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SINGULAR VALUE INEQUALITY AND GRAPH ENERGY CHANGE*

JANE DAY[†] AND WASIN SO[†]

Abstract. The energy of a graph is the sum of the singular values of its adjacency matrix. A classic inequality for singular values of a matrix sum, including its equality case, is used to study how the energy of a graph changes when edges are removed. One sharp bound and one bound that is never sharp, for the change in graph energy when the edges of a nonsingular induced subgraph are removed, are established. A graph is nonsingular if its adjacency matrix is nonsingular.

Key words. Singular value inequality, Graph energy.

AMS subject classifications. 15A45, 05C50.

1. Singular value inequality for matrix sum. Let X be an $n \times n$ complex matrix and denote its singular values by $s_1(X) \geq s_2(X) \geq \dots \geq s_n(X) \geq 0$. If X has real eigenvalues only, denote its eigenvalues by $\lambda_1(X) \geq \lambda_2(X) \geq \dots \geq \lambda_n(X)$. Define $|X| = \sqrt{XX^*}$ which is positive semi-definite, and note that $\lambda_i(|X|) = s_i(X)$ for all i . We write $X \geq 0$ to mean X is positive semi-definite. We are interested in the following singular value inequality for a matrix sum:

$$(1.1) \quad \sum_{i=1}^n s_i(A+B) \leq \sum_{i=1}^n s_i(A) + \sum_{i=1}^n s_i(B)$$

and its equality case. This inequality is well-known, and there are at least 4 different proofs in the literature. We briefly review them now.

The inequality (1.1) was first proved by Fan [4] using the variational principle:

$$\sum_{i=1}^n s_i(X) = \max \left\{ \left| \sum_{i=1}^n u_i^* U X u_i \right| : U \text{ is a unitary matrix} \right\},$$

where $\{u_i : 1 \leq i \leq n\}$ is a fixed orthonormal basis. This proof also appears in Gohberg and Krein [6], and Horn and Johnson [7]. No equality case was discussed in these references.

A different proof found in Bhatia [2] applied a related eigenvalue inequality for a sum of Hermitian matrices to Jordan-Wielandt matrices of the form $\begin{bmatrix} 0 & X^* \\ X & 0 \end{bmatrix}$, whose eigenvalues are $\{\pm s_i(X) : 1 \leq i \leq n\}$. Again, no equality case was discussed.

Another proof was provided by Thompson in [10]. He used polar decomposition and employed the inequalities due to Fan and Hoffman [5] (see Theorem 1.1 below) to establish the matrix-valued triangle inequality

$$|A+B| \leq U|A|U^* + V|B|V^*$$

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and its equality case was characterized in a later paper [11]. Inequality (1.1) and its equality case follow easily.

Still another proof was given by Cheng, Horn and Li in [3]. They used a result of Thompson [13] on the relationship between diagonal elements and singular values of a matrix. They also characterized the equality case in the same paper.

For the sake of completeness, we give the details of a proof of (1.1) and its equality case in Theorem 1.4. Our proof is a variation of the one given by Thompson.

THEOREM 1.1. *For any $n \times n$ complex matrix A ,*

$$\lambda_i\left(\frac{A + A^*}{2}\right) \leq s_i(A)$$

for all i .

Proof. Denote $\lambda_i = \lambda_i\left(\frac{A+A^*}{2}\right)$ and $s_i = s_i(A)$. Let v_1, \dots, v_n be orthonormal eigenvectors of $\frac{A+A^*}{2}$ such that $\frac{1}{2}(A + A^*)v_i = \lambda_i v_i$, and w_1, \dots, w_n be orthonormal eigenvectors of AA^* such that $AA^*w_i = s_i^2 w_i$. Now for a fixed $1 \leq i \leq n$, consider the subspace $S_1 = \text{span}\{v_1, \dots, v_i\}$ and $S_2 = \text{span}\{w_i, \dots, w_n\}$. By a dimension argument, the intersection $S_1 \cap S_2$ contains at least one unit vector x . Then

$$x^* \frac{A + A^*}{2} x \geq \lambda_i \quad \text{and} \quad x^* AA^* x \leq s_i^2.$$

Consequently,

$$\lambda_i \leq x^* \frac{A + A^*}{2} x = \text{Re } x^* A^* x \leq |x^* A^* x| \leq \|A^* x\| = \sqrt{x^* AA^* x} \leq s_i. \quad \square$$

REMARK 1.2. The inequality in Theorem 1.1 was first proved by Fan and Hoffman [5]. Our proof is taken from [12]. The equality case was discussed by So and Thompson [9]. We include a different proof of the equality case in Corollary 1.3.

COROLLARY 1.3. *For any $n \times n$ complex matrix A ,*

$$\text{tr}\left(\frac{A + A^*}{2}\right) \leq \text{tr}|A|.$$

Equality holds if and only if $\lambda_i\left(\frac{A+A^}{2}\right) = s_i(A)$ for all i if and only if $A \geq 0$.*

Proof. It follows from Theorem 1.1 that

$$\text{tr}\left(\frac{A + A^*}{2}\right) = \sum_{i=1}^n \lambda_i\left(\frac{A + A^*}{2}\right) \leq \sum_{i=1}^n s_i(A) = \text{tr}|A|.$$

Now if $A \geq 0$ then $\lambda_i\left(\frac{A+A^*}{2}\right) = \lambda_i(A) = s_i(A)$ for all i , and so $\text{tr}\left(\frac{A+A^*}{2}\right) = \text{tr}|A|$. Conversely, if the equality holds then $\sum_{i=1}^n \lambda_i\left(\frac{A+A^*}{2}\right) = \sum_{i=1}^n s_i(A)$, and so $\lambda_i\left(\frac{A+A^*}{2}\right) = s_i(A)$ for all i because of Theorem 1.1. Consequently, $\lambda_i^2\left(\frac{A+A^*}{2}\right) = s_i^2(A)$ for all i , and so $\text{tr}\left(\frac{A+A^*}{2}\right)^2 = \text{tr}(AA^*)$. Now we have

$$\text{tr}(A - A^*)(A^* - A) = \text{tr}(AA^* + A^*A - A^2 - (A^*)^2) = \text{tr}(4AA^* - (A + A^*)^2) = 0,$$

it follows that $A = A^*$. Then A is positive semi-definite because it is Hermitian and its eigenvalues are all non-negative. \square

THEOREM 1.4. *Let A and B be two $n \times n$ complex matrices. Then*

$$\sum_{i=1}^n s_i(A + B) \leq \sum_{i=1}^n s_i(A) + \sum_{i=1}^n s_i(B).$$

Moreover equality holds if and only if there exists a unitary matrix P such that PA and PB are both positive semi-definite.

Proof. By polar decomposition, there exists a unitary matrix P such that $P(A + B) \geq 0$. Then

$$\begin{aligned} \sum_{i=1}^n s_i(A + B) &= \sum_{i=1}^n s_i(P(A + B)) \\ &= \operatorname{tr} P(A + B) \\ &= \operatorname{tr} \left(\frac{PA + PB + (PA)^* + (PB)^*}{2} \right) \\ &= \operatorname{tr} \left(\frac{PA + (PA)^*}{2} \right) + \operatorname{tr} \left(\frac{PB + (PB)^*}{2} \right) \\ &\leq \operatorname{tr}|PA| + \operatorname{tr}|PB| \\ &= \operatorname{tr}|A| + \operatorname{tr}|B| \\ &= \sum_{i=1}^n s_i(A) + \sum_{i=1}^n s_i(B). \end{aligned}$$

Now equality holds if and only if $\operatorname{tr} \left(\frac{PA + (PA)^*}{2} \right) = \operatorname{tr}|PA|$ and $\operatorname{tr} \left(\frac{PB + (PB)^*}{2} \right) = \operatorname{tr}|PB|$ if and only if both PA and PB are positive semi-definite, by Corollary 1.3. \square

REMARK 1.5. If both A and B are real matrices then the unitary matrix P in the equality case of Theorem 1.4 can be taken to be real orthogonal.

2. Graph energy change due to edge deletion. Let G be a simple graph i.e., a graph without loops and multiple edges. Also let $V(G)$ and $E(G)$ denote the vertex set and edge set of G respectively, while denote $A(G)$ the adjacency matrix of G . The spectrum of G is defined as $Sp(G) = \{\lambda_i(A(G)) : 1 \leq i \leq n\}$ where n is the number of vertices of G . The energy of a graph G is defined as $\mathcal{E}(G) = \sum_{i=1}^n |\lambda_i(A(G))|$ [8]. Since $A(G)$ is a symmetric matrix, $\mathcal{E}(G)$ is indeed the sum of all singular values of $A(G)$, i.e., $\mathcal{E}(G) = \sum_{i=1}^n s_i(A(G))$ [14]. We are interested in how the energy of a graph changes when edges are deleted from a graph. Let us begin with a few examples.

EXAMPLE 2.1. Consider a graph H on 6 vertices with an adjacency matrix

$$A(H) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}.$$

We have $Sp(H) = \{1 + \sqrt{3}, \sqrt{2}, 0, 1 - \sqrt{3}, -\sqrt{2}, -2\}$ and $\mathcal{E}(H) = 2(1 + \sqrt{2} + \sqrt{3}) \approx 8.2925$.

EXAMPLE 2.2. Let H_1 be a graph obtained from H by deleting the edge $\{2, 3\}$. Then $Sp(H_1) = \{2.4383, 1.1386, 0.6180, -0.8202, -1.6180, -1.7566\}$ and $\mathcal{E}(H_1) \approx 8.3898 > \mathcal{E}(H)$.

EXAMPLE 2.3. Let H_2 be a graph obtained from H by deleting the edge $\{1, 2\}$. Then $Sp(H_2) = \{2.5395, 1.0825, 0.2611, -0.5406, -1.2061, -2.1364\}$ and $\mathcal{E}(H_2) \approx 7.7662 < \mathcal{E}(H)$.

EXAMPLE 2.4. Let H_3 be a graph obtained from H by deleting the edge $\{2, 5\}$. Then $Sp(H_3) = \{1 + \sqrt{2}, \sqrt{3}, 1 - \sqrt{2}, -1, -1, -\sqrt{3}\}$ and $\mathcal{E}(H_3) = 2(1 + \sqrt{2} + \sqrt{3}) = \mathcal{E}(H)$.

These examples show that the energy of a graph may increase, decrease, or remain the same when an edge is deleted. Theorem 2.6 gives bounds on the amount of change when edges are deleted, and characterizes the situation when the bounds are sharp. A graph is called *nonsingular* if its adjacency matrix is nonsingular. Let H be an induced subgraph of a graph G , which means that H contains all edges in G joining two vertices of H . Let $G - H$ denote the graph obtained from G by deleting all vertices of H and all edges incident with H . Let $G - E(H)$ denote the graph obtained from G by deleting all edges of H , but keeping all vertices of H . If G_1 and G_2 are two graphs without common vertices, let $G_1 \oplus G_2$ denote the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. Hence $A(G_1 \oplus G_2) = A(G_1) \oplus A(G_2)$. We need the next lemma, which appears as an exercise in [7, section 7.1, ex 2].

LEMMA 2.5. *If $A = [a_{ij}]$ is a positive semi-definite matrix and $a_{ii} = 0$ for some i , then $a_{ji} = a_{ij} = 0$ for all j .*

Our main result is

THEOREM 2.6. *Let H be an induced subgraph of a graph G . Then*

$$\mathcal{E}(G) - \mathcal{E}(H) \leq \mathcal{E}(G - E(H)) \leq \mathcal{E}(G) + \mathcal{E}(H).$$

Moreover,

(i) *if H is nonsingular then the left equality holds if and only if $G = H \oplus (G - H)$*

(ii) *the right equality holds if and only if $E(H) = \emptyset$.*

Proof. Note that

$$(2.1) \quad A(G) = \begin{bmatrix} A(H) & X^T \\ X & A(G-H) \end{bmatrix} = \begin{bmatrix} A(H) & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & X^T \\ X & A(G-H) \end{bmatrix}$$

where X represents edges connecting H and $G - H$. Indeed, $A(G - E(H)) = \begin{bmatrix} 0 & X^T \\ X & A(G-H) \end{bmatrix}$. By Theorem 1.4 to (2.1), we have $\mathcal{E}(G) \leq \mathcal{E}(H) + \mathcal{E}(G - E(H))$, which gives the left inequality. On the other hand,

$$(2.2) \quad A(G - E(H)) = A(G) + \begin{bmatrix} -A(H) & 0 \\ 0 & 0 \end{bmatrix}.$$

Again, by Theorem 1.4 to (2.2), we have $\mathcal{E}(G - E(H)) \leq \mathcal{E}(G) + \mathcal{E}(H)$, which gives the right inequality.

(i) Assume that $A(H)$ is a nonsingular matrix. For the sufficiency part, let $G = H \oplus (G - H)$ then

$$A(G) = \begin{bmatrix} A(H) & 0 \\ 0 & A(G - H) \end{bmatrix}$$

which gives $\mathcal{E}(G) = \mathcal{E}(H) + \mathcal{E}(G - H)$. On the other hand, if the left inequality becomes equality then, by applying Theorem 1.4 to (2.1), there exists an orthogonal matrix $P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix}$ such that both $P \begin{bmatrix} A(H) & 0 \\ 0 & 0 \end{bmatrix}$ and $P \begin{bmatrix} 0 & X^T \\ X & A(G - H) \end{bmatrix}$ are positive semi-definite. The symmetry of

$$\begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} A(H) & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} P_{11}A(H) & 0 \\ P_{21}A(H) & 0 \end{bmatrix}$$

gives $P_{21}A(H) = 0$ and so $P_{21} = 0$ because of the nonsingularity of $A(H)$. Since P is an orthogonal matrix, it follows that $P_{12} = 0$ and so P_{11} is nonsingular. Therefore

$$\begin{aligned} P \begin{bmatrix} 0 & X^T \\ X & A(G - H) \end{bmatrix} &= \begin{bmatrix} P_{11} & 0 \\ 0 & P_{22} \end{bmatrix} \begin{bmatrix} 0 & X^T \\ X & A(G - H) \end{bmatrix} \\ &= \begin{bmatrix} 0 & P_{11}X^T \\ P_{22}X & P_{22}A(G - H) \end{bmatrix}. \end{aligned}$$

Since this matrix is positive semi-definite with a zero diagonal block, by Lemma 2.5, $P_{11}X^T = 0$. Hence $X^T = 0$ because of the nonsingularity of P_{11} . Finally $X = 0$ implies that $G = H \oplus (G - H)$.

(ii) For the sufficiency part, let $E(H) = \emptyset$ then $G - E(H) = G$ and $\mathcal{E}(H) = 0$. Hence

$$\mathcal{E}(G - E(H)) = \mathcal{E}(G) = \mathcal{E}(G) + \mathcal{E}(H).$$

For the necessity part, assume that the right inequality becomes an equality, i.e.,

$$\mathcal{E}(G - E(H)) = \mathcal{E}(G) + \mathcal{E}(H).$$

By applying Theorem 1.4 to (2.2), there exists an orthogonal matrix

$Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}$ such that both $Q \begin{bmatrix} -A(H) & 0 \\ 0 & 0 \end{bmatrix}$ and $Q \begin{bmatrix} A(H) & X^T \\ X & A(G - H) \end{bmatrix}$ are positive semi-definite. We want to show that $E(H) = \emptyset$. Suppose not, i.e., $A(H)$ is nonzero.

Case 1. Suppose that $A(H)$ is nonsingular. As in the proof of (i), it follows that $Q_{21} = 0$ because $A(H)$ is nonsingular, and then $Q_{12} = 0$ because Q is orthogonal. Hence Q is block-diagonal. Therefore $Q_{11}A(H)$ and $-Q_{11}A(H)$ are both positive semi-definite, so $Q_{11}A(H)$ must be 0; but that implies $A(H) = 0$ since Q_{11} is orthogonal. This leads to a contradiction because $A(H)$ is nonsingular.

Case 2. Suppose that $A(H)$ is singular (but nonzero). Since it is symmetric and nonzero, there exist orthogonal R_1 and nonsingular symmetric A_1 such that

$A(H) = R_1 \begin{bmatrix} A_1 & 0 \\ 0 & 0 \end{bmatrix} R_1^T$. Let $A(H)$ be $(n-p) \times (n-p)$ and define $R = \begin{bmatrix} R_1 & 0 \\ 0 & I_p \end{bmatrix}$. Since both $Q \begin{bmatrix} -A(H) & 0 \\ 0 & 0 \end{bmatrix}$ and $Q \begin{bmatrix} A(H) & X^T \\ X & A(G-H) \end{bmatrix}$ are positive semi-definite, it follows that both

$$R^T Q R \begin{bmatrix} -A_1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad R^T Q R \begin{bmatrix} A_1 & X_1^T \\ X_1 & Y_1 \end{bmatrix}$$

are also positive semi-definite. This cannot happen, by Case 1, because A_1 is nonsingular and $R^T Q R$ is orthogonal. \square

COROLLARY 2.7. *Let e be an edge of a graph G . Then the subgraph with the edge set $\{e\}$ is induced and nonsingular, hence*

$$\mathcal{E}(G) - 2 \leq \mathcal{E}(G - \{e\}) \leq \mathcal{E}(G) + 2$$

Moreover, (i) the left equality holds if and only if e is an isolated edge of G , (ii) the right equality never holds.

REMARK 2.8. Corollary 2.7 answers two open questions on graph energy raised in the AIM workshop [1].

Question 1: If e is an edge of a connected graph G such that $\mathcal{E}(G) = \mathcal{E}(G - \{e\}) + 2$, then is it true that $G = K_2$?

Answer: YES. By (i) of Corollary 2.7, e is an isolated edge. Since G is connected, $G = K_2$.

Question 2: Are there any graphs G such that $\mathcal{E}(G - \{e\}) = \mathcal{E}(G) + 2$?

Answer: NO. By (ii) of Corollary 2.7.

3. More examples. In this section, we give examples to illuminate the significance of the condition on H and the tightness of the inequalities in Theorem 2.6. In particular, Examples 3.1 and 3.4 show that when H is singular, the equality

$$\mathcal{E}(G) - \mathcal{E}(H) = \mathcal{E}(G - E(H))$$

in Theorem 2.6 may or may not be true. Also, we know from Theorem 2.6 (ii) that $\mathcal{E}(G - H) < \mathcal{E}(G) + \mathcal{E}(H)$ for any graph G and any induced subgraph H which has at least one edge. Example 3.5 shows that this gap can be arbitrarily small.

EXAMPLE 3.1. This example shows that Theorem 2.6 (i) is not true for some singular graphs. The graph $H = K_2 \oplus K_1$ is singular, where K_i denotes a complete graph on i vertices. Let $G = K_2 \oplus K_2$, so H is an induced subgraph of G such that $\mathcal{E}(G) - \mathcal{E}(H) = \mathcal{E}(G - E(H))$. But $G \neq H \oplus (G - H)$.

LEMMA 3.2. *If u is a nonzero real vector such that uv^T is symmetric then $v = \lambda u$ for some λ .*

Proof. By symmetry, $uv^T = (uv^T)^T = vu^T$. Hence $u(v^T u) = v(u^T u)$, it follows that $v = \frac{v^T u}{u^T u} u$. \square

LEMMA 3.3. Let $K = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ and P_{11} be a 3×3 real matrix such that

$P_{11}K$ is positive semi-definite and $P_{11}^T P_{11}K = K$. Then $P_{11} = \begin{bmatrix} a_1 & \frac{1}{\sqrt{2}} & -a_1 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -a_1 & \frac{1}{\sqrt{2}} & a_1 \end{bmatrix}$

for some a_1 .

Proof. Write $P_{11} = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix}$. Since $P_{11}K = \begin{bmatrix} b_1 & a_1 + c_1 & b_1 \\ b_2 & a_2 + c_2 & b_2 \\ b_3 & a_3 + c_3 & b_3 \end{bmatrix}$ is positive semi-definite, it follows that $a_1 + c_1 = b_2 = a_3 + c_3$, $b_1 = b_3$, $b_1 \geq 0$, $a_2 + c_2 \geq 0$, and $b_1(a_2 + c_2) - b_2(a_1 + c_1) \geq 0$. Denote $a = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$, $b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$, and $c = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$. Since $\begin{bmatrix} a^T b & a^T(a+c) & a^T b \\ b^T b & b^T(a+c) & b^T b \\ c^T b & c^T(a+c) & c^T b \end{bmatrix} = P_{11}^T P_{11}K = K = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$, it follows that $a^T b = c^T b = 0$, $b^T b = 1$, $a^T(a+c) = c^T(a+c) = 1$, and so $b^T(a+c) = 0$, $a^T a = c^T c$. Also, note that $P_{11}^T P_{11}K = K$ does not have any zero column and so does $P_{11}K$, hence $a_2 + c_2 > 0$. These facts, with some algebraic manipulations, enable one to deduce that $b_2 = 0$, $b_1 = b_3 = \frac{1}{\sqrt{2}}$, $c_1 = -a_1$, $c_2 = a_2$, $c_3 = -a_3 = a_1$, and finally $a_2 = \frac{1}{\sqrt{2}}$. \square

EXAMPLE 3.4. This example shows that Theorem 2.6 (i) is true for some singular graphs. The path graph on 3 vertices P_3 is singular. If P_3 is an induced subgraph in a graph G , and $\mathcal{E}(G) - \mathcal{E}(P_3) = \mathcal{E}(G - E(P_3))$ then $G = P_3 \oplus (G - P_3)$.

Proof. Let $K = A(P_3) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ and $Y = A(G - P_3)$. Then $A(G) = \begin{bmatrix} K & X^T \\ X & Y \end{bmatrix}$ where X represents the edges between $G - P_3$ and P_3 . We want to show that $X = 0$ from the hypothesis that $\mathcal{E}(G) = \mathcal{E}(P_3) + \mathcal{E}(G - E(P_3))$. By Theorem 1.4, there exists an orthogonal matrix $P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix}$ such that both $P \begin{bmatrix} K & 0 \\ 0 & 0 \end{bmatrix}$ and $P \begin{bmatrix} 0 & X^T \\ X & Y \end{bmatrix}$ are positive semi-definite. The symmetry of

$$\begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} K & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} P_{11}K & 0 \\ P_{21}K & 0 \end{bmatrix}$$

gives $P_{21}K = 0$, and so $P_{21} = \beta k^T$ where β is an unknown vector and $k^T = \begin{bmatrix} 1 & 0 & -1 \end{bmatrix}$. The orthogonality of P gives $P^T P = I$, and it follows that

$$(3.1) \quad P_{11}^T P_{11} + P_{21}^T P_{21} = I$$

$$(3.2) \quad P_{12}^T P_{11} + P_{22}^T P_{21} = 0$$

Right-multiplying equation (3.1) by K , we have $P_{11}^T P_{11} K = K$. Together with the fact that $P_{11} K$ is positive semi-definite, Lemma 3.3 gives

$$P_{11} = \begin{bmatrix} a_1 & \frac{1}{\sqrt{2}} & -a_1 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -a_1 & \frac{1}{\sqrt{2}} & a_1 \end{bmatrix}.$$

Right-multiplying equation (3.2) by K , we have $P_{12}^T P_{11} K = 0$, and so $P_{12} = k\alpha^T$ where α is an unknown vector. Since

$$\begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} 0 & X^T \\ X & Y \end{bmatrix} = \begin{bmatrix} P_{12} X & P_{11} X^T + P_{12} Y \\ P_{22} X & P_{21} X^T + P_{22} Y \end{bmatrix}$$

is positive semi-definite, so is $P_{12} X = (k\alpha^T) X = k(X^T \alpha)^T$. By Lemma 3.2, $X^T \alpha = \mu k$, and so $P_{12} X = \mu k k^T$ which has a zero (2,2) entry. Consequently, by Lemma 2.5, the second row of $P_{11} X^T + P_{12} Y$ must be zero too because it is part of a positive semi-definite matrix. Let $X = [x_1 \ x_2 \ x_3]$, then $\frac{1}{\sqrt{2}}(x_1^T + x_3^T) = 0$. Since X is non-negative, $x_1 = x_3 = 0$ and so $P_{22} X = [0 \ P_{22} x_2 \ 0]$. By symmetry, the first and third rows of $P_{11} X^T + P_{12} Y$ must be zero, i.e.,

$$\begin{aligned} \frac{1}{\sqrt{2}} x_2^T + (Y^T \alpha)^T &= 0 \\ \frac{1}{\sqrt{2}} x_2^T - (Y^T \alpha)^T &= 0 \end{aligned}$$

and hence $x_2 = 0$. Finally, we have $X = 0$. \square

EXAMPLE 3.5. This example shows that the gap $\mathcal{E}(G) + \mathcal{E}(H) - \mathcal{E}(G - E(H))$ in the right inequality of Theorem 2.6 can be arbitrarily small if the set $E(H)$ is not empty. Consider the family of complete regular bipartite graphs $K_{n,n}$ with energy $\mathcal{E}(K_{n,n}) = 2n$ and $\mathcal{E}(K_{n,n} - \{e\}) = 2\sqrt{n^2 + 2n - 3}$ where e is any edge in $K_{n,n}$. Hence

$$\mathcal{E}(K_{n,n}) + 2 - \mathcal{E}(K_{n,n} - \{e\}) = \frac{8}{\sqrt{n^2 + 2n + 1} + \sqrt{n^2 + 2n - 3}},$$

which approaches 0 as n goes to infinity.

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