On Laplacian Eigenvalues of a Graph

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Let G be a connected graph with n vertices and m edges. The Laplacian eigenvalues are denoted by $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G) > \mu_n(G) = 0$. The Laplacian eigenvalues have important applications in theoretical chemistry. We present upper bounds for $\mu_1(G) + \cdots + \mu_k(G)$ and lower bounds for $\mu_{n-1}(G) + \cdots + \mu_{n-k}(G)$ in terms of n and m, where $1 \leq k \leq n-2$, and characterize the extremal cases. We also discuss a type of upper bounds for $\mu_1(G)$ in terms of degree and 2-degree.

Key words: Laplacian Eigenvalue; Line Graph; Bipartite Graph.

1. Introduction

Let $G = (V, E)$ be a simple finite, undirected graph with a vertex set V and an edge set E. For $u \in V$, the degree of u is denoted by $d_u(G)$ (or d_u). Let $A(G)$ be the $(0,1)$ adjacency matrix of G and $D(G)$ the diagonal matrix of vertex degrees. It turns out that the Laplacian matrix of G is $L(G) = D(G) - A(G)$, and $L(G)$ is positive semidefinite and singular. A Laplacian eigenvalue of G is an eigenvalue of $L(G)$. Denote the Laplacian eigenvalues of G by $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G) \geq \mu_n(G) = 0$. It is well known that $\mu_{n-1}(G) > 0$ if and only if G is connected. In the following we also write μ_i for $\mu_i(G)$ when G is given.

Laplacian eigenvalues play a significant role in theoretical chemistry. For example, the Wiener topological index W of alkanes can be express as $W = n\sum_{i=1}^{n-1} 1/\mu_i$, while within the Heilbronner model, the ionization potentials of alkanes are expressed as $\alpha + (\mu_i - \beta)$, $i = 1, 2, \ldots$, where α and β are pertinently chosen semiempirical constants [1]. In this article, we present upper bounds of the sum $\mu_1 + \cdots + \mu_k$ and lower bounds for the sum $\mu_{n-1} + \cdots + \mu_{n-k}$ in terms of n and m with $1 \leq k \leq n-2$, and discuss a type of upper bounds of μ_1.

2. Sums of Laplacian Eigenvalues

For $1 \leq k \leq n-2$, let $M_k(G) = \mu_1(G) + \cdots + \mu_k(G)$ and $N_k(G) = \mu_{n-1}(G) + \cdots + \mu_{n-k}(G)$. In this section we are interested in finding upper bounds of $M_k(G)$ and lower bounds of $N_k(G)$ in terms of n and m.

Lemma 1 [2]: *Let $G = (V, E)$ be a graph with n vertices and m edges. Then*

$$\sum_{u \in V} d_u^2 \leq m\left(\frac{2m}{n-1} + n - 2\right).$$

Moreover, if G is connected, then equality holds if and only if G is either a star $K_{1,n-1}$ or a complete graph K_n.

Theorem 1: *Let G be a connected graph with n vertices and m edges. Then for $1 \leq k \leq n-2$*

$$M_k(G) \leq \frac{2mk + \sqrt{mk(n-k-1)(n^2-n-2m)}}{n-1}, \quad (1)$$

and equality holds if and only if G is either a star $K_{1,n-1}$ or a complete graph K_n when $k = 1$, and G is a complete graph K_n when $2 \leq k \leq n-2$.

Proof: Let $M_k = M_k(G)$. Clearly

$$\mu_1 + \mu_2 + \cdots + \mu_{n-1} = \sum_{u \in V} d_u = 2m,$$

$$\mu_1^2 + \mu_2^2 + \cdots + \mu_{n-1}^2 = \sum_{u \in V}(d_u^2 + d_u) = 2m + \sum_{u \in V} d_u^2.$$

Then, by the Cauchy-Schwarz inequality, we have

$$\begin{aligned}(2m - M_k)^2 &= (\mu_{k+1} + \cdots + \mu_{n-1})^2 \\ &\leq (n-k-1)\left(\mu_{k+1}^2 + \cdots + \mu_{n-1}^2\right) \\ &= (n-k-1)\Big(2m + \sum_{u \in V} d_u^2 - (\mu_1^2 + \cdots + \mu_k^2)\Big) \\ &\leq (n-k-1)\Big(2m + \sum_{u \in V} d_u^2 - \frac{1}{k}M_k^2\Big).\end{aligned}$$

It follows that

$$M_k \leq \Big\{2mk + \Big[k(n-k-1)\big((n-1)(2m+\sum_{u\in V} d_u^2) - 4m^2\big)\Big]^{1/2}\Big\}\Big/(n-1).$$

By Lemma 1, (1) follows from the above inequality.

Now suppose the equality in (1) holds. Then, from the above proof, we have $\mu_1 = \cdots = \mu_k$ and $\mu_{k+1} = \cdots = \mu_{n-1}$ by the Cauchy-Schwarz inequality and G is either a star $K_{1,n-1}$ or a complete graph K_n by Lemma 1. Note that $\mu_1(K_{1,n-1}) = n$, $\mu_2(K_{1,n-1}) = \cdots = \mu_{n-1}(K_{1,n-1}) = 1$ and $\mu_1(K_n) = \cdots = \mu_{n-1}(K_n) = n$. Hence if $k = 1$, then G is either a star $K_{1,n-1}$ or a complete graph K_n, and if $2 \leq k \leq n-2$, then G is a complete graph K_n.

Conversely, it is easy to see that equality in (1) holds if G is a star $K_{1,n-1}$ or a complete graph K_n when $k = 1$, and G is a complete graph K_n when $2 \leq k \leq n-2$. □

Similar arguments lead to the following:

Theorem 2: *Let G be a connected graph with n vertices and m edges, $m > \frac{n-k-1}{n+k-1}\binom{n}{2}$ and $1 \leq k \leq n-2$. Then*

$$N_k(G) \geq \frac{2mk - \sqrt{mk(n-k-1)(n^2-n-2m)}}{n-1}, \quad (2)$$

and equality holds if and only if G is either a star $K_{1,n-1}$ or a complete graph K_n when $k = n-2$, and G is a complete graph K_n when $1 \leq k \leq n-3$.

Remark 1: Both

$$M_k(G) \leq \Big\{2mk + \Big[k(n-k-1)\big((n-1)(2m+\sum_{u\in V} d_u^2) -4m^2\big)\Big]^{1/2}\Big\}\Big/(n-1) \quad (3)$$

and

$$N_k(G) \geq \Big\{2mk - \Big[k(n-k-1)\big((n-1)(2m+\sum_{u\in V} d_u^2) -4m^2\big)\Big]^{1/2}\Big\}\Big/(n-1) \quad (4)$$

have been obtained in [3], Theorem 14. From the proof in Theorem 1 it is easy to see that the equality in (3) holds if and only if $\mu_1(G) = \cdots = \mu_k(G)$ and $\mu_{k+1}(G) = \cdots = \mu_{n-1}(G)$, while the equality holds in (4) holds if and only if $\mu_1(G) = \cdots = \mu_{n-k-1}(G)$ and $\mu_{n-k}(G) = \cdots = \mu_{n-1}(G)$.

Remark 2: Let G be a connected graph with n vertices and m edges, $1 \leq k \leq n-2$. By Theorem 1

$$\mu_1(G) \leq \frac{2m + \sqrt{m(n-2)(n^2-n-2m)}}{n-1},$$

and equality holds if and only if G is either a star $K_{1,n-1}$ or a complete graph K_n (which has been obtained in [2]). By Theorem 2, if $m > (n-1)(n-2)/2$,

$$\mu_{n-1}(G) \geq \frac{2m - \sqrt{m(n-2)(n^2-n-2m)}}{n-1},$$

and equality holds if and only if G is a complete graph K_n.

Remark 3: Since the upper bounds for the first Zagreb-Group index or Gutman index, $\sum_{u\in V} d_u^2$ in Lemma 1 can be sharpened [4], we can get better upper bounds for $M_k(G)$ and lower bounds for $N_k(G)$ by (3) and (4).

Now we consider a bipartite graph.

Lemma 2: *Let $G = (V,E)$ be a connected bipartite graph with n vertices and m edges. Then*

$$\sum_{u\in V} d_u^2 \leq mn,$$

and the equality holds if and only if G is a complete bipartite graph.

Proof: For any edge vw of G, $d_v + d_w \leq n$. Then $\sum_{u\in V} d_u^2 = \sum_{vw\in E}(d_v+d_w) \leq mn$. The equality holds if and only if $d_v + d_w = n$ for any edge vw of G, i. e., G is a complete bipartite graph. □

Theorem 3: *Let G be a connected bipartite graph with n vertices and m edges, $1 \leq k \leq n-2$. Then*

$$M_k(G) \leq \frac{2mk + \sqrt{mk(n-k-1)(n^2+n-2-4m)}}{n-1}, \quad (5)$$

and equality holds if and only if $k = 1$ and G is either a $K_{1,n-1}$ or a $K_{n/2,n/2}$.

Proof: By (3) and Lemma 2, (5) follows.

Suppose equality in (5) holds. Then $d_1^2 + d_2^2 + \cdots + d_n^2 = mn$ and hence, by Lemma 2, G is a complete bipartite graph, say $K_{r,n-r}$ with $1 \leq r \leq \lfloor n/2 \rfloor$. It is easy to see that $\mu_1 = n, \mu_2 = \cdots = \mu_r = n-r$, $\mu_{r+1} = \cdots = \mu_{n-1} = r$ and $\mu_n = 0$. By Remark 1, $\mu_1 = \cdots = \mu_k$ and $\mu_{k+1} = \cdots = \mu_{n-1}$. We have either $k = 1$ and $r = 1$ or

$k = 1$ and $r = n - r$ ($r \geq 2$). Hence $k = 1$ and G is either a $K_{1,n-1}$ or a $K_{n/2,n/2}$.

Conversely, if $k = 1$ and G is either a $K_{1,n-1}$ or a $K_{n/2,n/2}$, then clearly equality in (5) holds. □

Similar arguments lead to

Theorem 4: *Let G be a connected bipartite graph with n vertices and m edges, $m > \frac{(n-k-1)(n+2)}{4}$ and $1 \leq k \leq n-2$. Then*

$$N_k(G) > \frac{2mk - \sqrt{mk(n-k-1)(n^2+n-2-4m)}}{n-1}. \tag{6}$$

Remark 4: Let G be a connected bipartite graph with n vertices and m edges. By Theorem 3

$$\mu_1(G) \leq \frac{2m + \sqrt{m(n-2)(n^2+n-2-4m)}}{n-1},$$

and equality holds if and only if G is either a $K_{1,n-1}$ or a $K_{n/2,n/2}$.

3. A Type of Upper Bound for $\mu_1(G)$ in Terms of Degree and 2-degree

The 2-degree [5] of a vertex u in a graph G, denoted by $t_u(G)$ (or t_u), is the sum of degrees of vertices adjacent to u. For u, v in a graph G, $u \sim v$ means u and v are adjacent in G. Let L_G be the line graph of a graph G. An eigenvalue of G is an eigenvalue of $A(G)$. The spectral radius $\rho(G)$ of G is the largest eigenvalue of G.

Among the known upper bounds of $\mu_1(G)$ in terms of degree and 2-degree are the following:

1. Merris's bound [5]:

$$\mu_1(G) \leq \max\left\{\frac{d_u^2 + t_u}{d_u} : u \in V\right\}. \tag{7}$$

2. Li and Zhang's bound [6]:

$$\mu_1(G) \leq \max\left\{\frac{(d_u^2 + t_u) + (d_v^2 + t_v)}{d_u + d_v} : uv \in E\right\}. \tag{8}$$

When G is connected, it is known [7] that equality in (7) or (8) holds if and only if G is a semiregular bipartite graph.

Lemma 3 [8]: *Let G be a connected graph with an adjacency matrix A. Let P be any polynomial and $S_u(P(A))$ the row sum of $P(A)$ corresponding to vertex $u \in V$. Then $P(\rho(A)) \leq \max\{S_u(p(A)) : u \in V\}$, equality holds if and only if the row sums of $P(A)$ are all equal.*

Lemma 4 [9]: *Let G be a connected graph. Then $\mu_1(G) \leq 2 + \rho(L_G)$, and equality holds if and if G is a bipartite graph.*

Theorem 5: *Let $G = (V,E)$ be a connected graph. Then*

$$\mu_1(G) \leq \min\{2 + \sqrt{D_1}, \sqrt{D_2}\}, \tag{9}$$

where $D_1 = \max\{d_u^2 + d_v^2 + t_u + t_v - 4(d_u + d_v) + 4 : uv \in E\}$ and $D_2 = \max\{d_u^2 + d_v^2 + t_u + t_v : uv \in E\}$.

Proof: Let A and A_L be the adjacency matrices of G and L_G. It is easy to see that $S_v(A) = d_w$ and $S_w(A^2) = t_w$ for any $w \in V$. For any $e = uv \in E$

$$\begin{aligned} S_e(A_L^2) &= t_e(L_G) = \sum_{f \sim e} d_f(L_G) \\ &= \sum_{\substack{x \sim u \\ x \neq v}} (d_x + d_u - 2) + \sum_{\substack{x \sim v \\ x \neq u}} (d_x + d_v - 2) \\ &= (d_u - 2)(d_u - 1) + \sum_{x \sim u} d_x - d_v \\ &\quad + (d_v - 2)(d_v - 1) + \sum_{x \sim v} d_x - d_u \\ &= d_u^2 + d_v^2 - 4(d_u + d_v) + t_u + t_v + 4. \end{aligned}$$

By Lemma 3,

$$\rho^2(L_G) \leq \max\{d_u^2 + d_v^2 - 4(d_u + d_v) + t_u + t_v + 4 : uv \in E\},$$

and hence by Lemma 4,

$$\mu_1(G) \leq 2 + \rho(L_G) \leq 2 + \sqrt{D_1}.$$

On the other hand, note that $S_e(A_L) = d_e(L_G) = d_u + d_v - 2$. We have

$$S_e(A_L^2 + 4A_L + 4I) = d_u^2 + d_v^2 + t_u + t_v.$$

By Lemma 3,

$$\rho^2(L_G) + 4\rho(L_G) + 4 \leq \max\{d_u^2 + d_v^2 + t_u + t_v : uv \in E\},$$

and hence by Lemma 4,

$$\mu_1(G) \leq 2 + \rho(L_G) \leq \sqrt{D_2}.$$

Thus we have proved that

$$\mu_1(G) \leq \min\{2 + \sqrt{D_1}, \sqrt{D_2}\}.$$

Remark 5: The inequality $\mu_1(G) \leq \sqrt{D_2}$ has been obtained in [10], and it implies that $\mu_1(G) \leq \max\{\sqrt{2d_u + 2t_u} : u \in V\}$, which has also appeared in [2]. From the above argument and by Lemmas 3 and 4, we see that $\mu_1(G) = 2 + \sqrt{D_1}$ if and only if G is a bipartite graph such that each vertex in the same part of bipartition has the same value $d_u^2 + t_u - 4d_u$, while $\mu_1(G) = \sqrt{D_2}$ if and only if G is a bipartite graph such that each vertex in the same part of bipartition has the same value $d_u^2 + t_u$. If G is a semiregular bipartite graph, then $\mu_1(G) = 2 + \sqrt{D_1} = \sqrt{D_2}$, where a graph G is semiregular bipartite means it is bipartite and each vertex in the same part of bipartition has the same degree. Note also that $\mu_1(P_4) = 2 + \sqrt{D_1} = 2 + \sqrt{2}$.

Example: Let H be the graph obtained by adding two non-adjacent edges to a $K_{1,5}$. For P_5 and H, the actual values of μ_1 and the bounds (7), (8), $2 + \sqrt{D_1}$ and $\sqrt{D_2}$ give the following results (rounded to three decimal places):

	μ_1	(7)	(8)	$2+\sqrt{D_1}$	$\sqrt{D_2}$
P_4	3.414	3.500	3.500	3.414	3.742
H	6.000	6.800	6.667	6.583	6.708

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