjacency matrix. Note for instance that G must be regular, as the diagonal of A^2 is constant. Let $\mathcal{A}$ be the algebra generated by A and I — that is, the adjacency algebra of the graph G. This is obviously a matrix $*$-algebra. In fact, it is an algebra of symmetric and commuting matrices, therefore the decomposition of $\mathbb{R}^n$ into $\mathcal{A}$-modules is simply its simultaneous diagonalization.

Consider an orthogonal basis $I = A_0, A = A_1, A_2, \ldots, A_d$. For instance, this could have been obtained by applying Gram-Schmidt to $I, A, A^2, \ldots, A^d$. The relevant consequence of 1-walk regularity is that $A_k \circ I = 0$ and $A_k \circ A = 0$ for all $k \geq 2$, as the basis is orthogonal and all matrices of $\mathcal{A}$ are constant over the support of I and A.

Now let M and N be positive semidefinite matrices, and assume that (A) or (B) holds. Then $\langle M, A_k \rangle \langle A_k, N \rangle \leq 0$ for all $k \geq 1$. Thus M, N, $\mathcal{A}$ and its basis $\{A_0, \ldots, A_d\}$ satisfy the conditions of Lemmas 2.5 and 2.6, therefore we have the following theorem.

Theorem 3.2 *Let A be the adjacency matrix of a 1-walk regular graph. Let M and N be non-zero positive semidefinite matrices satisfying conditions (A) or (B) above. Then*

$$n \geq \frac{(\operatorname{tr} JM)(\operatorname{tr} JN)}{(\operatorname{tr} M)(\operatorname{tr} N)}.$$

Moreover, equality holds if and only if $M'N'$ is a scalar multiple of J, and either (A) holds or (B) holds in such way that $\langle M, A_r \rangle \langle A_r, N \rangle = 0$ for all $r \neq 0$, where $I = A_0, A = A_1, A_2, \ldots, A_d$ is an orthogonal basis of the adjacency algebra of G.

4 Thetas

The immediate corollaries to Theorems 3.1 and 3.2 are the so-called clique-coclique bounds. Assume S is a clique and T is a coclique in a graph which is either in a homogeneous coherent configuration or is 1-walk regular. Let χ_S and χ_T be their respective characteristic vectors, and define

$$N = \chi_S \chi_S^* \quad \text{and} \quad M = \chi_T \chi_T^*.$$

It follows that $M \circ A = 0$ and $N \circ \overline{A} = 0$. Thus Theorem 3.1 or Theorem 3.2 applies, and we obtain the following result, which has been stated before for graphs in association schemes or vertex-transitive graphs (see for instance [8, Theorem 3.8.4]).

Corollary 4.1 *Assume S is a clique and T is a coclique in a graph on n vertices which is either in a homogeneous coherent configuration or is 1-walk regular. Then*

$$|S||T| \leq n.$$

Proof. The inequality is immediate from Theorem 3.1 or Theorem 3.2.   □

The conditions on M and N being positive semidefinite and satisfying either (A) or (B) allow for a nice extension of this result. We write $X \succcurlyeq 0$ if X is a positive semidefinite matrix. The Lovász theta graph parameter $\vartheta(G)$ is defined (see [13]) as the optimum value of the following semidefinite program:

$$\vartheta(G) = \max \{\langle J, X \rangle : X \circ A = 0, \ \operatorname{tr} X = 1, \ X \succcurlyeq 0\}.$$

Upon making small variations in the formulations, one obtains, respectively, the Schrijver theta [15] and the Szegedy theta [17] functions:

$$\vartheta^-(G) = \max \{\langle J, X \rangle : X \circ A = 0, \ \operatorname{tr} X = 1, \ X \geq 0, \ X \succcurlyeq 0\}.$$

$$\vartheta^+(G) = \max \{\langle J, X \rangle : X \circ A \leq 0, \ \operatorname{tr} X = 1, \ X \succcurlyeq 0\}.$$

It is known since the first respective appearances of these thetas that, for all graphs G on n vertices, we have

$$\alpha(G) \leq \vartheta^-(G) \leq \vartheta(G) \leq \vartheta^+(G) \leq \chi(\overline{G}), \tag{2}$$

where $\chi(G)$ is the chromatic number of G; and that

$$\vartheta(G)\vartheta(\overline{G}) \geq n \quad \text{and} \quad \vartheta^-(\overline{G})\vartheta^+(G) \geq n, \tag{3}$$

with equality in both cases of (3) for vertex-transitive graphs.

The results in this paper extend the equality case in (3) for graphs in homogeneous coherent configurations and 1-walk regular graphs.

Corollary 4.2 *Let G be graph on n vertices that belongs to a homogeneous coherent configuration or that is 1-walk regular. Then*

$$\vartheta(G)\vartheta(\overline{G}) = n \quad \text{and} \quad \vartheta^-(\overline{G})\vartheta^+(G) = n.$$

Proof. Let M and N be positive semidefinite matrices that are optimal solutions for $\vartheta(G)$ and $\vartheta(\overline{G})$, respectively. They satisfy condition (A), and therefore Theorem 3.1 or 3.2 applies. Thus $n \geq \vartheta(G)\vartheta(\overline{G})$, and then (3) shows that equality holds. The same conclusion can be reached for matrices N and M which are respective optimal solutions for $\vartheta^-(\overline{G})$ and $\vartheta^+(G)$, by noting that they satisfy condition (B).□

Corollary 4.2 implies that, if M and N are optima for $\vartheta(G)$ and $\vartheta(\overline{G})$, or for $\vartheta^-(\overline{G})$ and $\vartheta^+(\overline{G})$, with G 1-walk regular or in a homogeneous coherent configuration, then the equality characterizations from Lemmas 2.5 and 2.6 hold.

It is interesting to consider if the tools and the framework we developed may be used to strengthen similar inequalities involving other variants of theta, such as the ones in [7] and in [14], and also for other hierarchies of semidefinite programs (see, e.g., [9]).

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