SHARP UPPER BOUNDS ON THE SPECTRAL RADIUS OF THE LAPLACIAN MATRIX OF GRAPHS

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Abstract. Let $G = (V, E)$ be a simple connected graph with n vertices and e edges. Assume that the vertices are ordered such that $d_1 \geq d_2 \geq \ldots \geq d_n$, where d_i is the degree of v_i for $i = 1, 2, \ldots, n$ and the average of the degrees of the vertices adjacent to v_i is denoted by m_i. Let $m_{\max}$ be the maximum of m_i's for $i = 1, 2, \ldots, n$. Also, let $\rho(G)$ denote the largest eigenvalue of the adjacency matrix and $\lambda(G)$ denote the largest eigenvalue of the Laplacian matrix of a graph G. In this paper, we present a sharp upper bound on $\rho(G)$:

$$\rho(G) \leq \sqrt{2e - (n-1)d_n + (d_n - 1)m_{\max}},$$

with equality if and only if G is a star graph or G is a regular graph.

In addition, we give two upper bounds for $\lambda(G)$:

$$1.\ \lambda(G) \leq \begin{cases} 2 + \sqrt{\sum_{i=1}^n d_i(d_i-1) - \left(\frac{1}{2}\sum_{i=1}^n d_i - 1\right)(2d_n - 2) + (2d_n-3)(2d_1-2)}, \\ \hfill \text{if } d_n \geq 2, \\ 2 + \sqrt{\sum_{i=1}^n d_i(d_i-1) - d_1 + 1}, \ \text{if } d_n = 1, \end{cases}$$

where the equality holds if and only if G is a regular bipartite graph or G is a star graph, respectively.

$$2.\ \lambda(G) \leq \frac{d_1 + \sqrt{d_1^2 + 4\left[\frac{2e}{n-1} + \frac{n-2}{n-1}d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right)\right] m_{\max}}}{2},$$

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with equality if and only if G is a regular bipartite graph.

1. Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and let e be the cardinality of the edge set E. To avoid trivialities we always assume that $n \geq 2$. We denote the line graph of G by L_G. Assume that the vertices are ordered such that $d_1 \geq d_2 \geq \ldots \geq d_n$, where d_i is the degree of v_i, for $i = 1, 2, \ldots, n$. The set of neighbors of v_i and the average of the degrees of the vertices adjacent to v_i are denoted by N_i and m_i, respectively. Let $m_{\max}$ be the maximum of m_i's for $i = 1, 2, \ldots, n$. Also, let $D(G)$=diag$\{d_1, d_2, \ldots, d_n\}$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$, where $A(G)$ is the $(0, 1)$-adjacency matrix of G. Both $A(G)$ and $L(G)$ are real symmetric matrices and they have real eigenvalues. The adjacency spectral radius, $\rho(G)$, of G is the largest eigenvalue of $A(G)$. The Laplacian spectral radius, $\lambda(G)$, of G is the largest eigenvalue of $L(G)$. It is known that the multiplicity of 0 as the eigenvalue of $L(G)$ is equal to the number of connected components of G. So a graph G is connected if and only if the second smallest Laplacian eigenvalue is strictly greater than 0.

The eigenvalues of the Laplacian matrix are important in graph theory, because they have relations to numerous graph invariants including connectivity, expanding property, isoperimetric number, maximum cut, independence number, genus, diameter, mean distance, and bandwidth-type parameters of a graph (see, for example, [**1**, **2**, **16**, **17**] and the references therein). Especially, the largest and the second smallest eigenvalues of $L(G)$ (for instance [**1**, **2**, **16**, **17**]) are probably the most important information contained in the spectrum of a graph. Since the sum of the second smallest Laplacian eigenvalue of a graph G and the largest Laplacian eigenvalue of the complement graph of G is equal to n, it is not surprising at all that the importance of one of these eigenvalues implies the importance of the other. In many applications good bounds for the largest Laplacian eigenvalue of G are needed (see, for instance, [**1**, **2**, **16**, **17**]).

In 2001, Y. Hong et al. (see [**12**], Section 1), there are plenty of upper bounds on the largest eigenvalue of the adjacency matrix of a graph G. We give another upper bound for $\rho(G)$ on n, e, m_{max} and d_n.

In 2000, Y. Hong et al. (see [11], Section 1), a large number of upper bounds on the sum of the spectral radius of a graph and its complement are presented. We also give one upper bound on the sum of the spectral radius of a graph and its complement in terms of n, d_1 and d_n.

Also we saw that a there is large number of upper bounds on the largest Laplacian eigenvalue of a graph G (see [3], [5]), but all of them are in terms of d_i's and m_i's.

However, in 2001, J.-S. Li and Y.-L. Pan [15] proved that

$$\lambda(G) \leq \sqrt{2d_1^2 + 4e - 2d_n(n-1) + 2d_1(d_n - 1)}, \tag{1}$$

with equality if and only if G is a regular bipartite graph, and in 2002, J.-L. Shu et al. [20] presented the following result:

$$\lambda(G) \leq d_n + \frac{1}{2} + \sqrt{\left(d_n - \frac{1}{2}\right)^2 + \sum_{i=1}^{n} d_i(d_i - d_n)}, \tag{2}$$

with equality if and only if G is a star graph or G is a regular bipartite graph.

Likewise, we give three new upper bounds for $\lambda(G)$, two depend only on the degree sequences and the other depends on n, e, d_1 and d_n. Also we determine its extremal graphs.

2. Lemmas and Results

The following result is of Perron-Frobenius in matrix theory ([8], p. 66).

Lemma 2.1. [8] *A non-negative matrix B always has a non-negative eigenvalue r such that the moduli of all the eigenvalues of B do not exceed r. To this 'maximal' eigenvalue r there corresponds a non-negative eigenvector*

$$B\mathbf{Y} = r\mathbf{Y} \qquad (\mathbf{Y} \geq 0,\ \mathbf{Y} \neq 0).$$

Lemma 2.2. [13] *Let $M = (m_{ij})$ be an $n \times n$ irreducible nonnegative matrix with spectral radius $\lambda_1(M)$, and let $R_i(M)$ be the ith row sum of M, i.e., $R_i(M) = \sum_{j=1}^{n} m_{ij}$. Then*

$$\min\{R_i(M) : \ 1 \le i \le n\} \le \lambda_1(M) \le \max\{R_i(M) : \ 1 \le i \le n\}. \tag{3}$$

Moreover, if the row sums of M are not all equal, then the both inequalities in (3) are strict.

Lemma 2.3. [20] *If G is a connected graph, then*

$$\lambda(G) \le 2 + \rho(L_G),$$

with equality if and only if G is a bipartite graph.

Lemma 2.4. *Let G be a simple connected graph. Then*

$$\sum_{k=1}^{n} |N_i \cap N_k| d_k = \sum_{j} \{d_j m_j : v_i v_j \in E\}, \ \textit{for } v_i \in V,$$

where d_i is the degree of the vertex v_i, m_i is the average of the degrees of the vertices adjacent to v_i and $|N_i \cap N_k|$ is the cardinality of the common neighbors of v_i and v_k.

Proof. For $v_i \in V$, we have

$$\begin{aligned}\sum_{k=1}^{n} |N_i \cap N_k| d_k &= \sum_{k=1, k\neq i}^{n} |N_i \cap N_k| d_k + d_i^2 \\ &= \sum_{i-j-k} d_k + d_i^2, \text{ summation is taken over all the paths } i-j-k, \\ &\qquad \text{starts from fixed vertex } v_i \\ &= \sum_j \left\{ \sum_k \{d_k : \ v_j v_k \in E\} : \ v_i v_j \in E \right\} \\ &= \sum_j \{d_j m_j : \ v_i v_j \in E\}.\end{aligned}$$

□

3. Upper bound for spectral radius of graphs

The largest eigenvalue $\rho(G)$ is often called the spectral radius of G. We now give some known important upper bounds for the spectral radius $\rho(G)$. Let G be a simple graph with n vertices and e edges. Also let d_1 and d_n be the highest degree and the lowest degree of G.

1. Hong [9]. If G is a connected graph, then

$$\rho(G) \leq \sqrt{2e - n + 1}, \tag{4}$$

with equality if and only if G is a star graph or G is a complete graph.

2. Hong, Shu and Fang [12]. If G is a connected graph, then

$$\rho(G) \leq \frac{d_n - 1 + \sqrt{(d_n+1)^2 + 4(2e - d_n n)}}{2}, \tag{5}$$

with equality if and only if G is a regular graph or G is a bidegreed graph in which each vertex is of degree either d_n or $n-1$.

3. Das and Kumar [7]. Let G be a connected graph and let $\rho(G)$ be the spectral radius of $A(G)$. Then

$$\rho(G) \leq \max\left\{\sqrt{\frac{TT_i}{d_i}} \ : \ 1 \leq i \leq n\right\}, \tag{6}$$

where $TT_i = \sum_j \{d_j m_j \ : \ v_i v_j \in E\}$ and the degree of the vertex v_i and the average of the degrees of the vertices adjacent to v_i are d_i and m_i, respectively.

Now we will extend our upper bound (6) to give a new upper bound for connected graphs. Our new upper bound (7) is in terms of n, e, d_n and $m_{\max}$. Moreover, we characterize the graphs for which the upper bound is attained.

Theorem 3.1. *Let G be a simple connected graph and $\rho(G)$ be the spectral radius of G, then*

$$\rho(G) \leq \sqrt{2e - (n-1)d_n + (d_n - 1)m_{\max}}, \tag{7}$$

where $m_{\max}$ is the maximum of m_i's, m_i is the average of the degrees of the vertices adjacent to v_i. Moreover, the equality in (7) holds if and only if G is a star graph or G is a regular graph.

Proof. If G is a path P_2 then the equality holds in (7). Now we have to show that Theorem 3.1 is true for $n > 2$. Since $\rho(G)$ is the spectral radius of $A(G)$, $\rho^2(G)$ is also the spectral radius of $D(G)^{-1}A^2(G)D(G)$.

Now the (i, j)-th element of $D(G)^{-1}A^2(G)D(G)$ is

$$\frac{d_j}{d_i}|N_i \cap N_j|.$$

Using Lemma 2.2 we conclude that

$$\rho^2(G) \leq \max_i \left\{ d_i + \frac{1}{d_i} \sum_{k:k\neq i} |N_i \cap N_k| d_k \right\} \tag{8}$$

$$= \max_i \left\{ \frac{1}{d_i} \sum_k |N_i \cap N_k| d_k \right\}$$

$$= \max_i \left\{ \frac{1}{d_i} \sum_j \{ d_j m_j : \ v_i v_j \in E \} \right\},$$

by Lemma 2.4

$$\leq \max_i \{2e - (n-1)d_n + (d_n - 1)m_i\}, \tag{9}$$

by $d_j m_j \leq 2e - d_j - (n - d_j - 1)d_n$

$$\leq 2e - (n-1)d_n + (d_n - 1)m_{\max}, \tag{10}$$

by $m_i \leq m_{\max}$.

Now suppose that equality in (7) holds. Then all inequalities in the above argument must be equalities. In particular, from equality in (8) and Lemma 2.2 we have that the row sums of $D(G)^{-1}A^2(G)D(G)$ are all equal.

Thus

$$(11)\quad \begin{aligned}\frac{1}{d_1}\sum_j\{d_jm_j : v_1v_j \in E\} &= \frac{1}{d_2}\sum_j\{d_jm_j : v_2v_j \in E\} = \dots \\ &= \frac{1}{d_n}\sum_j\{d_jm_j : v_nv_j \in E\}.\end{aligned}$$

From equality in (9) and using (11), we conclude that all vertices which are not adjacent to vertex v_i are of degree d_n as graph G is connected, for all $v_i \in V$.

From equality in (10), if $d_n > 1$ we have

$$m_{\max} = m_i, \text{ for all } v_i \in V.$$

Two cases arise viz., (i) $d_1 < n-1$,
(ii) $d_1 = n-1$.

Case (i): $d_1 < n-1$. In this case there exists at least one vertex which is not adjacent to the highest degree vertex v_1. Therefore the highest degree d_1 is equal to the lowest degree d_n as all the vertices which are not adjacent to vertex v_i are of degree d_n, for all $v_i \in V$. Hence $d_1 = d_n$ and graph G is regular.

Case (ii): $d_1 = n-1$. In this case graph G has only two type of degrees $n-1$ and d_n as all vertices which are not adjacent to vertex v_i are of degree d_n, for all $v_i \in V$. Two subcases arise viz., (a) $d_n = 1$,
(b) $d_n > 1$.

Subcase (a): $d_n = 1$. We have that the lowest degree vertex v_n of degree one is adjacent to the highest degree vertex v_1. Since all the vertices those are not adjacent to vertex v_n are of degree d_n, all the remaining vertices are of degree one. Hence G is a star graph.

Subcase (b): $d_n > 1$. We have $m_{\max} = m_1 = m_2 = \dots = m_n$. If possible, let $d_n \neq n-1$. Also, let p be the number of vertices of degree $n-1$. From $m_1 = m_n$ we get

$$\frac{2e-(n-1)}{n-1}=\frac{p(n-1)+(d_n-p)d_n}{d_n},$$

$$\text{i.e.,}\quad (n-1-d_n)(2e-(n-1)d_n)=0,\quad \text{as}\ \ 2e=p(n-1)+(n-p)d_n,$$

$$\text{i.e.,}\quad 2e=(n-1)d_n,\quad \text{as}\ \ d_n\neq n-1,$$

$$\text{i.e.,}\quad 2e<nd_n,\quad \text{as}\ \ nd_n>(n-1)d_n,$$

a contradiction. So our assumption is wrong and therefore all the vertices are of degree $n-1$. Hence G is a complete graph.

Conversely, let G be a star graph or G be a regular graph. Therefore we can easily see that the equality holds in (7). □

Corollary 3.2. [6]. *Let G be a simple connected graph with n vertices and e edges. Then*

$$\rho(G)\leq\sqrt{2e-(n-1)d_n+(d_n-1)d_1},\tag{12}$$

where d_1 and d_n are the highest degree and the lowest degree of G. Moreover, the equality holds if and only if G is a star graph or G is a regular graph.

Proof. The result follows by $d_n\geq 1$, $m_{\max}\leq d_1$, and Theorem 3.1. □

Remark. The upper bound obtained by applying (7) is always better than the bounds obtained by applying (4) and (12). But the upper bound given by (7) and (5) are not comparable. For the graph G_2 in Fig.1, the use of (7) and (5) gives $\rho(G_2)\leq 2.549$ and $\rho(G_2)\leq 2.561$, respectively. But for the graph G_4 in Fig. 1, the use of (7) and (5) gives $\rho(G_4)\leq 3.162$ and $\rho(G_4)\leq 3$, respectively.

4. Upper bound on the sum of the spectral radius of a graph and its complement

In this section we give an upper bound of the sum of the spectral radius of a graph and its complement in terms of n, d_1 and d_n only. First we give some known upper bounds of the sum of the spectral radius of a graph and its complement.

1. Nosal [18].
$$\rho(G) + \rho(G^c) \leq \sqrt{2}(n-1).$$
2. Li [14].
$$\rho(G) + \rho(G^c) \leq -1 + \sqrt{1 + 2n(n-1) - 4d_n(n-1-d_1)}.$$
3. Li [14] and Zhou [21].
$$\rho(G) + \rho(G^c) \leq \sqrt{2(n-1)(n-2)}.$$
4. Hong and Shu [10]. Let k be the chromatic number of a graph G and let $\bar{k}$ be the chromatic number of G^c. Then
$$\rho(G) + \rho(G^c) \leq \sqrt{(2 - \frac{1}{t})n(n-1)}$$
$$\text{and} \qquad \rho(G) + \rho(G^c) \leq \sqrt{(2 - \frac{1}{T})(n-1)},$$
where $t = \min\{k, \bar{k}\}$, $T = \max\{k, \bar{k}\}$.

5. Hong and Shu [11]. Let k be the chromatic number of a graph G and let $\bar{k}$ be the chromatic number of G^c. Then
$$\rho(G) + \rho(G^c) \leq \sqrt{(2 - \frac{1}{k} - \frac{1}{\bar{k}})n(n-1)},$$
with equality if and only if G is a complete graph or an empty graph.

Theorem 4.1. *Let G be a graph with n vertices. Also let both G and its complement G^c be connected. Then*
$$\rho(G) + \rho(G^c) \leq \sqrt{2[(n-1)^2 + 2d_1d_n - 2nd_n + 3d_n - d_1]}, \tag{13}$$
where d_1, d_n are respectively the highest degree and the lowest degree of G.

Proof. From Corollary 3.2, we have

$$\rho(G) \leq \sqrt{2e-(n-1)d_n+(d_n-1)d_1}$$

$$\text{and} \qquad \rho(G^c) \leq \sqrt{2e'-(n-1)d'_n+(d'_n-1)d'_1} = \sqrt{n(n-1)-2e-(n-1)(d_n+1)+d_n(d_1+1)},$$

where $2e' = n(n-1)-2e$, $d'_1 = n-1-d_n$ and $d'_n = n-1-d_1$.

Therefore

$$\begin{aligned}\rho(G)+\rho(G^c) &\leq \sqrt{2e-(n-1)d_n+(d_n-1)d_1} \\ &+ \sqrt{n(n-1)-2e-(n-1)(d_n+1)+d_n(d_1+1)}.\end{aligned}$$

Let

$$\begin{aligned}f(e) &= \sqrt{2e-(n-1)d_n+(d_n-1)d_1} \\ &+\sqrt{n(n-1)-2e-(n-1)(d_n+1)+d_n(d_1+1)}.\end{aligned}$$

It is easy to show that

$$f(e) \leq f\left(\frac{(n-1)^2+d_1+d_n}{4}\right) = \sqrt{2[(n-1)^2+2d_1d_n-2nd_n+3d_n-d_1]}.$$

Hence the theorem holds. □ □

5. Upper bounds on the spectral radius of Laplacian matrix

Let $G=(V,E)$. If V is the disjoint union of two nonempty sets V_1 and V_2 such that every vertex v_i in V_1 has the same vertex degree r and every vertex v_j in V_2 has the same vertex degree s, then G will be called a (r, s)-semiregular graph. In this section, we give two new upper bounds on $\lambda(G)$ for simple connected graphs.

Theorem 5.1. *Let G be a simple connected graph. Also, let $d_1 \geq d_2 \geq \ldots \geq d_n$ be the degree sequence of G and $\lambda(G)$ be the spectral radius of $L(G)$. Then*

$$(*) \qquad \lambda(G) \leq \begin{cases} 2+\sqrt{\sum_{i=1}^{n} d_i(d_i-1)|-\left(\frac{1}{2}\sum_{i=1}^{n} d_i-1\right)(2d_n-2)+(2d_n-3)(2d_1-2)}, \\ \qquad\qquad\qquad\qquad \text{if } d_n \geq 2, \\ 2+\sqrt{\sum_{i=1}^{n} d_i(d_i-1)-d_1+1}, \ \text{if } d_n = 1, \end{cases}$$

where the equality holds if and only if G is a regular bipartite graph or G is a star graph, respectively.

Proof. From the fact that G and L_G are connected graphs and Corollary 3.2, we have

$$\rho(L_G) \leq \sqrt{2e' - (n' - d'_1 - 1)d'_{n'} - d'_1}, \tag{14}$$

where $n' = e = \frac{1}{2}\sum_{i=1}^{n} d_i$, $\quad 2e' = \sum_{i=1}^{n} d_i(d_i-1)$, $\quad d_1 + d_n - 2 \leq d'_1 \leq 2d_1 - 2$, $\quad d'_{n'} \geq 2d_n - 2$.

Therefore

$$\begin{aligned} \rho(L_G) &\leq \sqrt{\sum_{i=1}^{n} d_i(d_i-1) - \left(\frac{1}{2}\sum_{i=1}^{n} d_i - d'_1 - 1\right) d'_{n'} - d'_1} \\ &\leq \sqrt{\sum_{i=1}^{n} d_i(d_i-1) - \left(\frac{1}{2}\sum_{i=1}^{n} d_i - d'_1 - 1\right)(2d_n-2) - d'_1}, \qquad (15) \end{aligned}$$

by $d'_{n'} \geq 2d_n - 2$

$$\leq \sqrt{\sum_{i=1}^{n} d_i(d_i-1) - \left(\frac{1}{2}\sum_{i=1}^{n} d_i - 1\right)(2d_n-2) + (2d_n-3)d'_1}. \tag{16}$$

Using $d_1 + d_n - 2 \leq d'_1 \leq 2d_1 - 2$ in (16), we get

$$\rho(L_G) \leq \begin{cases} \sqrt{\sum_{i=1}^{n} d_i(d_i-1) - \left(\frac{1}{2}\sum_{i=1}^{n} d_i-1\right)(2d_n-2) + (2d_n-3)(2d_1-2)}, & \text{if } d_n \geq 2, \\ \sqrt{\sum_{i=1}^{n} d_i(d_i-1) - d_1 + 1}, & \text{if } d_n = 1. \end{cases}$$

Using Lemma 2.3, we prove the first part of the theorem.

Now we suppose that

$$\begin{aligned} \lambda(G) &= 2 + \rho(L_G) \\ &= 2 + \sqrt{\sum_{i=1}^{n} d_i(d_i-1) - \left(\frac{1}{2}\sum_{i=1}^{n} d_i - 1\right)(2d_n-2) + (2d_n-3)(2d_1-2)}. \end{aligned}$$

Then we must have $d_n \geq 2$, $d'_1 = 2d_1 - 2$ and $d'_{n'} = 2d_n - 2$.

By Lemma 2.3 and $\lambda(G) = 2 + \rho(L_G)$, we conclude that G is a connected bipartite graph.

By Corollary 3.2, the equality holds in (14) then L_G is a star graph or L_G is a regular graph. But L_G is not a star graph as $d_n \geq 2$, that is, $d'_{n'} \geq 2$. Thus L_G is a regular graph, that is,

$$\begin{aligned} & d'_1 = d'_{n'}, \\ \text{i.e.,}\quad & 2d_1 - 2 = 2d_n - 2, \\ \text{i.e.,}\quad & d_1 = d_n. \end{aligned}$$

Hence G is a regular bipartite graph.

Next we suppose that

$$\begin{aligned} \lambda(G) &= 2 + \rho(L_G) \\ &= 2 + \sqrt{\sum_{i=1}^{n} d_i(d_i - 1) - d_1 + 1}. \end{aligned}$$

Then we must have $d_n = 1$ and $d'_1 = d_1 + d_n - 2$.

Now we have that G is a connected bipartite graph and either L_G is a star graph or L_G is a regular graph. If L_G is a star graph then using $d'_1 = d_1 - 1$, we get that G is a path P_3.

If L_G is a regular graph then G must be a connected semiregular graph as G is connected bipartite graph. Since $d_n = 1$, hence G is a star graph.

Conversely, it is easy to verify that equality in Theorem 5.1 holds for a regular bipartite graph or a star graph, respectively. □

Let $K(G) = D(G) + A(G)$. If G is a connected graph then $K(G)$ is a non-negative, symmetric and irreducible matrix. Let $\mu(G)$ be the largest eigenvalue of $K(G)$. Using Lemma 2.1 we have that all the eigencomponents of an eigenvector corresponding to the eigenvalue $\mu(G)$ of $K(G)$ are of the same sign (non-zero) if G is a connected graph. We can assume that all the eigencomponents are positive.

Lemma 5.2. [19] *Let $G = (V, E)$ be a connected graph with n vertices. Then $\lambda(G) \le \mu(G)$ with equality if and only if G is a bipartite graph.*

Lemma 5.3. [5] *Let G be a graph with n vertices, e edges. Then*

$$d_i + m_i \leq \frac{2e}{n-1} + \frac{n-2}{n-1}d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right), \tag{17}$$

holds for any non-isolated vertex v_i, where d_1 and d_n are the highest and the lowest degree of the graph G. Moreover, the equality holds in (17) if and only if $d_i = n-1$ or vertex v_i (degree is d_1) is adjacent to all vertices with degree d_1 and not adjacent to any vertex of degree d_n.

Now we give a new upper bound for $\lambda(G)$ in the following Theorem 5.4 and determine its extremal graphs.

Theorem 5.4. *Let G be a simple connected graph with n vertices and e edges. Also let d_1, d_n be respectively the highest degree and the lowest degree of G and let $\lambda(G)$ be the spectral radius of $L(G)$. Then*

$$\lambda(G) \leq \frac{d_1 + \sqrt{d_1^2 + 4\left[\frac{2e}{n-1} + \frac{n-2}{n-1}d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right)\right] m_{max}}}{2}, \tag{18}$$

where $m_{\max}$ is the maximum of $m_i's$, m_i is the average of the degrees of the vertices adjacent to v_i. Moreover, the equality in (18) holds if and only if G is a regular bipartite graph.

Proof. If G is a path P_2 then the equality holds in (18). Now we have to show that Theorem 5.4 is true for $n > 2$. Let $\mathbf{X}=(x_1, x_2, \ldots, x_n)^T$ be an eigenvector corresponding to the eigenvalue $\mu(G)$ of $D(G)^{-1}K(G)D(G)$. We can assume that one eigencomponent x_i is equal to 1 and the other eigencomponents are less than or equal to 1, that is, $x_i = 1$ and $0 < x_k \leq 1$, for all k.

Now the (i,j)-th element of $D(G)^{-1}K(G)D(G)$ is

$$\begin{cases} d_i & \text{if } v_i = v_j, \\ \dfrac{d_j}{d_i} & \text{if } v_iv_j \in E, \\ 0 & \text{otherwise.} \end{cases}$$

We have

$$\{D(G)^{-1}K(G)D(G)\}\mathbf{X} = \mu(G)\mathbf{X}. \tag{19}$$

From the i-th equation of (19),

$$\begin{aligned} \mu(G)x_i &= d_ix_i + \sum_j \left\{ \frac{d_jx_j}{d_i} : \ v_iv_j \in E \right\}, \\ \text{i.e., } \mu(G) &= d_i + \sum_j \left\{ \frac{d_jx_j}{d_i} : \ v_iv_j \in E \right\}. \end{aligned} \tag{20}$$

From the j-th equation of (19),

$$\mu(G)x_j = d_jx_j + \sum_k \left\{ \frac{d_kx_k}{d_j} : \ v_jv_k \in E \right\}. \tag{21}$$

Multiplying both sides of (20) by $\mu(G)$ and substituting this value $\mu(G)x_j$, we get

$$\begin{aligned}
\mu^2(G) &= d_i\mu(G) + \sum_j \left\{ \frac{d_j}{d_i} \left[d_j x_j + \sum_k \left\{ \frac{d_k x_k}{d_j} : v_j v_k \in E \right\} \right] : v_i v_j \in E \right\} \\
&= d_i\mu(G) + \sum_j \left\{ \frac{d_j^2 x_j}{d_i} : v_i v_j \in E \right\} \\
&\quad + \sum_j \left\{ \frac{1}{d_i} \sum_k \{ d_k x_k : v_j v_k \in E \} : v_i v_j \in E \right\} \\
&\leq d_i\mu(G) + \sum_j \left\{ \frac{d_j^2}{d_i} : v_i v_j \in E \right\} + \sum_j \left\{ \frac{d_j m_j}{d_i} : v_i v_j \in E \right\} \qquad (22) \\
&= d_i\mu(G) + \sum_j \left\{ \frac{d_j(d_j + m_j)}{d_i} : v_i v_j \in E \right\}.
\end{aligned}$$

Using (17),

$$\begin{aligned}
\mu^2(G) &\leq d_i\mu(G) + \left[\frac{2e}{n-1} + \frac{n-2}{n-1} d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right) \right] m_i \qquad (23) \\
&\leq d_1\mu(G) + \left[\frac{2e}{n-1} + \frac{n-2}{n-1} d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right) \right] m_{max}, \qquad (24) \\
\text{i.e., } \mu(G) &\leq \frac{d_1 + \sqrt{d_1^2 + 4\left[\frac{2e}{n-1} + \frac{n-2}{n-1} d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right) \right] m_{max}}}{2}.
\end{aligned}$$

Using Lemma 5.2 we get the required result (18).

Now suppose that equality in (18) holds. Then all inequalities in the above argument must be equalities. First we have $\lambda(G) = \mu(G)$. It follows from Lemma 5.2 that G is bipartite.

Since G is a bipartite graph, we can make a partition $V = U \cup W$ in such a way that U contains vertex v_i and each edges of G connected to the vertices, one contained in U and another contained in W. Hence graph G is connected and $n > 2$, $d_1 \geq 2$.

From equality in (22), we get $d_i = d_1$. We have $|W| \geq 2$, as $d_i = d_1 \geq 2$. So, $d_j \neq n-1$, $v_iv_j \in E$.

From equality in (23) and using Lemma 5.3, we conclude that either $d_j = n-1$ or all the vertices v_k adjacent to v_j (degree is d_1), are of degree d_1 and not adjacent to v_j are of degree d_n, where $v_iv_j \in E$. Using this result we conclude that all the vertices in W are of degree d_n as $d_j \neq n-1$ and $|W| \geq 2$.

From equality in (24), we get $m_i = m_{\max}$. Since all the vertices in W are of degree d_n, we get

$$m_{\max} = m_i = d_n,$$

which implies that all the vertices are of degree d_n. Hence G is a regular bipartite graph.

From equality in (22) we have that

$$x_j = 1 \text{ for all } j \text{ such that } v_iv_j \in E \text{ and } x_k = 1 \text{ for all } k \text{ such that } v_jv_k \in E.$$

Also it holds for regular bipartite graph.

Conversely, let G be a regular bipartite graph. Therefore we can see easily that the equality holds in (18). □

Corollary 5.5. *Let G be a simple connected graph with n vertices and e edges. Also let d_1, d_n be respectively the highest degree and the lowest degree of G and let $\lambda(G)$ be the spectral radius of $L(G)$. Then*

$$\lambda(G) \leq \frac{d_1 + \sqrt{d_1^2 + 4\left[\frac{2e}{n-1} + \frac{n-2}{n-1}d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right)\right]d_1}}{2}, \tag{25}$$

with equality if and only if G is a regular bipartite graph.

Lemma 5.6. [19] *Let G be a simple connected graph. Then*

$$\lambda(G) \leq \max\{d_i + m_i :\ 1 \leq i \leq n\},$$

with equality if and only if G is a regular bipartite graph or G is a semiregular bipartite graph.

Using Lemma 5.3 and Lemma 5.6, we get the following upper bound for $\lambda(G)$ on n, e, d_1 and d_n only.

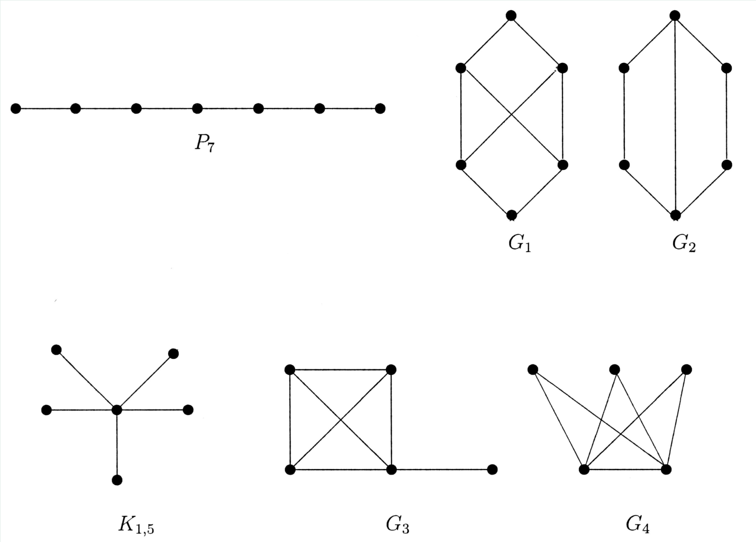

Figure 1.

Theorem 5.7. *Let G be a simple connected graph with n vertices and e edges. Then*

$$\lambda(G) \leq \frac{2e}{n-1} + \frac{n-2}{n-1}d_1 + (d_1 - d_n)\left(1 - \frac{d_1}{n-1}\right), \tag{26}$$

with equality if and only if G is a star graph or G is a regular bipartite graph.

Remark. The three bounds (∗), (18) and (26) are incomparable. Moreover, there is no comparability between any one of them and any one of the upper bounds (1) and (2). Also, we can construct a graph for which any one of the bound is better than any one of the other bounds. It is interesting that all the upper bounds are equal to $2(n-1)$ for a complete graph of order n. Let us consider five graphs P_7, $K_{1,5}$, G_1, G_2 and G_3 shown in Figure 1. Values of $\lambda(G)$ and the various bounds for the five graphs illustrated in Figure 1 are given (to two decimal places) in Fig. 2.

	$\lambda(G)$	(1)	(2)	(∗)	(18)	(25)	(26)
P_7	3.80	4.47	4.70	5.00	4.11	4.11	4.33
$K_{1,5}$	6.00	7.74	6.00	6.00	8.52	8.52	6.00
G_1	5.56	6.00	6.27	6.24	6.00	6.00	6.00
G_2	5.00	5.66	5.37	5.46	5.53	5.86	5.60
G_3	5.00	7.21	7.00	7.20	7.48	7.48	6.50

Figure 2.

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