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An Improved Upper Bound of the Energy of Some Graphs and Matrices

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Abstract

Considering a consequence of the Cauchy–Schwarz inequality we obtain a sharp upper bound of the energy of a bipartite graph and a large family graphs, namely those graphs whose adjacency matrix is partitioned into blocks with constant row sum.

1 Introduction

Let $G = (V, E)$ be an undirected simple graph with n vertices and m edges. The eigenvalues of G are the eigenvalues of its adjacency matrix, A_G. The multiset of the eigenvalues of a matrix M is the spectrum of M and will be denoted by σ_M. The spectrum of a graph G, is σ_{A_G}, for short we denote it by, σ_G. If G has at least one edge, then A_G has a negative eigenvalue, not greater than -1 and a positive eigenvalue not less than the average degree of the vertices of G (see [1,7]). Throughout the paper, the eigenvalues of a real symmetric matrix M of order n are ordered as follows: $\lambda_1(M) \geq \cdots \geq \lambda_n(M)$. In a similar way, $\lambda_1(G) \geq \cdots \geq \lambda_n(G)$ are ordered the eigenvalues of G. The energy of G is defined as

$$E\left(G\right) = \sum_{i=1}^{n} \left|\lambda_i\left(G\right)\right|.$$

This concept was introduced by Gutman and is intensively studied in chemistry, since it can be used to approximate the total π-electron energy of a molecule (see [5,6]).

Many upper bounds for the energy of a graph present in the literature (see, [8–10]) were obtained by using the Cauchy–Schwarz inequality (see [11].)

Lemma 1 *Let $x = (x_1, x_2, \ldots, x_n)^t$ and $y = (y_1, y_2, \ldots, y_n)^t$ in $\mathbb{C}^n$ then*

$$\left|\sum_{i=1}^{n} \overline{x}_i y_i\right| \leq \sqrt{\sum_{i=1}^{n} |x_i|^2} \sqrt{\sum_{i=1}^{n} |y_i|^2}\ . \tag{1}$$

Equality holds if and only if $y = \alpha x$, $\alpha \in \mathbb{C}$.

By taken $x_i = 1$, for all $1 \leq i \leq n$, we obtain

Lemma 2 *Let $y = (y_1, y_2, \ldots, y_n)^t$ in $\mathbb{C}^n$ then*

$$\sum_{i=1}^{n} |y_i| \leq \sqrt{n \sum_{i=1}^{n} |y_i|^2}\ . \tag{2}$$

Equality holds if and only if $|y_1| = \cdots = |y_n| = \sqrt{\frac{1}{n}\sum_{i=1}^{n} |y_i|^2}$.

Now we need to recall (see [3]) that a balanced incomplete block design (BIBD) consist of v elements and b subsets of these elements called blocks such that (i) each element is contained in r blocks, (ii) each block contains k elements, and (iii) each pair of elements is simultaneously contained in λ^* blocks. The integers (v, b, r, k, λ^*) are called the parameters of the design. In the particular case $r = k$ the design is called symmetric. The incidence matrix B of a design is the $v \times b$ matrix defined by setting for each x an element and N a block, $B_{x,N} := 0$ if $x \notin N$ and $B_{x,N} := 1$ otherwise. B satisfies $BB^T = (r - \lambda^*)I + \lambda^* J$ and $JB = kJ$, such that J denotes a square matrix whose all entries are equal to 1. The incidence graph of a design is defined to be the graph G with adjacency matrix

$$A_G = \begin{pmatrix} \mathbf{0} & B \\ B^T & \mathbf{0} \end{pmatrix}.$$

Clearly, the graph is bipartite with each vertex of degree r or k, and its eigenvalues are $0, \pm\sqrt{r-\lambda^*}$ and $\pm\sqrt{rk}$ with multiplicities $b-v$, $v-1$, and 1, respectively, where $vr = bk, \lambda^*(v-1) = r(k-1)$.

It is well known [3] that the eigenvalues of a bipartite graph G on $n = 2N$ vertices occur in pairs: $\pm\lambda_1, \pm\lambda_2, \ldots, \pm\lambda_N$. Let $q = \sum_{i=1}^{N} \lambda_i^4$. By the Cauchy–Schwarz inequality, $m^2 \leq Nq$.

Rada and Tineo showed the following [15]: Let G be a bipartite graph on 2N vertices. If $1 < m^2/q < N$, then

$$E(G) \leq \frac{2}{\sqrt{N}} \left[\left(m - \sqrt{(N-1)Q} \right) + (N-1) \left(m - \sqrt{\frac{q}{N-1}} \right) \right] \tag{3}$$

where $Q = Nq - m^2$. Equality holds if G is the graph of a *symmetric BIBD*. Conversely, if the equality holds and G is regular, then G is the graph of a *symmetric BIBD*.

In this paper, we obtain a sharp upper bound for the energy of connected bipartite graphs. We remark that the set of graphs that realize our upper bound contains all the connected graphs that realize the previous upper bound. Moreover, we have found two infinite families of graphs realizing our upper bound and not the previously.

The present paper is organized in four sections. In the second section we show an inequality which is a consequence of the Cauchy–Schwarz inequality and we study the equality case (see [16]). In the third section we apply the equality results obtained in the preceding section to an imprimitive symmetric matrix and we use these results to obtain a sharp upper bound of the energy of connected bipartite graphs. The most general result of this section is then used, in a subsection, to obtain tight upper bounds for the energy of a generalized Bethe tree (see [17]). In the fourth section we apply the results of the second one to an important family of graphs, namely those graphs whose adjacency matrix is given into block form with equitable partitions. We apply the result for energy of real symmetric equitable partitioned matrices to the H-join which is a generalization to more than two graphs of the join of two graphs.

2 A Consequence of the Cauchy–Schwarz Inequality

Now we obtain a new version of Eq. (2) (see [16]).

Lemma 3 *Let $y=(y_1,y_2,\ldots,y_n)^t$ in $\mathbb{C}^n$ and p an integer with $1\le p\le n$. Then*

$$\sum_{i=1}^{n}|y_i|\le\sqrt{\sum_{i=1}^{p}p\,|y_i|^2}+\sqrt{\sum_{i=p+1}^{n}(n-p)\,|y_i|^2}\le\sqrt{n\sum_{i=1}^{n}|y_i|^2}\,.$$

The left inequality is an equality if and only if $|y_1|=\cdots=|y_p|=a=\sqrt{\frac{1}{p}\sum_{i=1}^{p}|y_i|^2}$ and $|y_{p+1}|=\cdots=|y_n|=b=\sqrt{\frac{1}{n-p}\sum_{i=p+1}^{n}|y_i|^2}$.

Proof. For the left inequality we just apply two times the Cauchy–Schwarz inequality, firstly to $\sum_{i=1}^{p}|y_i|$ and thereafter to $\sum_{i=p+1}^{n}|y_i|$. For the right inequality we apply the Cauchy–Schwarz inequality to $x=(a_1,a_2)^t$ and $z=(b_1,b_2)^t$, where $a_1=\sqrt{p}$, $b_1=\sqrt{\sum_{i=1}^{p}|y_i|^2}$, $a_2=\sqrt{n-p}$ and $b_2=\sqrt{\sum_{i=p+1}^{n}|y_i|^2}$. It is evident that the left equality holds for the case in the statement. Reciprocally, if the left equality holds, then

$$\sum_{i=1}^{p}|y_i|+\sum_{i=p+1}^{n}|y_i|=\sum_{i=1}^{p}|y_i|+\sqrt{n-p}\sqrt{\sum_{i=p+1}^{n}|y_i|^2}=\sqrt{p}\sqrt{\sum_{i=1}^{p}|y_i|^2}+\sqrt{n-p}\sqrt{\sum_{i=p+1}^{n}|y_i|^2}.$$

In consequence, $\sum_{i=1}^{p}|y_i|=\sqrt{p}\sqrt{\sum_{i=1}^{p}|y_i|^2}$ and by Cauchy–Schwarz equality case we obtain $|y_1|=\cdots=|y_p|=a=\sqrt{\frac{1}{p}\sum_{i=1}^{p}|y_i|^2}$. By following analogous steps those above, now for the sum $\sum_{i=p+1}^{n}|y_i|$ we obtain $|y_{p+1}|=\cdots=|y_n|=b=\sqrt{\frac{1}{n-p}\sum_{i=p+1}^{n}|y_i|^2}$. ■

Let M be an $m_1\times m_2$ real matrix we denote by $|M|=\sqrt{trace\,(MM^t)}$ the Frobenius matrix norm of M. Nikiforov [13] defined the energy of M as the sum of its singular values. Let $p=\min\{m_1,m_2\}$ and consider $\sigma_1(M)\ge\sigma_2(M)\ge\cdots\ge\sigma_p(M)$ as the singular values of M. As a generalization of the result of Theorem 1 in [8], into the proof of Theorem 1 in [13], it is shown that

$$E(M)\le\sigma_1(M)+\sqrt{(p-1)\left(|M|^2-\sigma_1^2(M)\right)}\,. \tag{4}$$

Let M be a real symmetric $\ell \times \ell$ matrix. According to Nikiforov [14], the Ky Fan k-norm $\|M\|_{(k)}$ is the sum of the k largest absolute values of the eigenvalues of M. If $k=\ell$, the Ky Fan ℓ-norm and the energy of M coincide. Therefore,

$$E(M) = \|M\|_{(\ell)} = \sum_{j=1}^{\ell} |\lambda_j| \, .$$

The following inequality is an immediate consequence of the Cauchy–Schwarz result, for any real symmetric matrix M

$$E\,(M) \leq \sqrt{\ell}\,|M| \, . \tag{5}$$

3 Bipartite Graphs

Definition 1 *For an irreducible nonnegative matrix M with maximal eigenvalue r, with exactly h eigenvalues of modulus r, the number h is called the imprimitivity index of M (see [12, Ch. 3]). If $h=1$, then the matrix M is said to be primitive; otherwise it is imprimitive.*

Remark 1 *A symmetric imprimitive matrix M must have index 2. By the Frobenius Form of an Irreducible Matrix [12, Theorem 3.1], in those cases there exists a permutation matrix P such that*

$$M = P^t \begin{pmatrix} \mathbf{0} & M_{12} \\ M_{21} & \mathbf{0} \end{pmatrix} P \, . \tag{6}$$

We note that $M_{21}^t = M_{12}$.

In the next result we obtain an upper bound for the energy of an irreducible nonnegative imprimitive symmetric matrix M.

Theorem 1 *Let M be an imprimitive symmetric matrix whose Frobenius form is given in Eq. (6). If M_{12} has order $m_1 \times m_2$, and M_{21} has order $m_2 \times m_1$ and $\widetilde{m} = \min\{m_1, m_2\}$. Then*

$$E\,(M) \leq 2\lambda_1\,(M) + 2\sqrt{(\widetilde{m}-1)\left(|M|^2/2 - \lambda_1^2\,(M)\right)} \, .$$

Equality holds if and only if $\widetilde{m}=1$ or if M has $2\,(\widetilde{m}-1)$ eigenvalues distinct from $\pm\lambda_1\,(M)$ with the same modulus, namely $\sqrt{\left[\,|M|^2/2 - \lambda_1^2\,(M)\,\right]/(\widetilde{m}-1)}$ and $|m_2 - m_1|$ eigenvalues equal to 0.

Proof. Without loss of generality, we can assume that $\widetilde{m} = m_1$. Therefore,

$$M^2 = P^t \begin{pmatrix} M_{12}M_{21} & \mathbf{0} \\ \mathbf{0} & M_{21}M_{12} \end{pmatrix} P \, . \tag{7}$$

Since $M_{12}M_{21}$ and $M_{21}M_{12}$ share the same nonzero eigenvalues, the multiplicity of the eigenvalue 0 of M is at least $m_2 - m_1$. So the energy of M is the sum of absolute value of the $2m_1$ other eigenvalues. On the other hand, it is not difficult to prove that M and $-M$ are similar matrices. In consequence, the nonzero eigenvalues of M are on pairs, λ and $-\lambda$.

Let $\sigma_+(M) = \{\lambda \in \sigma_M : \lambda > 0\}$. Note that $0 < |\sigma_+(M)| \leq m_1$. Therefore,

$$|M|^2 = 2 \sum_{\lambda \in \sigma_+(M)} \lambda^2$$

and

$$E(M) = \sum_{\lambda \in \sigma_+(M)} 2|\lambda| \leq 2\lambda_1(M) + 2\sqrt{(m_1 - 1)\left(|M|^2/2 - \lambda_1^2(M)\right)}. \tag{8}$$

Thus, the inequality holds.

If $m_1 = 1$, it is clear that $E(M) = 2\lambda_1(M)$ and the equality holds in (8).

If M has $2(m_1 - 1)$ eigenvalues distinct from $\lambda_1(M)$ with the same modulus, say α, and the other $m_2 - m_1$ eigenvalues equal to 0, then

$$E(M) = \sum_{\lambda \in \sigma_M} |\lambda| = \lambda_1(M) + 2(m_1 - 1)\alpha$$

and the equality holds in (8). Conversely, if

$$\sum_{\lambda \in \sigma_M} |\lambda| = 2\lambda_1(M) + 2\sqrt{(m_1 - 1)\left(|M|^2/2 - \lambda_1^2(M)\right)},$$

then, $m_1 = 1$ or

$$\sum_{\lambda \in \sigma_+(M)} |\lambda| = \lambda_1(M) + \sqrt{(m_1 - 1)\left(|M|^2/2 - \lambda_1^2(M)\right)}.$$

and the result follows from Lemma 2 ■

In what follows we apply the above result to search an upper bound for the energy of a bipartite graph. Let G be a bipartite graph with bipartition $\{X, Y\}$, where $|X| = k$ and $|Y| = \ell$. We label the vertices of G so that

$$A_G = \begin{pmatrix} \mathbf{0} & A_{12} \\ A_{21} & \mathbf{0} \end{pmatrix}, \tag{9}$$

where A_{12} and A_{21} have order $k \times \ell$ and $\ell \times k$, respectively. If G is a connected graph, then A_G is an irreducible nonnegative symmetric matrix. We are now in a position to apply Theorem 1 to A_G.

Corollary 1 *Let G be a connected bipartite graph with n vertices and m edges and suppose that $\{X, Y\}$ is a bipartition of the vertices of G, with $|X| = k$ and $|Y| = \ell$. Let $\widetilde{k} = \min\{k, \ell\}$. Then*

$$E(G) \leq 2\lambda_1(G) + 2\sqrt{\left(\widetilde{k} - 1\right)(m - \lambda_1^2(G))}\ .$$

Equality holds if and only if $\widetilde{k} = 1$, or if A_G has $2\left(\widetilde{k} - 1\right)$ eigenvalues distinct from $\pm\lambda_1(M)$ with the same modulus, namely $\sqrt{(m - \lambda_1^2(M)) / \left(\widetilde{k} - 1\right)}$, and $|k - \ell|$ eigenvalues equal to 0.

Proof. By considering $P = I_n$, the identity matrix, in Eq. (6) it is possible identify A_G in Eq. (9) with M. In this case $\widetilde{k}$ and $\widetilde{m}$ coincide. Moreover, $\frac{|M|^2}{2}$ and $\lambda_1(M)$ correspond to m and $\lambda_1(G)$, respectively, and the inequality holds. Considering further that the order of the adjacency matrix coincides with the number of vertices we see the case of equality in the statement reproduces the case for equality in Theorem 1. Thus, the result is proved. ■

Remark 2 *The set of connected bipartite graphs that realize the upper bound in Corollary 1 contains all connected graphs that realize the upper bound in equation (3).*

Remark 3 *The set of incidence graph of a BIBD (*symmetric or not*) is a family of graphs that is extremal in the sense of Corollary 1.*

The subdivision of a graph G is the graph obtained by inserting a new vertex on every edge of G. We denote by S_{2k+1} the subdivision of the star $K_{1,k}$. According to Ghorbani [4], $\sigma_{S_{2k+1}} = \{\pm\sqrt{k+1}, 0, \pm 1^{(k-1)}\}$.

Remark 4 *For $k \geq 3$, the graphs S_{2k+1} are not the incidence graph of a design (because of the degree of its vertices) and they are extremal in the sense of Corolllary 1.*

In the Remarks 3 and 4 we exhibit two infinite families of graphs that are extremal to our upper bound in Corollary 1 and are not extremal to the upper bound for bipartite graphs in Eq. (3): the set of incidence graph of a BIBD that are not symmetric and the graphs S_{2k+1}.

3.1 Generalized Bethe Trees

We now continue with the application of the result of Theorem 1 to search an upper bound for the energy of some balanced trees, namely the generalized Bethe trees. Let $\mathcal{T}$ be an unweighted rooted tree of k levels, where the root is the only vertex at first level and such that, if we consider the decreasing order, all the vertices in the $(k-j+1)$-th level have equal degree, d_j. Thus d_k and d_1 $(=1)$ are the degrees of the root vertex and the vertices at level k (pendant vertices), respectively. By a suitable labeled, the authors in [18] have characterized the eigenvalues of the adjacency matrix of $\mathcal{T}$. Define

$$R_k = \begin{pmatrix} 0 & \sqrt{d_2-1} & 0 & \cdots & \cdots & 0 \\ \sqrt{d_2-1} & 0 & \sqrt{d_3-1} & \ddots & & \vdots \\ 0 & \sqrt{d_3-1} & \ddots & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \sqrt{d_{k-1}-1} & 0 \\ \vdots & & \ddots & \sqrt{d_{k-1}-1} & 0 & \sqrt{d_k} \\ 0 & \cdots & \cdots & 0 & \sqrt{d_k} & 0 \end{pmatrix}. \tag{10}$$

For $1 \le j \le k$, let denote by n_j the total number of vertices at level $k-j+1$. Thus $n_k = 1$.

Theorem 2 *[18] For $1 \le j \le k-1$, let R_j, be the principal submatrix of order j of R_k. If $\Omega = \{j : 1 \le j \le k-1,\ n_j - n_{j+1} > 0\}$. Then*

1. $\sigma(A_{\mathcal{T}}) = \sigma(R_k) \cup \bigcup_{j\in\Omega} \sigma(R_j)$.
2. *For $j \in \Omega$ the multiplicity of each eigenvalue of the matrix R_j, as an eigenvalue of $A_{\mathcal{T}}$, is at least $n_j - n_{j+1}$ and equal to 1 for $j = k$.*

Remark 5 *¿From interlacing Theorem we immediately note that the spectral radius of $\mathcal{T}$ corresponds to the spectral radius of R_k. Moreover, for the energy of $\mathcal{T}$ it is holds*

$$E(\mathcal{T}) = E(R_k) + \sum_{j\in\Omega} (n_j - n_{j+1}) E(R_j). \tag{11}$$

For $a \in \mathbb{R}$ we denote by $[a]$ the greater integer less than or equal to a.

Remark 6 *It is well known that for $1 \le j \le k$, the matrix R_j is a symmetric imprimitive matrix and it has at most $[j/2]$ nonzero eigenvalues. By Theorem 1 we derive that*

$$E(R_j) \le 2\lambda_1(R_j) + 2\sqrt{([j/2]-1)\left(|R_j|^2/2 - \lambda_1^2(R_j)\right)}, \tag{12}$$

where

$$\frac{1}{2}\left|R_j\right|^2 = \begin{cases} \sum\limits_{t=1}^{j}\left(d_t-1\right), & j<k \\ 1+\sum\limits_{t=1}^{k}\left(d_t-1\right), & j=k\ . \end{cases} \tag{13}$$

Our aim here is to give an upper bound for the energy of $\mathcal{T}$. By Eqs. (11) and (12) we establish.

Theorem 3 *Let $\mathcal{T}$ be a Bethe tree as described above. Then*

$$\begin{aligned} E\left(\mathcal{T}\right)/2 \le \lambda_1\left(\mathcal{T}\right) &+ \sqrt{\left([k/2]-1\right)\left(\left|R_k\right|^2/2-\lambda_1^2\left(\mathcal{T}\right)\right)} \\ &+ \sum_{j\in\Omega}\left(n_j-n_{j+1}\right)\left(\lambda_1\left(R_j\right)+\sqrt{\left([j/2]-1\right)\left(\left|R_j\right|^2/2-\lambda_1^2\left(R_j\right)\right)}\right). \end{aligned} \tag{14}$$

Equality in (14) holds if and only if $k\in\{2,3,4,5\}$ or if for each $j\in\Omega\cup\{k\}$, $j\ge 6$, the matrix R_j has $2\left([j/2]-1\right)$ nonzero eigenvalues with the same modulus, namely $\sqrt{\left(\left|R_j\right|^2/2-\lambda_1^2\left(R_j\right)\right)/\left([j/2]-1\right)}$.

4 Equitable Partitions

For $1\le i,j\le k$, let us consider the $n_i\times n_j$ matrices M_{ij}. Let $n=\sum\limits_{i=1}^{k}n_i$ and suppose that $M_{ij}=M_{ji}^t$ for all (i,j). We consider the $n\times n$ symmetric matrix having the block form

$$M=\begin{pmatrix} M_{11} & M_{12} & \dots & & M_{1k} \\ M_{21} & M_{22} & & & M_{2k} \\ \vdots & & \ddots & \ddots & \vdots \\ & & \ddots & & \\ M_{k1} & \dots & & & M_{kk} \end{pmatrix}. \tag{15}$$

Let denote by $\mathbb{J}_{pq}$ the all one matrix of order $p\times q$ and simply by $\mathbb{J}_p$ the all one vector of order $p\times 1$. The quotient matrix B^M of M is the $k\times k$ matrix whose (i,j)-entry, b_{ij} is the average of the row sums of M_{ij}. More precisely

$$b_{ij}=\frac{1}{n_i}\left(\mathbb{J}_{n_i}^t\, M_{ij}\, \mathbb{J}_{n_j}\right) \qquad 1\le i,j\le k. \tag{16}$$

The partition into blocks of M is called regular (or equitable) if each block M_{ij} of M has constant row sum. Note that in this case B^M corresponds to the row sums matrix. According to Lemma 2.3.1 in [1], *if M is regular then all the eigenvalues of B^M are eigenvalues of M*. Let $q_{ij}=\mathbb{J}_{n_i}^t M_{ij}\mathbb{J}_{n_j}=q_{ji}$. Note that $n_ib_{ij}=q_{ij}$, for all $1\le i,j\le k$. Let

$$F=diag\left(\sqrt{n_1},\dots,\sqrt{n_k}\right). \tag{17}$$

Lemma 4 *Let B^M and F defined as in Eqs. (16) and (17), respectively. If $FB^MF^{-1} = S$, then S is a symmetric matrix whose (i,j)-entry is $s_{ij} = q_{ij}/\sqrt{n_i n_j}$.*

Proof. It is clear that the (i,j)-entry of S is $\frac{\sqrt{n_i}b_{ij}}{\sqrt{n_j}} = \sqrt{n_i}\left(\frac{q_{ij}}{n_i}\right)\frac{1}{\sqrt{n_j}} = \frac{q_{ij}}{\sqrt{n_i n_j}}$. On the other hand the (j,i)-entry of FB^MF^{-1} is $\frac{\sqrt{n_j}b_{ji}}{\sqrt{n_i}} = \sqrt{n_j}\left(\frac{q_{ji}}{n_j}\right)\frac{1}{\sqrt{n_i}} = \frac{q_{ji}}{\sqrt{n_j n_i}} = \frac{q_{ij}}{\sqrt{n_i n_j}}$, and the result holds. ■

Remark 7 *If M is a symmetric regular partitioned matrix and B^M and S are defined as in Eq. 16 and Lemma 4 respectively, then all the eigenvalues of S are eigenvalues of M. Therefore, $\sigma_S \subset \sigma_M$ (as multisets), and*

$$E(M) = E(S) + \sum_{\lambda \in \sigma_M \setminus \sigma_S} |\lambda|. \tag{18}$$

At follows we present an upper bound for the energy of symmetric matrices regular partitioned into blocks.

Theorem 4 *Let M be the real symmetric regular partitioned matrix of order $n = \sum_{i=1}^{k} n_i$ and B^M and S defined as in (16) and Lemma 4 respectively. Then*

$$E(M) \le E(S) + \sqrt{(n-k)\left(|M|^2 - |S|^2\right)}. \tag{19}$$

Equality holds if and only if M has $n-k$ eigenvalues, distinct to those from S, with the same modulus, we say α, where $\alpha = \sqrt{\left(|M|^2 - |S|^2\right)/(n-k)}$.

Proof. Note that $\sum_{\lambda \in \sigma(M)} |\lambda|^2 = \sum_{\lambda \in \sigma_M \setminus \sigma_S} |\lambda|^2 + \sum_{\lambda \in \sigma(S)} |\lambda|^2$ or equivalently

$$\sum_{\lambda \in \sigma_M \setminus \sigma_S} |\lambda|^2 = |M|^2 - |S|^2. \tag{20}$$

The inequality in Eq. (19) is an immediate consequence of Eq. (18) and Cauchy–Schwarz inequality. It is evident that the equality holds for the case in the statement. Reciprocally if the equality holds, then

$$E(M) = \sum_{i=1}^{k} |\lambda_i(S)| + \sum_{\lambda_i(M) \in \sigma_M \setminus \sigma_S} |\lambda_i(M)| = \sum_{i=1}^{k} |\lambda_i(S)| + \sqrt{n-k}\sqrt{\sum_{\lambda_i(M) \in \sigma_M \setminus \sigma_S} |\lambda_i^2(M)|}.$$

In consequence,

$$\sum_{\lambda_i(M) \in \sigma_M \setminus \sigma_S} |\lambda_i(M)| = \sqrt{n-k}\sqrt{\sum_{\lambda_i(M) \in \sigma_M \setminus \sigma_S} |\lambda_i^2(M)|}$$

and by Cauchy–Schwarz equality case we obtain $\alpha_{k+1}(M) = \cdots = \alpha_n(M) = a = \sqrt{\left(|M|^2 - |S|^2\right)/(n-k)}$, where $\{\alpha_{k+1}(M), \ldots, \alpha_n(M)\} = \sigma_M \setminus \sigma_S$. ■

An exact analogue of Lemma 3 for symmetric matrices partitioned into blocks with constant row sum is given below.

Theorem 5 *Let M be the real symmetric regular partitioned matrix of order $n = \sum_{i=1}^{k} n_i$ as in (15) and S the matrix defined in Lemma (4) then*

$$E(M) \le \sqrt{k}\,|S| + \sqrt{(n-k)\left(|M|^2 - |S|^2\right)} \le \sqrt{n}\,|M|. \tag{21}$$

Equality in the left inequality holds if and only if M has k eigenvalues with the same modulus, namely $\sqrt{|S|^2/k}$ and the others $n-k$ eigenvalues of M have the same modulus, namely $\sqrt{\left(|M|^2 - |S|^2\right)/(n-k)}$.

Proof. ¿From (5), $E(S) \le \sqrt{k}\,|S|$. Now we use Eq. (19) and result holds. The equality case is a direct consequence of the equality case in the Lemma 3. ■

Theorem 6 *Let M be the real irreducible nonnegative symmetric regular partitioned matrix of order $n = \sum_{i=1}^{k} n_i$ and consider S in Lemma 4. Then*

$$E(M) \le \lambda_1(M) + \sqrt{(k-1)\left(|S|^2 - \lambda_1^2(M)\right)} + \sqrt{(n-k)\left(|M|^2 - |S|^2\right)}. \tag{22}$$

Equality holds if and only if S has $k-1$ eigenvalues distinct to $\lambda_1(M)$ with the same modulus, namely $\sqrt{\left(|S|^2 - \lambda_1^2(M)\right)/(k-1)}$ and the others $n-k$ eigenvalues of M have the same modulus, namely $\sqrt{\left(|M|^2 - |S|^2\right)/(n-k)}$.

Proof. It is well known that for a irreducible nonnegative matrix, the only eigenvalue with a nonnegative eigenvector is its maximal eigenvalue (see [12]). Since M is nonnegative then B^M it is hence its maximal eigenvalue $\lambda_1\left(B^M\right)$ has a nonnegative eigenvector, we say $\mathbf{x}$. Since M is regular partitioned, all the eigenvalues of B^M (hence of S) are eigenvalues of M. By Theorem 2.5.1 in [1] there exists a $n \times k$ nonnegative matrix T such that $\mathbf{y} = T\mathbf{x}$ is an eigenvector of M. Hence, $\mathbf{y}$ nonnegative imply that $\lambda_1\left(B^M\right) = \lambda_1(M)$, hence $\lambda_1(S) = \lambda_1(M)$.

By Eq. (4)

$$E(S) \le \lambda_1(S) + \sqrt{(k-1)\left(|S|^2 - \lambda_1^2(S)\right)}\ .$$

By Eq. (19) the inequality in the statement follows. The equality case is a direct consequence of the equality case in the Lemma 3. ■

Remark 8 *Let M be the real irreducible nonnegative symmetric regular partitioned matrix of order $n = \sum_{i=1}^{k} n_i$ and consider S as in Lemma 4. By Lemma 3 the upper bound in Eq. (19) is sharper than the upper bound in Eq. (22) and we confirm that the upper bound in Eq. (22) is sharper than its analogue in Eqs. (21) and (4).*

4.1 Join graph operations

A generalization of the join operation was introduced in [2] as follows: Consider a family of k graphs, $\mathcal{F} = \{G_1, \ldots, G_k\}$, where each graph G_i has order n_i, for $1 \leq i \leq k$, and a graph H such that $\mathcal{V}(H) = \{v_1, \ldots, v_k\}$. Each vertex $v_i \in \mathcal{V}(H)$ is assigned to the graph $G_i \in \mathcal{F}$. The H-join of $G_1, \ldots, G_k$ is the graph $G = H[G_1, \ldots, G_k]$ such that $\mathcal{V}(G) = \bigcup_{i=1}^{k} \mathcal{V}(G_i)$ and edge set:

$$\mathcal{E}(G) = \left(\bigcup_{i=1}^{k} \mathcal{E}(G_i)\right) \cup \left(\bigcup_{uv\in\mathcal{E}(H)} \{v_i v_j \colon v_i \in \mathcal{V}(G_u), v_j \in \mathcal{V}(G_v)\}\right).$$

This operation, where H is an arbitrary graph of order k, is the same as the so called generalized composition, was studied in [19] with the notation $H[G_1, \ldots, G_k]$.

Consider a family of k regular graphs, $\mathcal{F} = \{G_1, \ldots, G_k\}$, where each graph G_i has order n_i, and vertex degree p_i for $1 \leq i \leq k$, and a graph H such that $\mathcal{V}(H) = \{v_1, \ldots, v_k\}$. Suppose that $A_H = (a_{ij}) \in \mathbb{R}^{k\times k}$. For $1 \leq i, j \leq k$, let, $h_{ij} = a_{ij}\sqrt{n_i n_j}$ and define

$$C = \begin{pmatrix} p_1 & h_{12} & \cdots & & h_{1k} \\ h_{12} & p_2 & \cdots & & h_{2k} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{1k} & h_{2p} & \cdots & p_{k-1} & h_{k,k-1} \\ h_{1k} & h_{2k} & \cdots & h_{k,k-1} & p_k \end{pmatrix}.$$

Let $G = H[G_1, \ldots, G_k]$. Since,

$$A_G = \begin{pmatrix} A_{G_1} & a_{12}\mathbb{J}_{n_1 n_2} & \cdots & & a_{1k}\mathbb{J}_{n_1 n_k} \\ a_{12}\mathbb{J}_{n_2 n_1} & A_{G_2} & \cdots & & a_{2k}\mathbb{J}_{n_2 n_k} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{1k}\mathbb{J}_{n_{k-1} n_1} & a_{2p}\mathbb{J}_{n_{p-1} n_2} & \cdots & A_{G_{k-1}} & a_{k,k-1}\mathbb{J}_{n_{k-1} n_k} \\ a_{1k}\mathbb{J}_{n_k n_1} & a_{2k}\mathbb{J}_{n_k n_2} & \cdots & a_{k,k-1}\mathbb{J}_{n_k n_{k-1}} & A_{G_k} \end{pmatrix}$$

in [2] it was proven that

$$\sigma(G) = \bigcup_{j=1}^{k} \sigma(G_j) \diagdown \{p_j\} \cup \sigma(C).$$

In consequence,

$$E(G) = E(C) + \sum_{j=1}^{k} (E(G_j) - p_j).$$

By Theorem 4 we obtain.

Corollary 2 *Let $\mathcal{F} = \{G_1, \ldots, G_k\}$ a family of k regular graphs, where each graph G_i has order n_i and vertex degree p_i, for $1 \leq i \leq k$, and a graph H such that $\mathcal{V}(H) = \{v_1, \ldots, v_k\}$. Let $n = \sum_{i=1}^{k} n_i$ and let consider $G = H[G_1, \ldots, G_k]$. Then*

$$E(G) \leq E(C) + \sqrt{\sum_{i=1}^{k} p_i(n_i - p_i)(n-k)}\ .$$

Equality holds if and only if A_G has $n-k$ eigenvalues, distinct to those from C, with the same modulus, namely $\sqrt{\sum_{i=1}^{k} p_i(n_i - p_i)/(n-k)}$.

Proof. If in Theorem 4 we replace M by A_G we obtain $S = C$. Therefore following the result in Theorem 4 we derive that

$$E(G) \leq E(C) + \sqrt{(n-k)\left(|A_G|^2 - |C|^2\right)}\ .$$

Equality holds if and only if A_G has $n-k$ eigenvalues, which are not shared with C, with the same absolute value. Now by noticing that $|A_G|^2 - |C|^2 = \sum_{i=1}^{k} p_i(n_i - p_i)$, the result follows. ■

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