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On the Sum of Powers of Normalized Laplacian Eigenvalues of Graphs

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Abstract

For a graph G without isolated vertices and a real $\alpha \neq 0$, we introduce a new graph invariant $s_{\alpha}^{*}(G)$- the sum of the αth power of the non-zero normalized Laplacian eigenvalues of G. Recently, the cases $\alpha = 2$ and -1 have appeared in various problems in the literature. Here, we present some lower and upper bounds of $s_{\alpha}^{*}(G)$ for a connected graph G, where $\alpha \neq 0, 1$. We also discuss the case $\alpha = -1$.

1 Introduction

Topological indices (molecular structure descriptors) based on graph distance are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules [26, 27]. They provide correlations with physical, chemical and thermodynamic parameters of chemical compounds.

Let G be a simple connected graph with n vertices and m edges on the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For $v_i \in V(G)$, the degree of the vertex v_i, denoted by $d(v_i)$, is the number of vertices adjacent to v_i. Let $d(v_i, v_j)$ be the distance (i.e., the length of the shortest path [17]) between the vertices v_i and v_j of G.

The *Wiener index* of a graph G is defined as the sum of all distances between unordered

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pairs of vertices v_i and v_j, i.e.,

$$W(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} d(v_i, v_j). \tag{1}$$

This molecular structure descriptor is one of the most utilized topological indices in high correlation with many physical and chemical indices of molecular compounds. For survey and detailed information, see [1].

The *degree distance* of a graph G is defined as [2]

$$D'(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} [d(v_i) + d(v_j)]\, d(v_i, v_j). \tag{2}$$

This quantity was mentioned in the paper [28] under the name *Schultz index*. In fact, in [23] Schultz put forward a *molecular topological index*, $MTI(G)$, of G which turns out to be

$$MTI(G) = Zg(G) + D'(G) \tag{3}$$

where $Zg(G)$ is equal to the sum of squares of the vertex degrees of G, which is also known as the first *Zagreb index* in mathematical chemistry [29].

The degree distance of graphs has been studied thoroughly in the literature. For instance, the minimum degree distance of graphs with given order and size was established in [41]. In [42] Dankelmann et al. obtained an asymptotically sharp upper bound on degree distance of graphs with given order and diameter. In [3] bicyclic graphs with maximum degree distance were determined. In [4] Ilić et al. obtained the degree distance of partial Hamming graphs. In [5] the minimum degree distance of unicyclic and bicyclic graphs were determined. In [24] Yuan and An determined the maximum degree distance among unicyclic graphs with n vertices. In [30] Tomescu reported further properties of the degree distance.

In [28] Gutman defined the multiplicative variant of the degree distance as

$$S(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} d(v_i)\, d(v_j)\, d(v_i, v_j). \tag{4}$$

He also called $S(G)$ as the *Schultz index of the second kind*, but for which the name *Gutman index* has also been used in [47].

The Gutman index of graphs has attracted great attention recently. In [43] Dankelmann et al. obtained an asymptotically upper bound for the Gutman index and also established the relations between the edge-Wiener index and Gutman index of graphs. The maximal and minimal Gutman indices of bicyclic graphs were determined in [35] and [48], respectively. Some bounds for the Gutman index were also established in [11, 49].

In [16] Klein and Randić proposed a new distance function named resistance distance based on the theory of electrical networks. They consider the graph G as an electrical network N by replacing each edge of G with a unit resistor. Then the resistance distance between the vertices v_i and v_j of G, denoted by $R(v_i, v_j)$, is defined to be the effective resistance distance between the nodes v_i and v_j in N. The resistance distance concept has been studied intensely in graph theory, study of Laplacian and of normalized Laplacian, electric networks and chemistry. For detailed information, see [16, 21, 36, 50].

The *Kirchhoff index* (or resistance index) of a graph G is defined in analogy to the Wiener index as [14]

$$Kf(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} R(v_i, v_j) . \tag{5}$$

The Kirchhoff index has been studied thoroughly in the literature. For instance, in [12] the extremal graphs with given matching number, connectivity and minimal Kirchhoff index were characterized. In unicyclic graphs extremal with respect to the Kirchhoff index were determined in [51, 52]. Deng examined the Kirchhoff index of fully loaded unicyclic graphs [45] and graphs with many cut edges [22]. Some lower bounds for the Kirchhoff index of a connected (molecular) graph in terms of its structural parameters such as the number of vertices (atoms), the number of edges (bonds), maxmimum vertex degree (valency), connectivity and chromatic number were also reported in [13].

Recently, Chen and Zhang introduced a new index named *degree Kirchhoff index* as [21]

$$Kf^*(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} d(v_i)\, d(v_j)\, R(v_i, v_j) . \tag{6}$$

The degree Kirchhoff index has also been studied extensively in the literature. In [34] unicyclic graphs having maximum, second-maximum, minimum and second-minimum degree Kirchhoff index were characterized. In [10, 21] some bounds on the degree Kirchhoff index and relations between the degree Kirchhoff index and Kirchhoff index were established. The degree Kirchhoff index was further studied in [32]. From (4) and (6), we can conclude that the degree Kirchhoff index is the resistance-distance analogue of the Gutman index. However, there is a strong reason for the introduction of this novel structure descriptor.

Let $L(G) = D(G) - A(G)$ be the Laplacian matrix of the graph G, where $A(G)$ and $D(G)$ are the $(0,1)$-adjacency matrix and the diagonal matrix of the vertex degrees of G, respectively. The Laplacian eigenvalues of G are the eigenvalues of $L(G)$. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n = 0$ be the Laplacian eigenvalues of G. The multiplicity of $\mu_n = 0$ is equal to the number of connected components of G [38]. For more details on Laplacian eigenvalues, see [46]. A long time known result for the Kirchhoff index is [25]

$$Kf(G) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i}. \tag{7}$$

Let $L = D(G)^{-1/2} L(G) D(G)^{-1/2}$ be the normalized Laplacian matrix of the graph G, where $D(G)^{-1/2}$ is the matrix which is obtained by getting $\left(-\frac{1}{2}\right)$-power of each entry of $D(G)$. The normalized Laplacian eigenvalues of G are the eigenvalues of its normalized Laplacian matrix. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n = 0$ be the normalized Laplacian eigenvalues of G. The multiplicity of $\lambda_n = 0$ is equal to the number of connected components of G [18]. For detailed information on the normalized Laplacian eigenvalues, see [18, 33].

An interesting analogy between the Kirchhoff and degree Kirchhoff indices is given as [21]

$$Kf^*(G) = 2m\sum_{i=1}^{n-1}\frac{1}{\lambda_i}. \tag{8}$$

From (7) and (8), we can conclude that the degree Kirchhoff index is the normalized Laplacian analogue of the ordinary Kirchhoff index.

For a non-zero real number α, in [7] Zhou defined the *sum of the αth power of the non-zero Laplacian eigenvalues,* $s_\alpha(G)$, of a graph G as

$$s_\alpha(G) = \sum_{i=1}^{h}\mu_i^\alpha \tag{9}$$

where h is the number of non-zero Laplacian eigenvalues of G. The case $\alpha = 1$ is trivial as $s_1(G) = 2m$. Some properties of $s_{\frac{1}{2}}(G)$ and $s_2(G)$ were establised in [31] and [39], respectively. Note that for a connected graph G with n vertices $ns_{-1}(G)$ is equal to the Kirchhoff index. Recently, $s_\alpha(G)$ and its bounds have been studied intensely. For instance, in [7] Zhou established some properties of $s_\alpha(G)$ for $\alpha \neq 0, 1$. He also discussed further properties for $s_{\frac{1}{2}}(G)$ and $s_2(G)$. The results obtained in [7] were improved in [19] and [40]. Some bounds for $s_\alpha(G)$ related to degree sequences were establised in [8]. In [9] some bounds of $s_\alpha(G)$ for a bipartite graph G were given from which lower and upper bounds for incidence energy and lower bounds for Kirchhoff index and Laplacian Estrada index were also deduced.

Now paralel to Zhou's definition, we define a new graph invariant $s_{\alpha}^{*}(G)$-the *sum of the α-th power of the non-zero normalized Laplacian eigenvalues* of a graph G without isolated vertices as

$$s_{\alpha}^{*}(G)=\sum_{i=1}^{h}\lambda_i^{\alpha} \tag{10}$$

where h is the number of non-zero normalized Laplacian eigenvalues of G. The case $\alpha=1$ is trivial as $s_1^{*}(G)=n$. Note that for a connected graph G, $2ms_{-1}^{*}(G)$ is equal to the degree Kirchhoff index of G, where m is the number of edges of G. There is an interesting relation between $s_{\alpha}^{*}(G)$ and the *general Randić index,* $R_{\alpha}(G)$, of G defined by

$$R_{\alpha}(G)=\sum_{v_i\sim v_j}\left(d(v_i)\,d(v_j)\right)^{\alpha} \tag{11}$$

where the summation is over all (unordered) edges v_iv_j in G and $\alpha\neq 0$ is a fixed real number [6]. Note that $s_2^{*}(G)$ is equal to the trace of L^2, from which it may be shown that [44]

$$s_2^{*}(G)=n+2\sum_{v_i\sim v_j}\frac{1}{d(v_i)\,d(v_j)}=n+2R_{-1}(G)\,.$$

For more information on $R_{-1}(G)$ and its importance to the normalized Laplacian eigenvalues, see [20, 37].

In this paper, we present some lower and upper bounds of $s_{\alpha}^{*}(G)$ for a connected graph G, where $\alpha\neq 0,1$. We also discuss the case $\alpha=-1$.

2 Preliminary Lemmas

In this section, we give some working lemmas which will be needed later. Firstly, we introduce two auxiliary quantities of a graph G on the vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ as

$$\Delta=\prod_{i=1}^{n}d(v_i)\quad\text{and}\quad P=1+\sqrt{\frac{2}{n(n-1)}\sum_{v_i\sim v_j}\frac{1}{d(v_i)\,d(v_j)}}$$

where $d(v_i)$ is the degree of the vertex v_i of G. Recall that $R_{-1}(G)=\sum_{v_i\sim v_j}1/d(v_i)\,d(v_j)\,.$

Lemma 2.1 *[15] Let G be a graph with n vertices and m edges. Then the number of spanning trees t of G is given as*

$$t=\frac{\Delta}{2m}\prod_{i=1}^{n-1}\lambda_i.$$

Lemma 2.2 *[18] Let G be a graph with n vertices and normalized Laplacian eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$. Then*

$$\lambda_1 \geq \frac{n}{n-1}. \tag{12}$$

Moreover, the equality holds in (12) if and only if G is a complete graph K_n.

Lemma 2.3 ***[33]*** *Let G be a graph with n vertices and normalized Laplacian eigenvalues*

$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$. Then

$$\lambda_1 \geq P. \tag{13}$$

Moreover, the equality holds in (13) if and only if G is a complete graph K_n.

Lemma 2.4 *[33] The lower bound (13) is always better than the lower bound (12).*

Lemma 2.5 ***[33]*** *Let G be a connected graph of order $n > 2$. Then $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$ if and only if $G \cong K_n$ or $G \cong K_{p,q}$.*

Lemma 2.6 *[18] Let G be a graph with n vertices and normalized Laplacian eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$. Then*

$$0 \leq \lambda_i \leq 2.$$

Moreover, $\lambda_1 = 2$ if and only if a connected component of G is bipartite and nontrivial.

3 Main Results

Now we present the main results of this paper using the ideas in [7]. Note that Δ and P were defined earlier in the previous section.

Theorem 3.1 *Let α be a real number with $\alpha \neq 0, 1$, and let G be a connected graph with $n \geq 3$ vertices, m edges and t spanning trees. Then*

$$s_\alpha^*(G) \geq P^\alpha + (n-2)\left(\frac{2mt}{\Delta P}\right)^{\alpha/(n-2)} \tag{14}$$

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

Proof. By Lemma 2.1, we have $\prod_{i=1}^{n-1} \lambda_i = \frac{2mt}{\Delta}$. Using the arithmetic-geometric mean inequality, we obtain

$$\begin{aligned} s_\alpha^*(G) &= \lambda_1^\alpha + \sum_{i=2}^{n-1} \lambda_i^\alpha \\ &\geq \lambda_1^\alpha + (n-2)\left(\prod_{i=2}^{n-1} \lambda_i^\alpha\right)^{1/(n-2)} \\ &= \lambda_1^\alpha + (n-2)\left(\frac{2mt}{\Delta\lambda_1}\right)^{\alpha/(n-2)} \end{aligned}$$

with equality if and only if $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$. Let

$$f(x) = x^\alpha + (n-2)\left(\frac{2mt}{\Delta x}\right)^{\alpha/(n-2)}.$$

Solving $f'(x) = \alpha\left(x^{\alpha-1} - \left(\frac{2mt}{\Delta}\right)^{\frac{\alpha}{n-2}} x^{-\frac{\alpha}{n-2}-1}\right) \geq 0$, we can easily see that $f(x)$ is increasing for $x \geq \left(\frac{2mt}{\Delta}\right)^{1/(n-1)}$ whether $\alpha > 0$ or $\alpha < 0$. Using Lemma 2.3, Lemma 2.4 and the arithmetic-geometric mean inequality, we get

$$\lambda_1 \geq P \geq \frac{n}{n-1} = \frac{\sum_{i=1}^{n-1} \lambda_i}{n-1} \geq \left(\prod_{i=1}^{n-1} \lambda_i\right)^{1/(n-1)} = \left(\frac{2mt}{\Delta}\right)^{1/(n-1)}.$$

Therefore we obtain

$$s_\alpha^*(G) \geq f(P) = P^\alpha + (n-2)\left(\frac{2mt}{\Delta P}\right)^{\alpha/(n-2)}.$$

Hence (14) follows and the equality holds in (14) if and only if

$$\lambda_1 = P \text{ and } \lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}.$$

Then, by Lemma 2.3 and Lemma 2.5, we conclude that $G = K_n$. ■

As mentioned in Section 1, we have $Kf^*(G) = 2ms_{-1}^*(G)$. Considering this information and Theorem 3.1, we can give the following result.

Corollary 3.2 *Let G be a connected graph with $n \geq 3$ vertices, m edges and t spanning trees. Then*

$$Kf^*(G) \geq \frac{2m}{P} + 2(n-2)m\left(\frac{\Delta P}{2mt}\right)^{1/(n-2)} \tag{15}$$

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

Theorem 3.3 *Let G be a connected graph with $n \geq 3$ vertices:*

(i) If $\alpha < 0$ or $\alpha > 1$, then

$$s_{\alpha}^{*}(G) \geq P^{\alpha} + \frac{(n-P)^{\alpha}}{(n-2)^{\alpha-1}} \tag{16}$$

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

(ii) If $0 < \alpha < 1$, then

$$s_{\alpha}^{*}(G) \leq P^{\alpha} + \frac{(n-P)^{\alpha}}{(n-2)^{\alpha-1}} \tag{17}$$

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

Proof. Note that x^{α} is concave up when $x > 0$ and $\alpha < 0$ or $\alpha > 1$. Therefore we obtain

$$\left(\sum_{i=2}^{n-1} \frac{1}{n-2}\lambda_i\right)^{\alpha} \leq \sum_{i=2}^{n-1} \frac{1}{n-2}\lambda_i^{\alpha}$$

i.e.,

$$\sum_{i=2}^{n-1} \lambda_i^{\alpha} \geq \frac{1}{(n-2)^{\alpha-1}} \left(\sum_{i=2}^{n-1} \lambda_i\right)^{\alpha}$$

with equality if and only if $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$. It follows that

$$\begin{aligned} s_{\alpha}^{*}(G) &\geq \lambda_1^{\alpha} + \frac{1}{(n-2)^{\alpha-1}} \left(\sum_{i=2}^{n-1} \lambda_i\right)^{\alpha} \\ &= \lambda_1^{\alpha} + \frac{(n-\lambda_1)^{\alpha}}{(n-2)^{\alpha-1}}. \end{aligned}$$

Let

$$g(x) = x^{\alpha} + \frac{(n-x)^{\alpha}}{(n-2)^{\alpha-1}}.$$

By solving $g'(x) = \alpha\left(x^{\alpha-1} - \frac{(n-x)^{\alpha-1}}{(n-2)^{\alpha-1}}\right) \geq 0$, we can easily see that $g(x)$ is increasing for $x \geq \frac{n}{n-1}$. By Lemma 2.3 and Lemma 2.4, we have

$$\lambda_1 \geq P \geq \frac{n}{n-1}.$$

Therefore

$$s_{\alpha}^{*}(G) \geq g(P) = P^{\alpha} + \frac{(n-P)^{\alpha}}{(n-2)^{\alpha-1}}$$

with equality if and only if $\lambda_1 = P$ and $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$. Then, by Lemma 2.3 and 2.5, we conclude that the equality holds in (16) if and only if $G = K_n$. Now we suppose that $0 < \alpha < 1$. Note that x^{α} is concave down when $x > 0$ and $0 < \alpha < 1$. Thus we have

$$\left(\sum_{i=2}^{n-1} \frac{1}{n-2}\lambda_i\right)^{\alpha} \geq \sum_{i=2}^{n-1} \frac{1}{n-2}\lambda_i^{\alpha}$$

with equality if and only if $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$. Note further that the function $g(x) = x^\alpha + \frac{(n-x)^\alpha}{(n-2)^{\alpha-1}}$ is decreasing for $x \geq \frac{n}{n-1}$. By similar arguments mentioned above, we get the second part of the theorem. ■

From Theorem 3.3 (i), we obtain the following result.

Corollary 3.4 *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then*

$$Kf^*(G) \geq \frac{2m}{P} + \frac{2(n-2)^2 m}{n-P} \tag{18}$$

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

Now we consider bipartite graphs.

Theorem 3.5 *Let α be a real number with $\alpha \neq 0, 1$, and let G be a connected bipartite graph with $n \geq 3$ vertices, m edges and t spanning trees. Then*

$$s_\alpha^*(G) \geq (2)^\alpha + (n-2)\left(\frac{mt}{\Delta}\right)^{\alpha/(n-2)} \tag{19}$$

with equality if and only if $G \cong K_{p,q}$.

Proof. Using the similar arguments in the proof of Theorem 3.1, we derive

$$s_\alpha^*(G) \geq \lambda_1^\alpha + (n-2)\left(\frac{2mt}{\Delta\lambda_1}\right)^{\alpha/(n-2)}.$$

Since G is a connected bipartite graph, by Lemma 2.6, we have $\lambda_1 = 2$ and then (19) follows. The equality holds in (19) if and only if $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$.

Now we suppose that the equality holds in (19). Then, by Lemma 2.5, we conclude that $G \cong K_{p,q}$.

Conversely, we can easily see that the equality holds in (19) for the complete bipartite graph $K_{p,q}$. ■

From Theorem 3.5, we get the following result.

Corollary 3.6 *Let G be a connected bipartite graph with $n \geq 3$ vertices, m edges and t spanning trees. Then*

$$Kf^*(G) \geq m + 2(n-2)\,m\left(\frac{\Delta}{mt}\right)^{1/(n-2)} \tag{20}$$

with equality if and only if $G \cong K_{p,q}$.

Theorem 3.7 *Let G be a connected bipartite graph with $n \geq 3$ vertices:*

(i) If $\alpha < 0$ or $\alpha > 1$, then

$$s_{\alpha}^{*}(G) \geq n + 2\left(2^{\alpha-1} - 1\right) \tag{21}$$

with equality if and only if $G \cong K_{p,q}$.

(ii) If $0 < \alpha < 1$, then

$$s_{\alpha}^{*}(G) \leq n + 2\left(2^{\alpha-1} - 1\right) \tag{22}$$

with equality if and only if $G \cong K_{p,q}$.

Proof. Using the similar arguments in the proof of Theorem 3.3, we derive

$$s_{\alpha}^{*}(G) \geq \lambda_1^{\alpha} + \frac{(n-\lambda_1)^{\alpha}}{(n-2)^{\alpha-1}}.$$

Since G is a connected bipartite graph, by Lemma 2.6, we have $\lambda_1 = 2$ and then (21) follows.

From the proof of Theorem 3.3, we also obtain

$$s_{\alpha}^{*}(G) \leq \lambda_1^{\alpha} + \frac{(n-\lambda_1)^{\alpha}}{(n-2)^{\alpha-1}}$$

for $0 < \alpha < 1$. Since $\lambda_1 = 2$, (22) follows.

Either equality in (21) or (22) holds if and only if $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$. By similar arguments as in the proof of Theorem 3.5, we get $G \cong K_{p,q}$. ■

From Theorem 3.7 (i), we have the following result.

Corollary 3.8 *[10] Let G be a connected bipartite graph with $n \geq 3$ vertices and m edges. Then*

$$Kf^{*}(G) \geq (2n-3)\,m \tag{23}$$

with equality if and only if $G \cong K_{p,q}$.

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