

Sharp Bounds on the Spectral Radius and the Energy of Graphs

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Abstract

Let $G = (V, E)$ be a simple graph of order n with $V(G) = \{v_1, v_2, \dots, v_n\}$ and degree sequence d_1, d_2, \dots, d_n . Let $\rho(G)$ be the largest eigenvalue of adjacency matrix of G , and let $E(G)$ be the energy of G . Denote $(^\alpha t)_i = \sum_{i \sim j} d_j^\alpha$ and $(^\alpha m)_i = (^\alpha t)_i / d_i^\alpha$, where α is a real number. In this paper, we obtain two sharp bounds on $\rho(G)$ in terms of $(^\alpha m)_i$ or $(^\alpha t)_i$, respectively. Also, we present some sharp bounds on the energy $E(G)$. From which, we can derive some known results.

1. Introduction

Let $G = (V, E)$ be a simple graph of order n . Let $V(G) = \{v_1, v_2, \dots, v_n\}$. For any two vertices $v_i, v_j \in V(G)$, we will use the symbol $i \sim j$ to denote the edge $v_i v_j$. For $v_i \in V(G)$, $N_G(v_i)$ denotes the neighbors of v_i . The degree of v_i , written by $d(v_i)$ or d_i , is the number of edges incident with v_i . The 2-degree of v_i [2] is the sum of the degrees of the vertices adjacent to v_i and denoted by t_i , and the average-degree of v_i is $m_i = \frac{t_i}{d_i}$. Here we define

$$({}^\alpha t)_i = \sum_{i \sim j} d_j^\alpha \quad \text{and} \quad ({}^\alpha m)_i = \frac{\sum_{i \sim j} d_j^\alpha}{d_i^\alpha},$$

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where α is a real number. Note that $d_i = ({}^0t)_i = ({}^0m)_i$, $t_i = ({}^1t)_i$ and $m_i = ({}^1m)_i$.

Let $A(G) = (a_{ij})$ be the adjacency matrix of G with $a_{ij} = 1$ if v_i is adjacent to v_j , and $a_{ij} = 0$ otherwise. It follows immediately that if G is a simple graph, then $A(G)$ is a symmetric $(0, 1)$ matrix in which every diagonal entry is zero. Since $A(G)$ is real and symmetric, its eigenvalues are real. The *spectral radius* of G , denoted by $\rho(G)$, is the largest eigenvalue of $A(G)$. Note that if G is connected, then $A(G)$ is irreducible, and so by the Perron-Frobenius theory of non-negative matrices, $\rho(G)$ has multiplicity one and there exists a unique positive unit eigenvector (also called Perron-eigenvector) corresponding to $\rho(G)$.

The *energy* of G , denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^n |\lambda_i|$, where $\rho(G) = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ are the eigenvalues of the adjacency matrix of G .

Up to now, many bounds for $\rho(G)$ and $E(G)$ were given (see for example, [1]–[11], [16]–[24]).

In this paper, we present two sharp upper and lower bounds on the spectral radius of a graph G , and give an upper bound for the energy of G by using this new lower bound of spectral radius. From which, we can derive some known results.

2. Upper Bounds for the Spectral Radius of Graphs

Throughout this section, let G be a simple graph of order n with degree sequence (d_1, d_2, \dots, d_n) . Let $A(G)$ be the adjacency matrix of G . Let $\tilde{D} = \text{diag}(d_1^\alpha, \dots, d_n^\alpha)$.

Lemma 2.1 [12]. *Let $M = (m_{ij})$ be an $n \times n$ irreducible nonnegative matrix with spectral radius $\rho(M)$, and let $R_i(M)$ be the i th row sum of M , i.e., $R_i(M) = \sum_{j=1}^n m_{ij}$. Then*

$$\min\{R_i(M) : 1 \leq i \leq n\} \leq \rho(M) \leq \max\{R_i(M) : 1 \leq i \leq n\}.$$

Moreover, if the row sums of M are not all equal, then the both inequalities in the above are strict.

Now, we give our main result of this section.

Theorem 2.2. *Let G be a connected graph. Then*

$$\rho(G) \leq \min_{\alpha} \max_{i \sim j} \left\{ \sqrt{{}^\alpha m_i {}^\alpha m_j} \right\}. \tag{1}$$

Moreover, the equality holds in (1) for a particular value of α if and only if $({}^\alpha m)_1 = ({}^\alpha m)_2 = \dots = ({}^\alpha m)_n$ or G is a bipartite graph with the partition $\{v_1, \dots, v_{n_1}\} \cup \{v_{n_1+1}, \dots, v_n\}$ and $({}^\alpha m)_1 = \dots = ({}^\alpha m)_{n_1}$, $({}^\alpha m)_{n_1+1} = \dots = ({}^\alpha m)_n$.

Proof. Note that $\rho(G) = \rho(A) = \rho(\tilde{D}^{-1}A\tilde{D})$. Now, the (i, j) th element of $\tilde{D}^{-1}A\tilde{D}$ is

$$\begin{cases} \frac{d_j^\alpha}{d_i^\alpha} & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

Let $X = (x_1, x_2, \dots, x_n)^T$ be the eigenvector corresponding to the eigenvalue $\rho(G)$ of $\tilde{D}^{-1}A\tilde{D}$. We can assume that one eigencomponent, say x_i , is equal to 1 and the other eigencomponents are less than or equal to 1 in magnitude, that is, $x_i = 1$ and $|x_k| \leq 1$ for $v_k \in V(G)$. Let $x_j = \max_{i \sim k} \{x_k\}$.

Since

$$\tilde{D}^{-1}A\tilde{D}X = \rho(A)X,$$

we have

$$\rho(G)x_i = \sum_{k \sim i} \frac{d_k^\alpha}{d_i^\alpha} x_k \leq (\alpha m)_i x_j \tag{2}$$

$$\rho(G)x_j = \sum_{k \sim j} \frac{d_k^\alpha}{d_j^\alpha} x_k \leq (\alpha m)_j \tag{3}$$

Eliminating x_j from (2) and (3), we obtain

$$\rho(G) \leq \sqrt{(\alpha m)_i (\alpha m)_j}. \tag{4}$$

Now suppose that equality in (1) holds for a particular value of α . Then all inequalities in the above argument must be equalities. In particular, we have, from (2), that $x_k = x_j$ for $k \sim i$. Also from (3) that $x_k = 1$ for $k \sim j$. Let $U = \{v_k \in V(G) : x_k = 1\}$. Then $v_i \in U$.

If $x_j = 1$, then we will show $U = V(G)$. Otherwise, if $U \neq V(G)$, there exist vertices $v_a, v_b \in U, v_c \notin U$ such that $a \sim b, b \sim c$ since G is connected. Therefore, from

$$\rho(G)x_a = \sum_{k \sim a} \frac{d_k^\alpha}{d_a^\alpha} x_k \leq (\alpha m)_a$$

and

$$\rho(G)x_b = \sum_{k \sim b} \frac{d_k^\alpha}{d_b^\alpha} x_k < (\alpha m)_b,$$

we have $\rho(G) < \sqrt{(\alpha m)_a (\alpha m)_b}$, which contradicts that the equality holds in (1). Thus $U = V(G)$ and $(\alpha m)_1 = (\alpha m)_2 = \dots = (\alpha m)_n = \rho(G)$.

If $x_j < 1$. Let $W = \{v_k \in V(G) : x_k = x_j\}$. So $N_G(v_j) \subseteq U$ and $N_G(v_i) \subseteq W$. Now we show that $N_G(N_G(v_i)) \subseteq U$. Let $v_r \in N_G(N_G(v_i))$, there exists a vertex v_p

such that $i \sim p$ and $r \sim p$. Therefore, $x_p = x_j$ and $\rho(G)x_p = \sum_{w \sim p} \frac{d_w^\alpha}{d_p^\alpha} x_w \leq (\alpha m)_p$. Using (2), we obtain $\rho^2(G) \leq (\alpha m)_i (\alpha m)_p$. Note that $\rho^2(G) \geq (\alpha m)_i (\alpha m)_p$, and hence $\rho^2(G) = (\alpha m)_i (\alpha m)_p$, which shows that $x_r = 1$. Hence $N_G(N_G(v_i)) \subseteq U$. By a similar argument, we can show that $N_G(N_G(v_j)) \subseteq W$. Continuing the procedure, it is easy to see, since G is connected, that $V = U \cup W$ and that the subgraphs induced by U, W are empty. Hence G is bipartite. Moreover, $(\alpha m)_p$ are the same for $v_p \in U$ and $(\alpha m)_q$ are the same for $v_q \in W$.

Conversely, if G is a graph with $(\alpha m)_1 = (\alpha m)_2 = \dots = (\alpha m)_n$, then the equality in (1) is satisfied. Let G be a bipartite graph with bipartition $V = U \cup W$ and $(\alpha m)_i = a$ for $v_a \in U$, $(\alpha m)_i = b$ for $v_b \in W$. Let $M = \tilde{K}^{-1}(\tilde{D}^{-1}A\tilde{D})\tilde{K}$, where $\tilde{K} = \text{diag}\{\sqrt{(\alpha m)_1}, \dots, \sqrt{(\alpha m)_n}\}$. Note that the (i, j) th element of M is

$$\begin{cases} \sqrt{\frac{b}{a}} \frac{d_j^\alpha}{d_i^\alpha} & \text{if } i \sim j, v_i \in U, \\ \sqrt{\frac{a}{b}} \frac{d_i^\alpha}{d_j^\alpha} & \text{if } i \sim j, v_i \in W, \\ 0 & \text{otherwise.} \end{cases}$$

Using Lemma 2.1 on M , we have $\rho(G) = \rho(M) = \sqrt{ab}$. ■

Note 2.3. If $\alpha = 0$, then the inequality (1) is the Berman and Zhang's bound (see [1]); If $\alpha = 1$, then the inequality (1) is the Das and Kummer's bound (Theorem 2.3, [5]). It was shown that in [5] Das and Kummer's bound is better than Berman and Zhang's bound. Here, we give an example to show that (1) is better than the Das and Kummer's bound in some case. Let G be a graph shown in Fig. 1. Then the bound (6) is $\sqrt{6}$ when $\alpha = 0.5$, and the Das and Kummer's bound is 2.5. Thus in that case, (1) is better than the Das and Kummer's bound.



G
Fig. 1

From Theorem 2.2, we have the following result.

Corollary 2.4. *Let G be a connected graph. Then*

$$\rho(G) \leq \min_{\alpha} \max_{1 \leq i \leq n} \{(\alpha m)_i\}. \tag{5}$$

Moreover, the equality holds for a particular value of α if and only if $(\alpha m)_1 = (\alpha m)_2 = \dots = (\alpha m)_n$.

Note 2.5. If $\alpha = 1$, then the bound (5) is the Favaron et.al's bound (see [6]).

3. Lower Bounds for the Spectral Radius of Graphs

In this section, we give a lower bound for the largest eigenvalue of the adjacent matrix of a graph. Now we define a sequence

$$N_i^{(1)}, N_i^{(2)}, \dots, N_i^{(k)}, \dots,$$

with $N_i^{(1)} = d_i^\alpha$, $N_i^{(2)} = \sum_{i \sim j} N_j^{(1)}$ and $N_i^{(k)} = \sum_{i \sim j} N_j^{(k-1)}$ for $k \geq 3$, where α is a real number. Note that $(\alpha t)_i = N_i^{(2)}$.

First we state the following lemma.

Lemma 3.1 [11]. *Let A be a nonnegative symmetric matrix and x be a unit vector of \mathcal{R}^n . If $\rho(G) = x^T A x$, then $Ax = \rho(A)x$.*

Theorem 3.2. *Let G be a connected graph of order n with degree sequence d_1, \dots, d_n . Then*

$$\rho(G) \geq \max_k \max_{\alpha \in \mathbb{R}} \left\{ \sqrt{\frac{\sum_{i=1}^n \left(N_i^{(k+1)}\right)^2}{\sum_{i=1}^n \left(N_i^{(k)}\right)^2}} \right\} \quad (6)$$

Moreover, the equality holds in (6) for a particular values of α and k if and only if $\frac{N_1^{(k+1)}}{N_1^{(k)}} = \frac{N_2^{(k+1)}}{N_2^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}}$ or G is a bipartite graph with the partition $\{v_1, \dots, v_{n_1}\} \cup \{v_{n_1+1}, \dots, v_n\}$ and $\frac{N_1^{(k+1)}}{N_1^{(k)}} = \dots = \frac{N_{n_1}^{(k+1)}}{N_{n_1}^{(k)}}$, $\frac{N_{n_1+1}^{(k+1)}}{N_{n_1+1}^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}}$.

Proof. Let $X = (x_1, x_2, \dots, x_n)^T$ be the unit positive eigenvector of A corresponding to $\rho(A)$. Take

$$C = \sqrt{\frac{1}{\sum_{i=1}^n \left(N_i^{(k)}\right)^2}} (N_1^{(k)}, N_2^{(k)}, \dots, N_n^{(k)})^T.$$

Then

$$\rho(G) = \sqrt{\rho(A^2)} = \sqrt{X^T A^2 X} \geq \sqrt{C^T A^2 C}.$$

Since

$$\begin{aligned} AC &= \sqrt{\frac{1}{\sum_{i=1}^n \left(N_i^{(k)}\right)^2}} \left(\sum_{j=1}^n a_{1j} N_j^{(k)}, \sum_{j=1}^n a_{2j} N_j^{(k)}, \dots, \sum_{j=1}^n a_{nj} N_j^{(k)} \right)^T \\ &= \sqrt{\frac{1}{\sum_{i=1}^n \left(N_i^{(k)}\right)^2}} \left(N_1^{(k+1)}, N_2^{(k+1)}, \dots, N_n^{(k+1)} \right)^T, \end{aligned}$$

we have

$$\rho(G) \geq \sqrt{\frac{\sum_{i=1}^n \left(N_i^{(k+1)}\right)^2}{\sum_{i=1}^n \left(N_i^{(k)}\right)^2}}. \tag{7}$$

If the equality holds, then $\rho(A^2) = C^T A^2 C$. By Lemma 3.1, $A^2 C = \rho(A^2) C$. If the multiplicity of $\rho(A^2)$ is one, then $X = C$, which implies $N_i^{(k+1)} = \rho(G) N_i^{(k)} (1 \leq i \leq n)$. Hence $\frac{N_i^{(k+1)}}{N_i^{(k)}} = \rho(G)$. Otherwise, the multiplicity of $\rho(A^2) = (\rho(A))^2$ is two, which implies that $-\rho(A)$ is also an eigenvalue of G . Then G is a connected bipartite graph (see Theorem 3.4 in [4]). Without loss of generality, we assume $A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$, where $B = (b_{i,j})$ is an $n_1 \times n_2$ matrix with $n_1 + n_2 = n$. Let $X = (X_1, X_2)^T$ and $C = \sqrt{\frac{1}{\sum_{i=1}^n (N_i^{(k)})^2}} (C_1, C_2)^T$, where $X_1 = (x_1, \dots, x_{n_1})^T$ and $X_2 = (x_{n_1+1}, \dots, x_n)^T$, $C_1 = (N_1^{(k)}, N_2^{(k)}, \dots, N_{n_1}^{(k)})^T$ and $C_2 = (N_{n_1+1}^{(k)}, N_{n_1+2}^{(k)}, \dots, N_n^{(k)})^T$. Since $A^2 = \begin{pmatrix} BB^T & 0 \\ 0 & BB^T \end{pmatrix}$, we have $BB^T C_1 = \rho(A^2) C_1$, $B^T B C_2 = \rho(A^2) C_2$ and $BB^T X_1 = \rho(A^2) X_1$, $B^T B X_2 = \rho(A^2) X_2$. Noting that BB^T and $B^T B$ have the same nonzero eigenvalues, $\rho(A^2)$ is the spectral radius of BB^T and its multiplicity is one. So $X_1 = p_1 C_1$ (p_1 is a constant), which implies $\frac{N_1^{(k+1)}}{N_1^{(k)}} = \dots = \frac{N_{n_1}^{(k+1)}}{N_{n_1}^{(k)}}$. Similarly, $X_2 = p_2 C_2$ (p_2 is a constant), which implies $\frac{N_{n_1+1}^{(k+1)}}{N_{n_1+1}^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}}$.

Conversely, if $\frac{N_1^{(k+1)}}{N_1^{(k)}} = \frac{N_2^{(k+1)}}{N_2^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}} = p$, then $AC = pC$. It is known that for any positive eigenvector of a nonnegative matrix, the corresponding eigenvalue is the spectral radius of that matrix. Hence $\rho(G) = p = \sqrt{\frac{\sum_{i=1}^n \left(N_i^{(k+1)}\right)^2}{\sum_{i=1}^n \left(N_i^{(k)}\right)^2}}$.

Now assume that G is a bipartite graph with the partition $\{v_1, \dots, v_{n_1}\} \cup \{v_{n_1+1}, \dots, v_n\}$ and its adjacency matrix

$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$, $\frac{N_1^{(k+1)}}{N_1^{(k)}} = \dots = \frac{N_{n_1}^{(k+1)}}{N_{n_1}^{(k)}} = p_1$, $\frac{N_{n_1+1}^{(k+1)}}{N_{n_1+1}^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}} = p_2$, where $B = (b_{i,j})$ is an $n_1 \times n_2$ matrix with $n_1 + n_2 = n$. Let $C_1 = (N_1^{(k)}, N_2^{(k)}, \dots, N_{n_1}^{(k)})^T$ and $C_2 = (N_{n_1+1}^{(k)}, N_{n_1+2}^{(k)}, \dots, N_n^{(k)})^T$. Then for each i ($1 \leq i \leq n_1$), the i th element of $BB^T C_1$ is

$$r_i(BB^T C_1) = \sum_{j=1}^{n_1} \sum_{l=1}^{n_2} b_{il} b_{jl} N_j^{(k)} = \sum_{l=1}^{n_2} b_{il} \sum_{j=1}^{n_1} b_{jl} N_j^{(k)}$$

$$= \sum_{i=1}^{n_2} b_{ii} p_2 N_{n_1+i}^{(k)} = p_1 p_2 N_i^{(k)}.$$

Similarly, $r_j(B^T B C_2) = p_1 p_2 N_{n_1+j}^{(k)}$ for j ($n_1 + 1 \leq j \leq n$). Hence $A^2 C = p_1 p_2 C$, where $C = \sqrt{\frac{1}{\sum_{i=1}^n (N_i^{(k)})^2}} (N_1^{(k)}, N_2^{(k)}, \dots, N_n^{(k)})^T$. It is known that for any positive eigenvector of a nonnegative matrix, the corresponding eigenvalue is the spectral radius of that matrix. So $\rho(A^2) = p_1 p_2 = C^T A^2 C$. It follows that $\rho(G) = \sqrt{C^T A^2 C} = \sqrt{p_1 p_2} = \sqrt{\frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}}$. ■

Note 3.3. If $\alpha = 1$, then the bound (6) is the Hou et.al’s bound (Theorem 5, [13]). If $\alpha = 1$ and $k = 2$, then the bound (6) is the Hong and Zhang’s bound (Theorem 3.1, [11]).

Note that $(\alpha t)_i = N_i^{(2)}$ and $(\alpha m)_i = \frac{(\alpha t)_i}{d_i^\alpha} = \frac{N_i^{(2)}}{N_i^{(1)}}$, and hence we have the following result by Theorem 3.2.

Corollary 3.4. *Let G be a connected bipartite graph of order n with degree sequence d_1, \dots, d_n . Then*

$$\rho(G) \geq \max_{\alpha \in \mathbb{R}} \left\{ \sqrt{\frac{\sum_{i=1}^n (\alpha t)_i^2}{\sum_{i=1}^n d_i^{2\alpha}}} \right\} \tag{8}$$

Moreover, the equality holds for a particular value of α if and only if $(\alpha m)_1 = (\alpha m)_2 = \dots = (\alpha m)_n$ or G is a bipartite graph with the partition $\{v_1, \dots, v_{n_1}\} \cup \{v_{n_1+1}, \dots, v_n\}$ and $(\alpha m)_1 = \dots = (\alpha m)_{n_1}$, $(\alpha m)_{n_1+1} = \dots = (\alpha m)_n$.

Note 3.5. If $\alpha = \frac{1}{2}$, then the inequality (8) is the Shi’s bound (Theorem 2.3, [19]); if $\alpha = 1$, then the inequality (8) is the Yu et.al’s bound (Theorem 4, [22]); if $\alpha = 0$, then the inequality (8) is the Hofmeister’s bound [7] (also see Corollary 6, [22]).

Theorem 3.6. *Let G be a connected graph of order n and*

$$f(k) = \sqrt{\frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}}, \quad \text{for } k \geq 1.$$

Then

$$\rho(G) = \lim_{k \rightarrow \infty} f(k). \tag{9}$$

Proof. Let $A(G) = (a_{ij})$ be the adjacent matrix of G . By Cauchy-Schwarz's inequality, we have

$$\begin{aligned} \left(\sum_{i=1}^n \left(N_i^{(k+1)} \right)^2 \right) \left(\sum_{i=1}^n \left(N_i^{(k-1)} \right)^2 \right) &\geq \left(\sum_{i=1}^n N_i^{(k+1)} N_i^{(k-1)} \right)^2 \\ &= \left(\sum_{i=1}^n \sum_{j=1}^n a_{ij} N_i^{(k)} N_i^{(k-1)} \right)^2 \\ &= \left(\sum_{j=1}^n \left(\sum_{i=1}^n a_{ij} N_i^{(k-1)} \right) N_i^{(k)} \right)^2 \\ &= \left(\sum_{j=1}^n \left(N_i^{(k)} \right)^2 \right)^2 \end{aligned}$$

with equality if and only if

$$\frac{N_1^{(k+1)}}{N_1^{(k)}} = \frac{N_2^{(k+1)}}{N_2^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}}.$$

Hence

$$\frac{\sum_{i=1}^n \left(N_i^{(k+1)} \right)^2}{\sum_{i=1}^n \left(N_i^{(k)} \right)^2} \geq \frac{\sum_{i=1}^n \left(N_i^{(k)} \right)^2}{\sum_{i=1}^n \left(N_i^{(k-1)} \right)^2}. \tag{10}$$

That is, $f(k+1) \geq f(k)$ for $k \geq 1$.

Since the sequence $f(k)$ is monotonically increasing and has an upper bound $\rho(G)$, the limit $\lim_{k \rightarrow \infty} f(k)$ must exist. In order to show the limit it suffices to prove $\rho(G) = \lim_{k \rightarrow \infty} f(2k)$.

Let $\rho(G) = \lambda_1 > \lambda_2 \geq \dots \geq \lambda_n$ be all the eigenvalues of G and X_1, X_2, \dots, X_n be unit eigenvectors corresponding to these eigenvalues of G . Then X_1, X_2, \dots, X_n consist of a orthonormal basis of \mathcal{R}^n . Thus $X_i^T X_j = 1$ if $i = j$ and $X_i^T X_j = 0$ if $i \neq j$. In order to show that $\rho(G) = \lim_{k \rightarrow \infty} f(2k)$, it suffices to prove $C^* = \frac{1}{\sqrt{\sum_{i=1}^n (N_i^{(2k)})^2}} (N_1^{(2k)}, N_2^{(2k)}, \dots, N_n^{(2k)})^T$ approaches a unit eigenvector corresponding to the eigenvalue $\rho^2(G)$ of $A^2(G)$ when $k \rightarrow \infty$. Denote $J^* = (d_1^\alpha, d_2^\alpha, \dots, d_n^\alpha)^T$. Note that the inner product $\langle A^{2k} J^*, A^{2k} J^* \rangle = \sum_{i=1}^n (N_i^{(2k)})^2$. Thus

$$C^* = \frac{A^{2k} J^*}{\sqrt{\langle A^{2k} J^*, A^{2k} J^* \rangle}}.$$

Assume that $J^* = \sum_{i=1}^n \theta_i X_i$. Then $\theta_i = (J^*)^T X_i$, $i = 1, 2, \dots, n$. Thus

$$A^{2k} J^* = A^{2k} \sum_{i=1}^n \theta_i X_i = \sum_{i=1}^n \theta_i (A^{2k} X_i) = \sum_{i=1}^n \theta_i \lambda_i^{2k} X_i,$$

and hence

$$\sum_{i=1}^n (N_i^{(2k)})^2 = \langle A^{2k} J^*, A^{2k} J^* \rangle = \sum_{i=1}^n \theta_i^2 \lambda_i^{4k}.$$

If G is nonbipartite, then $\theta_1 > 0$ and $\lambda_1 > |\lambda_i|$ for all $i = 2, 3, \dots, n$. Thus the vector $\frac{\theta_i \lambda_i^{2k} X_i}{\sqrt{\sum_{i=1}^n \theta_i^2 \lambda_i^{4k}}}$ approaches X_1 if $i = 1$; 0 if $i = 2, 3, \dots, n$ when $k \rightarrow \infty$. Therefore the eigenvector C^* approached X_1 , and the result follows.

If G is bipartite, then $\theta_1 > 0$ and $\lambda_1 > |\lambda_i|$ for all $i = 2, 3, \dots, n-1$, $\lambda_n = -\lambda_1$. Thus the vector $\frac{\theta_i \lambda_i^{2k} X_i}{\sqrt{\sum_{i=1}^n \theta_i^2 \lambda_i^{4k}}}$ approaches $\frac{\theta_1 X_1}{\sqrt{\theta_1^2 + \theta_n^2}}$ if $i = 1$; 0 if $i = 2, 3, \dots, n-1$; $\frac{\theta_n X_n}{\sqrt{\theta_1^2 + \theta_n^2}}$ if $i = n$ when $k \rightarrow \infty$. Therefore, when $k \rightarrow \infty$, the eigenvector C^* approached $\frac{\theta_1 X_1 + \theta_n X_n}{\sqrt{\theta_1^2 + \theta_n^2}}$, which is a unit eigenvector corresponding to the eigenvalue $\rho^2(G)$ of $A^2(G)$ and the result follows. ■

By Theorem 3.2, we have the following corollary.

Corollary 3.7. (i) Let G be a graph of order n with $\frac{N_i^{(k+1)}}{N_i^{(k)}} = p$, $1 \leq i \leq n$. Then $\rho(G) = p$;

(ii) Let G be a bipartite graph of order n with the bipartition (X, Y) , where $X = \{v_1, \dots, v_{n_1}\}$ and $Y = \{v_{n_1+1}, \dots, v_n\}$. If $\frac{N_i^{(k+1)}}{N_i^{(k)}} = p_1$, $1 \leq i \leq n_1$, and $\frac{N_j^{(k+1)}}{N_j^{(k)}} = p_2$, $n_1 \leq j \leq n$. Then $\rho(G) = \sqrt{p_1 p_2}$.

4. The Energy of a (Bipartite) Graph

In this section, we give some upper bounds for the energy of a (bipartite) graph and characterize those graphs for which these bounds are best possible. Recall that $N_i^{(1)} = d_i^\alpha$, $N_i^{(2)} = \sum_{i \sim j} N_j^{(1)}$ and $N_i^{(k)} = \sum_{i \sim j} N_j^{(k-1)}$ for $k \geq 3$, where α is a real number.

Theorem 4.1. Let G be a nonempty simple connected graph with n vertices and e edges. Then

$$E(G) \leq \min_k \min_{\alpha \in \mathbb{R}} \left\{ \sqrt{\frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}} + \sqrt{(n-1) \left(2e - \frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2} \right)} \right\} \quad (11)$$

Equality holds for a particular value of α if and only if $G \cong K_n$ or G is a non-bipartite connected graph satisfying $\frac{N_i^{(k+1)}}{N_i^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}}$ and has three distinct eigenvalues $\left(p, \sqrt{\frac{2e-p^2}{n-1}}, -\sqrt{\frac{2e-p^2}{n-1}} \right)$, where $p = \frac{N_i^{(k+1)}}{N_i^{(k)}} > \sqrt{\frac{2e}{n}}, 1 \leq i \leq n$.

Proof. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be the eigenvalues of G . By the Cauchy-Schwartz inequality, we have

$$E(G) \leq \lambda_1 + \sum_{i=2}^n |\lambda_i| \leq \lambda_1 + \sqrt{(n-1) \sum_{i=2}^n \lambda_i^2} = \lambda_1 + \sqrt{(n-1)(2e - \lambda_1^2)}.$$

By Theorem 3.2 and (10), we have

$$\lambda_1(G) \geq \max_{\alpha} f(k) \geq \max_{\alpha=1} f(k) \geq \sqrt{\frac{\left(\sum_{i=1}^n t_i\right)^2}{n \sum_{i=1}^n d_i^2}} = \sqrt{\frac{1}{n} \sum_{i=1}^n d_i^2} \geq \sqrt{\frac{2e}{n}}.$$

Let $g(x) = x + \sqrt{(n-2)(2e-x^2)}$, $x \leq \sqrt{2e}$. Then $g(x)$ is monotonously decreasing in $x \geq \sqrt{\frac{2e}{n}}$. Hence $g(\lambda_1(G)) \leq g\left(\sqrt{\frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}}\right)$, which implies

$$E(G) \leq \sqrt{\frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}} + \sqrt{(n-1) \left(2e - \frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}\right)}.$$

If G is one of the two graphs shown in the third part of Theorem 3.2, it is easy to check that the equality (11) holds. Conversely, if the equality (11) holds, then by the same method of the proof for Theorem 2.5 in [17], G is one of the two graphs shown in the third part of Theorem 3.2. ■

By (12) and the same method of the proof for Theorem 3.1 in [17], we have the following result.

Theorem 4.2. *Let $G = (X, Y)$ be a connected bipartite graph with $n > 2$ vertices and e edges. Then*

$$E(G) \leq \min_k \min_{\alpha \in \mathbb{R}} \left\{ 2 \sqrt{\frac{\sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}} + \sqrt{(n-2) \left(2e - \frac{2 \sum_{i=1}^n (N_i^{(k+1)})^2}{\sum_{i=1}^n (N_i^{(k)})^2}\right)} \right\}$$

Equality holds if and only if $G \cong K_{r_1, r_2} \cup (n - r_1 - r_2)K_1$, where $r_1 r_2 = e$; or G is a connected bipartite graph with $X = \{v_1, \dots, v_{n_1}\}$, $Y = \{v_{n_1+1}, \dots, v_n\}$ such that $\frac{N_1^{(k+1)}}{N_1^{(k)}} = \dots = \frac{N_{n_1}^{(k+1)}}{N_{n_1}^{(k)}}$, $\frac{N_{n_1+1}^{(k+1)}}{N_{n_1+1}^{(k)}} = \dots = \frac{N_n^{(k+1)}}{N_n^{(k)}}$ and has four distinct eigenvalues $(\sqrt{p_x p_y}, \sqrt{\frac{2e-2p_x p_y}{n-2}}, -\sqrt{\frac{2e-2p_x p_y}{n-2}}, -\sqrt{p_x p_y})$, where $p_x = \frac{N_i^{(k+1)}}{N_i^{(k)}}$, $1 \leq i \leq n_1$ and $p_y = \frac{N_j^{(k+1)}}{N_j^{(k)}}$, $n_1 + 1 \leq j \leq n$, $\sqrt{p_x p_y} > \sqrt{\frac{2e}{n}}$.

Note 4.3. Our results in Theorems 4.3 and 4.4, for $\alpha = 1$, are the Hou et al's bounds [13]. Moreover, for $k = 2$, are the Liu et.al's bounds (see [17]); and for $k = 1$, are the Yu et.al's bounds (see [23]).

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