MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 611-619

ISSN 0340 - 6253

ON SUM OF POWERS OF LAPLACIAN EIGENVALUES AND LAPLACIAN ESTRADA INDEX OF GRAPHS

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(Received June 30, 2008)

Abstract

Let G be a simple graph and α a real number. The quantity $s_\alpha(G)$ defined as the sum of the α-th power of the non-zero Laplacian eigenvalues of G generalizes several concepts in the literature. The Laplacian Estrada index is a newly introduced graph invariant based on Laplacian eigenvalues. We establish bounds for s_α and Laplacian Estrada index related to the degree sequences.

1. INTRODUCTION

Let G be a simple graph possessing n vertices. The Laplacian spectrum of G, consisting of the numbers $\mu_1, \mu_2, \ldots, \mu_n$ (arranged in non-increasing order), is the spectrum of the Laplacian matrix of G. It is known that $\mu_n = 0$ and the multiplicity of 0 is equal to the number of connected components of G. See [1, 2] for more details for the properties of the Laplacian spectrum.

Let α be a real number and let G be a graph with n vertices. Let $s_\alpha(G)$ be the sum of the α-th power of the non-zero Laplacian eigenvalues of G, i.e.,

$$s_\alpha(G) = \sum_{i=1}^{h} \mu_i^\alpha,$$

where h is the number of non-zero Laplacian eigenvalues of G. The cases $\alpha = 0, 1$ are trivial as $s_0(G) = h$ and $s_1(G) = 2m$, where m is the number of edges of G. For a nonnegative integer k, $t_k(G) = \sum_{i=1}^{n} \mu_i^k$ is the k-th Laplacian spectral moment of G. Obviously, $t_0(G) = n$ and $t_k(G) = s_k(G)$ for $k \geq 1$. Properties of s_2 and $s_{\frac{1}{2}}$ were studied respectively in [3] and [4]. For a connected graph G with n vertices, $ns_{-1}(G)$ is equal to its Kirchhoff index, denoted by $Kf(G)$, which found applications in electric circuit, probabilistic theory and chemistry [5, 6]. Some properties of s_α for $\alpha \neq 0, 1$, including further properties of s_2 and $s_{\frac{1}{2}}$ have been established recently in [7]. Now we give further properties of s_α, that is, bounds related to the degree sequences of the graphs. As a by-product, a lower bound for the Kirchhoff index is given.

Note that lots of spectral indices were proposed in [8] recently, and since the Laplacian eigenvalues are all nonnegative, for $\alpha \neq 0$, s_α is equal to the spectral index $SpSum^\alpha(L)$ with L being the Laplacian matrix of the graph.

The Estrada index of a graph G with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. It is a very useful descriptors in a large variety of problems, including those in biochemistry and in complex networks [9–11], for recent results see [12–14]. The Laplacian Estrada index of a graph G with n vertices is defined as [15]

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

We also give bounds for the Laplacian Estrada index related to the degree sequences of the graphs.

2. PRELIMINARIES

For two non-increasing sequences $x = (x_1, x_2, \ldots, x_n)$ and $y = (y_1, y_2, \ldots, y_n)$, x is majorized by y, denoted by $x \preceq y$, if

$$\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i \text{ for } j = 1, 2, \ldots, n-1, \text{ and}$$
$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.$$

For a real-valued function f defined on a set in $\mathbb{R}^n$, if $f(x) < f(y)$ whenever $x \preceq y$ but $x \neq y$, then f is said to be strictly Schur-convex [16].

Lemma 1. *Let α be a real number with $\alpha \neq 0, 1$.*

(i) For $x_i \geq 0$, $i = 1, 2, \ldots, h$, $f(x) = \sum_{i=1}^{h} x_i^\alpha$ is strictly Schur-convex if $\alpha > 1$, and $f(x) = -\sum_{i=1}^{h} x_i^\alpha$ is strictly Schur-convex if $0 < \alpha < 1$.

(ii) For $x_i > 0$, $i = 1, 2, \ldots, h$, $f(x) = \sum_{i=1}^{h} x_i^\alpha$ is strictly Schur-convex if $\alpha < 0$.

Proof. From [16, p. 64, C.1.a] we know that if the real-valued function g defined on an interval in $\mathbb{R}$ is a strictly convex then $\sum_{i=1}^{h} g(x_i)$ is strictly Schur-convex.

If $x_i \geq 0$, then x_i^α is strictly convex if $\alpha > 1$ and $-x_i^\alpha$ is strictly convex if $0 < \alpha < 1$, and thus (i) follows.

If $x_i > 0$ and $\alpha < 0$, then x_i^α is strictly convex, and thus (ii) follows. $\square$

Let K_n and S_n be respectively the complete graphs and the star with n vertices. Let $K_n - e$ be the graph with one edge deleted from K_n.

Recall the the degree sequence of a graph G is a list of the degrees of the vertices in non-increasing order, denoted by $(d_1, d_2, \ldots, d_n)$, where n is the number of vertices of G. Then d_1 is the maximum vertex degree of G.

3. BOUNDS FOR s_α RELATED TO DEGREE SEQUENCES

We need the following lemmas.

Lemma 2. [17] *Let G be a connected graph with $n \geq 2$ vertices. Then $(d_1 + 1, d_2, \ldots, d_{n-1}, d_n - 1) \preceq (\mu_1, \mu_2, \ldots, \mu_n)$.*

Lemma 3. [7] *Let G be a connected graph with $n \geq 2$ vertices. Then $\mu_2 = \cdots = \mu_{n-1}$ and $\mu_1 = 1 + d_1$ if and only if $G = K_n$ or $G = S_n$.*

Now we provide bounds for s_α using degree sequences.

Proposition 1. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$s_\alpha(G) \geq (d_1 + 1)^\alpha + \sum_{i=2}^{n-1} d_i^\alpha + (d_n - 1)^\alpha \ if \ \alpha > 1$$

$$s_\alpha(G) \leq (d_1 + 1)^\alpha + \sum_{i=2}^{n-1} d_i^\alpha + (d_n - 1)^\alpha \ if \ 0 < \alpha < 1$$

with either equality if and only if $G = S_n$.

Proof. If $\alpha > 1$, then by Lemma 1 (i), $f(x) = \sum_{i=1}^{n} x_i^{\alpha}$ is strictly Schur-convex, which, together with Lemma 2, implies that

$$s_\alpha(G) = \sum_{i=1}^{n} \mu_i^\alpha \geq (d_1+1)^\alpha + \sum_{i=2}^{n-1} d_i^\alpha + (d_n-1)^\alpha$$

with equality if and only if $(\mu_1, \mu_2, \ldots, \mu_n) = (d_1+1, d_2, \ldots, d_{n-1}, d_n-1)$.

If $0 < \alpha < 1$, then by Lemma 1 (i), $f(x) = -\sum_{i=1}^{h} x_i^{\alpha}$ is strictly Schur-convex, which, together with Lemma 2, implies that

$$-s_\alpha(G) = -\sum_{i=1}^{n} \mu_i^\alpha \geq -\left[(d_1+1)^\alpha + \sum_{i=2}^{n-1} d_i^\alpha + (d_n-1)^\alpha\right],$$

i.e.,

$$s_\alpha(G) = \sum_{i=1}^{n} \mu_i^\alpha \leq (d_1+1)^\alpha + \sum_{i=2}^{n-1} d_i^\alpha + (d_n-1)^\alpha$$

with equality if and only if $(\mu_1, \mu_2, \ldots, \mu_n) = (d_1+1, d_2, \ldots, d_{n-1}, d_n-1)$.

By Lemma 3, we have $(\mu_1, \mu_2, \ldots, \mu_n) = (d_1+1, d_2, \ldots, d_{n-1}, d_n-1)$ if and only if $G = S_n$. □

We note that the result for $\alpha = \frac{1}{2}$ has been given in [4].

Proposition 2. *Let G be a connected graph with $n \geq 3$ vertices. If $\alpha < 0$, then*

$$s_\alpha(G) \geq (d_1+1)^\alpha + \sum_{i=2}^{n-2} d_i^\alpha + (d_{n-1}+d_n-1)^\alpha$$

with equality if and only if $G = S_n$ or $G = K_3$.

Proof. By Lemma 1 (ii), $f(x) = \sum_{i=1}^{n-1} x_i^{\alpha}$ is strictly Schur-convex for $x_i > 0$, $i = 1, 2, \ldots, n-1$. By Lemma 2, $(d_1+1, d_2, \ldots, d_{n-2}, d_{n-1}+d_n-1) \preceq (\mu_1, \mu_2, \ldots, \mu_{n-1})$. Thus

$$s_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha \geq (d_1+1)^\alpha + \sum_{i=2}^{n-2} d_i^\alpha + (d_{n-1}+d_n-1)^\alpha$$

with equality if and only if $(\mu_1, \mu_2, \ldots, \mu_{n-1}) = (d_1+1, d_2, \ldots, d_{n-2}, d_{n-1}+d_n-1)$, which, by Lemma 3, is equivalent to $G = S_n$ or $G = K_3$. □

Let G be a connected graph with $n \geq 3$ vertices. Then by Proposition 2,

$$Kf(G) \geq n\left(\frac{1}{d_1+1} + \sum_{i=2}^{n-2} \frac{1}{d_i} + \frac{1}{d_{n-1}+d_n-1}\right)$$

with equality if and only if $G = S_n$ or $G = K_3$. Note that we have already shown in [18] that

$$Kf(G) \geq -1 + (n-1)\sum_{i=1}^{n} \frac{1}{d_i}.$$

These two lower bounds are incomparable as for K_n with $n \geq 4$ the latter is better but for $K_n - e$ with $n \geq 7$ the former is better.

Remark 1. For the degree sequence $(d_1, d_2, \ldots, d_n)$ of a graph, its conjugate sequence is $(d_1^*, d_2^*, \ldots, d_n^*)$, where d_i^* is equal to the cardinality of the set $\{j : d_j \geq i\}$. Note that $(d_1, d_2, \ldots, d_n) \preceq (d_1^*, d_2^*, \ldots, d_n^*)$ [1, 19]. It was conjectured in [19] that

$$(\mu_1, \mu_2, \ldots, \mu_n) \preceq (d_1^*, d_2^*, \ldots, d_n^*).$$

Though still open, it has been proven to be true for a class of graphs including trees [20]. Let G be a tree with $n \geq 2$ vertices. Then $d_1^* = n$, $d_{d_1+1}^* = 0$, and by similar arguments as in the proof of Proposition 1, we have

$$s_\alpha(G) \leq \sum_{i=1}^{d_1} (d_i^*)^\alpha \ \text{ if } \alpha > 1 \text{ or } \alpha < 0$$
$$s_\alpha(G) \geq \sum_{i=1}^{d_1} (d_i^*)^\alpha \ \text{ if } 0 < \alpha < 1$$

with either equality if and only if $(\mu_1, \mu_2, \ldots, \mu_n) = (d_1^*, d_2^*, \ldots, d_n^*)$, which, is equivalent to $G = S_n$ since if $G \neq S_n$, then $d_{n-1}^* = 0$ but $\mu_{n-1} > 0$.

To end this section, we mention a result of Rodriguez and Petingi concerning the Laplacian spectral moments in [21]:

Proposition 3. *For a graph G with n vertices and any positive integer k, we have*

$$s_k(G) \geq \sum_{i=1}^{n} d_i(1 + d_i)^{k-1}$$

and for $k \geq 3$, equality occurs if and only if G is a vertex–disjoint union of complete subgraphs.

4. BOUNDS FOR LAPLACIAN ESTRADA INDEX RELATED TO DEGREE SEQUENCES

Let G be a graph with n vertices. Obviously,

$$LEE(G) = \sum_{k \geq 0} \frac{t_k(G)}{k!} = n + \sum_{k \geq 1} \frac{s_k(G)}{k!}.$$

Thus, properties of the Laplacian moments in previous section may be converted into properties of the Laplacian Estrada index.

Proposition 4. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$LEE(G) \geq e^{d_1+1} + \sum_{i=2}^{n-1} e^{d_i} + e^{d_n-1}$$

with equality if and only if $G = S_n$.

Proof. Note that $t_0(G) = n$, $t_1(G) = \sum_{i=1}^{n} d_i$, and $t_k(G) = s_k(G)$ for $k \geq 1$. By Proposition 1,

$$t_k(G) \geq (d_1+1)^k + \sum_{i=2}^{n-1} d_i^k + (d_n-1)^k$$

for $k = 0, 1, \ldots$, with equality for $k = 0, 1$, and if $k \geq 2$ then equality occurs if and only if $G = S_n$. Thus

$$\begin{aligned} LEE(G) &= \sum_{k\geq 0} \frac{t_k(G)}{k!} \\ &\geq \sum_{k\geq 0} \frac{(d_1+1)^k + \sum_{i=2}^{n-1} d_i^k + (d_n-1)^k}{k!} \\ &= e^{d_1+1} + \sum_{i=2}^{n-1} e^{d_i} + e^{d_n-1} \end{aligned}$$

with equality if and only if $G = S_n$. □

Similarly, if G be a tree with $n \geq 2$ vertices, Then by similar arguments as in the proof of Proposition 4, we have

$$LEE(G) \leq \sum_{i=1}^{n} e^{d_i^*} = n - d_1 + \sum_{i=1}^{d_1} e^{d_i^*}$$

with equality if and only if $G = S_n$.

Proposition 5. *Let G be a graph with $n \geq 2$ vertices. Then*

$$LEE(G) \geq n + \sum_{i=1}^{n} \frac{d_i}{1+d_i}\left(e^{1+d_i} - 1\right)$$

with equality if and only if G is a vertex–disjoint union of complete subgraphs.

Proof. By Proposition 3,

$$t_k(G) \geq \sum_{i=1}^{n} d_i(1+d_i)^{k-1}$$

for $k = 1, 2 \ldots$, and for $k \geq 3$ equality occurs if and only if G is a disjoint union of cliques. The inequality above is an equality for $k = 1, 2$. Thus

$$\begin{aligned} LEE(G) &= \sum_{k \geq 0} \frac{t_k(G)}{k!} \\ &\geq n + \sum_{k \geq 1} \frac{\sum_{i=1}^{n} d_i (1+d_i)^{k-1}}{k!} \\ &= n + \sum_{i=1}^{n} \frac{d_i}{1+d_i} \sum_{k \geq 1} \frac{(1+d_i)^k}{k!} \\ &= n + \sum_{i=1}^{n} \frac{d_i}{1+d_i} \left(e^{1+d_i} - 1\right) \end{aligned}$$

with equality if and only if G is a vertex–disjoint union of complete subgraphs. $\square$

Remark 2. We note that lower bounds on the Laplacian spectral moments in [7] may also be converted to the bounds of Laplacian Estrada index.

(a) Let G be a connected graph with $n \geq 3$ vertices, m edges. Then

$$LEE(G) \geq 1 + e^{1+d_1} + (n-2)e^{\frac{2m-1-d_1}{n-2}}$$

$$LEE(G) \geq 1 + e^{1+d_1} + (n-2)e^{\left(\frac{tn}{1+d_1}\right)^{\frac{1}{n-2}}}$$

with either equality if and only if $G = K_n$ or $G = S_n$, where t is the number of spanning trees in G.

(b) Let G be a graph with $n \geq 2$ vertices and m edges. Let $\overline{G}$ be the complement of the graph G. By the arithmetic–geometric inequality, we have $LEE(G) = 1 + \sum_{i=1}^{n-1} e^{\mu_i} \geq 1 + (n-1)e^{\frac{2m}{n-1}}$ with equality if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$, i.e., $G = K_n$ or $G = \overline{K_n}$ [7]. Let $\overline{m}$ be the number of edges of $\overline{G}$. Thus

$$\begin{aligned} LEE(G) + LEE(\overline{G}) &\geq 2 + (n-1)\left(e^{\frac{2m}{n-1}} + e^{\frac{2\overline{m}}{n-1}}\right) \\ &\geq 2 + 2(n-1)e^{\frac{2m+2\overline{m}}{2(n-1)}} \\ &= 2 + 2(n-1)e^{\frac{n}{2}}, \end{aligned}$$

and then $LEE(G) + LEE(\overline{G}) > 2 + 2(n-1)e^{\frac{n}{2}}$.

(c) Let G be a connected bipartite graph with $n \geq 3$ vertices and m edges. Recall that the first Zagreb index of a graph G, denoted by $M_1(G)$, is defined as the sum of the squares of the degrees of the graph [22–24]. Then

$$LEE(G) \geq 1 + e^{2\sqrt{\frac{M_1(G)}{n}}} + (n-2)e^{\frac{2m-2\sqrt{\frac{M_1(G)}{n}}}{n-2}}$$

$$LEE(G) \geq 1 + e^{2\sqrt{\frac{M_1(G)}{n}}} + (n-2)e^{\left(\frac{tn\sqrt{n}}{2\sqrt{M_1(G)}}\right)^{\frac{1}{n-2}}}$$

with either equality if and only if n is even and $G = K_{\frac{n}{2},\frac{n}{2}}$, where t is the number of spanning trees in G.

Acknowledgement. This work was supported by the National Natural Science Foundation (no. 10671076) and the Guangdong Provincial Natural Science Foundation (no. 8151063101000026) of China.

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