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Research Article

Spectral properties of the atom-bond sum-connectivity matrix

Jiangtong Liu[1], Yarong Hu[2], Xiangyu Ren[1,*]

[1]*School of Mathematics and Statistics, Shanxi University, Taiyuan 030006, P.R. China*
[2]*School of Mathematics and Information Technology, Yuncheng University, Yuncheng 044000, P.R. China*

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Abstract

The atom-bond sum-connectivity index (ABS index) is a topological index introduced in 2022. For a graph G, this index is defined as $ABS(G) = \sum_{v_iv_j \in E(G)} \sqrt{(d_i + d_j - 2)/(d_i + d_j)}$, where d_i is the degree of a vertex v_i of G and $E(G)$ is the set of edges of G. The ABS-matrix is defined as $S(G) = [a_{ij}]_{n\times n}$, where a_{ij} equals $\sqrt{(d_i + d_j - 2)/(d_i + d_j)}$ when $v_iv_j \in E(G)$ and $a_{ij} = 0$ otherwise. Furthermore, the Laplacian ABS-matrix is defined as $\tilde{L}(G) = \tilde{D}(G) - S(G)$, where $\tilde{D}(G) = [\tilde{d}_{ij}]_{n\times n}$ is the ABS-diagonal matrix with $\tilde{d}_{ij} = \sum_{k=1}^{n} a_{ik}$ when $i = j$ and $\tilde{d}_{ij} = 0$ when $i \neq j$. In this paper, we first present several bounds on the ABS index. We then explore several properties of the eigenvalues of the ABS-matrix and Laplacian ABS-matrix. Finally, inspired by the definition of the convex linear combination of the adjacency matrix and diagonal matrix proposed by Nikiforov, we also define the convex linear combination of the ABS-matrix and ABS-diagonal matrix, and present some of its fundamental properties.

Keywords: ABS index; ABS-matrix; ABS eigenvalues.

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1. Introduction

Let $G = (V(G), E(G))$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. We use the notation $i \sim j$ to indicate that the vertices v_i and v_j are adjacent; that is, $v_iv_j \in E(G)$. For $v_i \in V(G)$, the degree of v_i, denoted by d_i, is the number of edges incident with v_i. The maximum and minimum degrees of G are denoted by Δ and δ, respectively.

The study of chemical structures using graphs is known as chemical graph theory. Atoms and bonds are replaced with vertices and edges, respectively, to represent a chemical structure as a graph. This makes it feasible to explore the properties of chemical structures using the concepts of graph theory. In chemical graph theory, the graph invariants that take quantitative values are commonly referred to as topological indices.

In the 1970s, Randić [10] put forward a topological index for studying molecular branching and named it the "branching index", which is now referred to as the Randić index. For a graph G, the Randić index is defined as

$$R(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_id_j}}.$$

The Randić index is one of the most-studied and most-applied topological indices. The atom-bond connectivity (ABC) index [5] and the sum-connectivity (SC) index [12] are the variants of the Randić index. These indices have the following definitions for a graph G:

$$ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_id_j}}$$

and

$$SC(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_i + d_j}}.$$

In [1], by amalgamating the main idea of the ABC and SC indices, a new topological index, namely the atom-bond sum-connectivity index (ABS index), was proposed. This index is defined as

$$ABS(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}}.$$

*Corresponding author (renxy@sxu.edu.cn).

The graphs with the maximum and minimum values of the ABS index were found in [1] over particular classes of graphs and (chemical) trees. Unicyclic graphs with extremum ABS index were studied in [3], where chemical uses of the ABS index were also reported. The problems of finding graphs that achieve the minimum ABS index among all trees of a
(i) specific number of pendent vertices,
(ii) fixed order and a specific number of pendent vertices,
were addressed in [4]; see also [8], where one of these two problems was addressed independently. For further details about the ABS index, the reader is referred to [2].

We define the ABS-matrix as $S(G) = [a_{ij}]_{n\times n}$, where

$$a_{ij} = \begin{cases} \sqrt{\dfrac{d_i + d_j - 2}{d_i + d_j}} & \text{if } v_iv_j \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

The eigenvalues of $S(G)$ are called the ABS eigenvalues of G and are denoted by $\xi_1(G), \xi_2(G), \dots, \xi_n(G)$ with the assumption that $\xi_1(G) \geq \xi_2(G) \geq \cdots \geq \xi_n(G)$. We define the Laplacian ABS-matrix of G as $\tilde{L}(G) = \tilde{D}(G) - S(G)$, where $\tilde{D}(G) = [\tilde{d}_{ij}]_{n\times n}$ is the ABS-diagonal matrix with

$$\tilde{d}_{ij} = \begin{cases} \sum_{k=1}^{n} a_{ik} & \text{if } i = j, \\ 0, & \text{otherwise.} \end{cases}$$

The eigenvalues of $\tilde{L}(G)$ are called the Laplacian ABS eigenvalues of G and are denoted by $\mu_1(G), \mu_2(G), \dots, \mu_n(G)$ such that $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$.

For any real number $\alpha \in [0, 1]$, Nikiforov [9] defined the matrix

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G), \tag{1}$$

where $A(G)$ and $D(G)$ are the adjacency and diagonal matrices, respectively. Inspired by (1), for $\alpha \in [0, 1]$, we define the following matrix:

$$S_\alpha(G) = \alpha\tilde{D}(G) + (1 - \alpha)S(G).$$

The eigenvalues of the matrix $S_\alpha(G)$ are denoted by $\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)$ provided that $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$. It is easy to see $S(G) = S_0(G)$, $\tilde{D}(G) = S_1(G)$, $\tilde{Q}(G) = 2S_{\frac{1}{2}}(G)$, where $\tilde{Q}(G) = S(G) + \tilde{D}(G)$.

The rest of this paper is organized as follows. In Section 2, some preliminary results are presented. Section 3 provides some bounds for the ABS index. Section 4 explores some properties of the ABS eigenvalues and Laplacian ABS eigenvalues. In Section 5, some basic properties of the matrix $S_\alpha(G)$ are obtained.

2. Preliminaries

This section gives some preliminary results that will be used in the subsequent sections.

Theorem 2.1 (see [7,11])**.** *Let A and B be Hermitian matrices of order n. Let $\xi_i(M)$ denote the i-th largest eigenvalue of the matrix $M \in \{A, B, A + B\}$. For $1 \leq i \leq n$ and $1 \leq j \leq n$, the following inequalities hold:*

$$\xi_i(A) + \xi_j(B) \begin{cases} \leq \xi_{i+j-n}(A + B) & \text{when } i + j \geq n + 1, \\ \geq \xi_{i+j-1}(A + B) & \text{when } i + j \leq n + 1. \end{cases}$$

In either of these inequalities, equality holds if and only if a nonzero n-vector exists that is an eigenvector to each of the three eigenvalues involved. The two inequalities given above yield

$$\xi_k(A) + \xi_n(B) \leq \xi_k(A + B) \leq \xi_k(A) + \xi_1(B).$$

Lemma 2.1. *Let G be a graph with n vertices and M_k be the k-th spectral moment of the ABS-matrix $S = S(G)$; that is,*

$$M_k = \sum_{i=1}^{n} (\xi_i^k(G)) = tr((S)^k).$$

Then $M_0 = n$, $M_1 = 0$, and $M_2 = 2\sum_{\substack{v_iv_j \in E(G) \\ 1\leq i,j\leq n}} \frac{d_i+d_j-2}{d_i+d_j}$.

Proof. Note that $M_0 = \sum_{i=1}^{n}(\xi_i^0(G)) = n$ and $M_1 = \sum_{i=1}^{n} \xi_i(G) = tr(S) = 0$. Next, we consider M_2. We observe that

$$(S^2)_{ij} = \sum_{k=1}^{n} a_{ki}a_{kj} = \sum_{\substack{k\sim i, k\sim j\\ 1\le k\le n}} a_{ki}a_{kj} = \sum_{\substack{k\sim i, k\sim j\\ 1\le k\le n}} \sqrt{\frac{d_i+d_k-2}{d_i+d_k}}\sqrt{\frac{d_j+d_k-2}{d_j+d_k}},$$

for any $1 \le i, j \le n$ and $i \ne j$, where $a_{ij} = \sqrt{\frac{d_i+d_j-2}{d_i+d_j}}$. If $1 \le i \le n$, then

$$(S^2)_{ii} = \sum_{j=1}^{n} a_{ij}a_{ji} = \sum_{\substack{v_iv_j\in E(G)\\ 1\le j\le n}} a_{ij}^2 = \sum_{\substack{v_iv_j\in E(G)\\ 1\le j\le n}} \frac{d_i+d_j-2}{d_i+d_j}.$$

Thus, we have

$$M_2 = tr(S^2) = \sum_{i=1}^{n}\left(\sum_{\substack{v_iv_j\in E(G)\\ 1\le j\le n}} \frac{d_i+d_j-2}{d_i+d_j}\right) = 2\sum_{\substack{v_iv_j\in E(G)\\ 1\le i,j\le n}} \frac{d_i+d_j-2}{d_i+d_j}.$$

□

In what follows, we provide two obvious lemmas without proof.

Lemma 2.2. *Let* $f(x,y) = \sqrt{\frac{x+y-2}{x+y}}$. *If* $x, y \ge 0$ *and* $x+y \ge 2$, *then* $f(x,y)$ *is an increasing function for* x *and* y.

We denote the eigenvalues of the adjacency matrix of G by $\eta_1(G), \eta_2(G), \ldots, \eta_n(G)$ such that $\eta_1(G) \ge \eta_2(G) \ge \cdots \ge \eta_n(G)$.

Lemma 2.3. *Let* G *be an* r*-regular graph with* m *edges,* $n \ge 3$ *vertices, and no isolated vertices. Then*

$$\xi_i(G) = \sqrt{\frac{r-1}{r}}\eta_i(G), \quad \text{for } i = 1, 2, \ldots, n.$$

Also, for any real number $\alpha \in [0,1]$, *it holds that*

$$\lambda_i(G) = \alpha\sqrt{r(r-1)} + (1-\alpha)\xi_i(G) = \alpha\sqrt{r(r-1)} + (1-\alpha)\sqrt{\frac{r-1}{r}}\eta_i(G).$$

3. Bounds for the ABS index

This section is concerned with determining some bounds for the ABS index.

Lemma 3.1. *Let* G *be a nontrivial graph with* n *vertices. Then*

$$ABS(G) \le \frac{n}{2}\sqrt{(n-1)(n-2)},$$

where the equality holds if and only if $G = K_n$.

Theorem 3.1. *Let* G *be a graph with* $m \ge 1$ *edges and* M_2 *be the 2nd spectral moment of the* ABS*-matrix. Then*

$$\sqrt{\frac{1}{2}M_2 + m(m-1)\frac{\delta-1}{\delta}} \le ABS(G) \le \sqrt{\frac{1}{2}M_2 + m(m-1)\frac{\triangle-1}{\triangle}},$$

where either of the equalities holds if and only if G *is a regular graph.*

Proof. By Lemmas 2.1 and 2.2, we have

$$\begin{aligned}(ABS(G))^2 &= \left(\sum_{v_iv_j\in E(G)} \sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\right)^2\\ &= \sum_{v_iv_j\in E(G)} \frac{d_i+d_j-2}{d_i+d_j} + \sum_{\substack{i\sim j, k\sim l\\ v_iv_j\ne v_kv_l}} \sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\sqrt{\frac{d_k+d_l-2}{d_k+d_l}}\\ &\le \frac{1}{2}M_2 + m(m-1)\frac{\triangle-1}{\triangle}.\end{aligned}$$

Thus,

$$ABS(G) \leq \sqrt{\frac{1}{2}M_2 + m(m-1)\frac{\triangle - 1}{\triangle}},$$

with equality if and only if G is a regular graph. Similarly, we have

$$\sqrt{\frac{1}{2}M_2 + m(m-1)\frac{\delta - 1}{\delta}} \leq ABS(G),$$

where the equality holds if and only if G is a regular graph. □

Theorem 3.2. *Let G be a graph with minimum degree at least 2 and M_2 be the 2nd spectral moment of the ABS-matrix. Then*

$$\frac{1}{2}\sqrt{\frac{\triangle}{\triangle - 1}}M_2 \leq ABS(G) \leq \frac{1}{2}\sqrt{\frac{\delta}{\delta - 1}}M_2,$$

where the equality holds if and only if G is a regular graph.

Proof. By Lemmas 2.1 and 2.2, we have

$$\begin{aligned} M_2 &= 2\sum_{v_iv_j \in E(G)} \frac{d_i + d_j - 2}{d_i + d_j} \\ &= 2\sum_{v_iv_j \in E(G)} \left(\sqrt{\frac{d_i + d_j - 2}{d_i + d_j}}\right)^2 \\ &\geq 2\sqrt{\frac{\delta - 1}{\delta}} \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}} \\ &= 2\sqrt{\frac{\delta - 1}{\delta}} ABS(G). \end{aligned}$$

Thus,

$$ABS(G) \leq \frac{1}{2}\sqrt{\frac{\delta}{\delta - 1}}M_2,$$

where the equality holds if and only if G is a regular graph. Similarly, we have

$$ABS(G) \geq \frac{1}{2}\sqrt{\frac{\triangle}{\triangle - 1}}M_2,$$

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

Theorem 3.3. *Let G be a graph with n vertices and maximum degree at least 2. Then*

$$\frac{n}{2(n-1)}\sqrt{\frac{\triangle}{\triangle - 1}}\xi_1^2 \leq ABS(G) \leq \frac{n\xi_1}{2}.$$

If $G = K_n$, the left equality holds. If G is a regular graph, the right equality holds.

Proof. Let A be the adjacency matrix of G and $\eta_1(G), \eta_2(G), \cdots, \eta_n(G)$ be its eigenvalues such that

$$\eta_1(G) \geq \eta_2(G) \geq \cdots \geq \eta_n(G).$$

Note that $e = (1, 1, \ldots, 1)^T \in R^n$. Thus, by the Courant-Fischer Minimax theorem, we have

$$\xi_1(G) = \xi_1 = \max_{x \neq 0}\left(\frac{x^TSx}{x^Tx}\right) \geq \frac{e^TSe}{e^Te} = \frac{2}{n}ABS(G),$$

and hence $ABS(G) \leq \frac{n\xi_1}{2}$. If G is a k-regular graph, then by Lemma 2.3, we have $\xi_1(G) = \eta_1(G)\sqrt{\frac{k-1}{k}} = k\sqrt{\frac{k-1}{k}}$, and

$$ABS(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}} = \frac{kn}{2}\sqrt{\frac{k-1}{k}} = \frac{n}{2}k\sqrt{\frac{k-1}{k}} = \frac{n\xi_1}{2}.$$

Now, by Cauchy's inequality, we have

$$\xi_1^2 = \left(\sum_{i=2}^{n}\xi_i\right)^2 \leq (n-1)\left(\sum_{i=2}^{n}\xi_i^2\right).$$

Hence, by Theorem 3.2, we have

$$\frac{n\xi_1^2}{n-1} = \xi_1^2 + \frac{\xi_1^2}{n-1} \le \xi_1^2 + \sum_{i=2}^{n} \xi_i^2 = \sum_{i=1}^{n} \xi_i^2 = M_2 \le 2\sqrt{\frac{\Delta-1}{\Delta}} ABS(G).$$

Consequently, we have

$$ABS(G) \ge \frac{\xi_1^2 n}{2(n-1)} \sqrt{\frac{\Delta}{\Delta-1}}.$$

If $G = K_n$, then by Lemma 2.3, we have $\xi_1 = \sqrt{(n-2)(n-1)}$ and

$$ABS(G) = \frac{n(n-1)}{2}\sqrt{\frac{n-2}{n-1}} = \frac{n}{2(n-1)}\sqrt{\frac{\Delta}{\Delta-1}}\xi_1^2.$$

□

4. The ABS eigenvalues and the Laplacian ABS eigenvalues

In this section, we establish some basic properties and bounds for the ABS eigenvalues and Laplacian ABS eigenvalues. The harmonic index [6] of a graph G is defined as

$$H(G) = \sum_{v_i v_j \in E(G)} \frac{2}{d_i + d_j}.$$

Proposition 4.1. *Let G has $n \ge 3$ vertices, m edges, and no isolated vertices. Then*

$$\sum_{i=1}^{n} \xi_i(G) = 0,$$

$$\sum_{i=1}^{n} \xi_i^2(G) = 2(m - H(G)),$$

and

$$\sum_{1 \le i < j \le n} \xi_i(G)\xi_j(G) = H(G) - m.$$

Proof. Using the fundamental properties of $S(G)$, we have

$$\sum_{i=1}^{n} \xi_i(G) = tr(S(G)) = 0.$$

Also, it holds that

$$\sum_{i=1}^{n} \xi_i^2(G) = tr(S(G)^2) = 2\sum_{v_i v_j \in E(G)} \left(1 - \frac{2}{d_i + d_j}\right) = 2(m - H(G)).$$

Furthermore,

$$\sum_{1 \le i < j \le n} \xi_i(G)\xi_j(G) = \frac{1}{2}\left((\sum_{i=1}^{n} \xi_i(G))^2 - \sum_{i=1}^{n} \xi_i^2(G) \right) = H(G) - m.$$

□

Theorem 4.1. *Let G be a graph of order $n \ge 3$ with no isolated vertices. Then $S(G)$ has only one (distinct) eigenvalue if and only if n is even and $G = (\frac{n}{2})K_2$.*

Proof. Proposition 4.1 gives $\sum_{i=1}^{n} \xi_i(G) = 0$. Therefore, all the ABS eigenvalues of G are equal to 0 if there is merely one distinct ABS eigenvalue. This suggests that $S(G) = \mathbf{0}$, which leads to the conclusion that $G = (\frac{n}{2})K_2$ and n is even.

On the other hand, if n is even and $G = (\frac{n}{2})K_2$, then $S(G) = \mathbf{0}$ and therefore all of its eigenvalues equal to 0. □

Proposition 4.2. *Let G be a graph with order $n \ge 3$. Then G has two different eigenvalues of $S(G)$ if and only if $G = K_n$.*

Proposition 4.3. *Assume that G has m edges, $n \ge 3$ vertices, and no isolated vertices. Then*

$$\xi_1(G) \ge \sqrt{\frac{2\,(m - H(G))}{n}}, \tag{2}$$

where the equality holds if and only if n is even and $G = (\frac{n}{2})K_2$.

Proof. By Proposition 4.1, we have

$$n\xi_1^2(G) \geq \sum_{i=1}^{n} \xi_i^2(G) = 2\left(m - H(G)\right). \tag{3}$$

Hence, we have

$$\xi_1(G) \geq \sqrt{\frac{2\left(m - H(G)\right)}{n}}.$$

Now, we give a characterization for the equality in (2). First, assume that n is even and $G = (\frac{n}{2})K_2$. Then $S(G) = \mathbf{0}$ and hence $\xi_1(G) = \xi_2(G) = \cdots = \xi_n(G) = 0$. Note that $H(G) = \frac{n}{2}$, and as a result, we have

$$\sqrt{\frac{2\left(m - H(G)\right)}{n}} = \sqrt{\frac{2(\frac{n}{2} - H(G))}{n}} = 0.$$

Thus, the equality in (2) is satisfied. Conversely, we suppose that the equality in (2) is satisfied. According to the equality in (3), we have $\xi_1^2(G) = \xi_2^2(G) = \cdots = \xi_n^2(G)$. Hence, G has at most two different eigenvalues. By Proposition 4.1, if $G = (\frac{n}{2})K_2$ and n is even, then G has only one eigenvalue for $S(G)$. If G has two distinct eigenvalues of $S(G)$, then Proposition 4.2 implies that G has a component $C = K_t$ having two different ABS eigenvalues and $|V(C)| = t \geq 3$. Thus, by Lemma 2.3, we have $\xi_1(C) = \sqrt{(t-2)(t-1)}$ and $\xi_2(C) = \xi_3(C) = \cdots = \xi_t(C) = -\sqrt{\frac{t-2}{t-1}}$; but, $\xi_1^2(C) \neq \xi_2^2(C)$ if $t \geq 3$. This leads to a contradiction, along with the fact that $\xi_1(C), \xi_2(C), \ldots, \xi_t(C)$ are part of the eigenvalues of $S(G)$. □

Lemma 4.1. *Let G be a connected graph with $n \geq 3$ vertices. Then $\tilde{L}(G)$ has t $(2 \leq t \leq n)$ distinct eigenvalues if and only if there exist $t-1$ distinct nonzero numbers $\ell_1, \ell_2, \ldots, \ell_{t-1}$ such that*

$$\prod_{i=1}^{t-1}(\tilde{L}(G) - \ell_i I) = (-1)^{t-1}\frac{\prod_{i=1}^{t-1}\ell_i}{n}J,$$

where I is the unit matrix of order n and J is all 1 matrix of order n.

Theorem 4.2. *Let G be a graph with $n \geq 3$ vertices. Then G has exactly two different Laplacian ABS eigenvalues if and only if $G = K_n$.*

Proof. According to Lemma 4.1, G has exactly two different Laplacian ABS eigenvalues if and only if there is a number $\ell \neq 0$ such that

$$\tilde{L}(G) - \ell I = -\frac{\ell}{n}J.$$

That is, $\tilde{L}(G) = \ell I - \frac{\ell}{n}J$. Clearly, all of the off-diagonal entries of $\tilde{L}(G)$ are nonzero. Thus, we have $G = K_n$ and

$$\ell = n\sqrt{\frac{n-2}{n-1}}.$$

□

Proposition 4.4. *Let G be a graph of order $n \geq 3$. Then*

$$\mu_1(G) \leq n\sqrt{\frac{n-2}{n-1}} \text{ and } \mu_n(G) = 0.$$

Every eigenvector of $\tilde{L}(G)$ corresponding to the eigenvalue 0 is constant if G is connected.

Theorem 4.3. *Let G be a graph with order $n \geq 3$. Then*

$$\mu_{n-1}(G) \leq n\sqrt{\frac{n-2}{n-1}}, \tag{4}$$

where the equality holds if and only if $G = K_n$.

Proof. We have

$$tr\left(\tilde{L}(G)\right) = \mu_1(G) + \mu_2(G) + \cdots + \mu_n(G) = 2ABS(G). \tag{5}$$

Note that $\mu_n(G) = 0$. By Lemma 3.1, we have

$$\mu_{n-1}(G) \leq \frac{2ABS(G)}{n-1} \leq n\sqrt{\frac{n-2}{n-1}}. \tag{6}$$

By (5) and $\mu_1(G) \geq \cdots \geq \mu_{n-1}(G)$, we have $\mu_1(G) = \cdots = \mu_{n-1}(G)$. Thus, if the equality in (4) holds, then by Theorem 4.2, we have $G = K_n$. Conversely, if $G = K_n$ then we obtain the equality in (4). □

5. Basic properties of the matrix $S_\alpha(G)$

By using the definition of $S_\alpha(G)$, for $1 < k \le n$, we obtain the eigenequations given as follows:

$$\begin{aligned}\lambda x_k = S_\alpha(G)x_k &= \alpha \sum_{v_iv_k\in E(G)} a_{ki}x_k + (1-\alpha)\sum_{v_iv_k\in E(G)} a_{ki}x_i \\ &= \alpha \sum_{v_iv_k\in E(G)} \sqrt{\frac{d_i+d_k-2}{d_i+d_k}}x_k + (1-\alpha)\sum_{v_iv_k\in E(G)} \sqrt{\frac{d_i+d_k-2}{d_i+d_k}}x_i.\end{aligned} \tag{7}$$

Let $a_{ij} = \sqrt{\frac{d_i+d_j-2}{d_i+d_j}}$. By using Lemma 2.2, we have the following two results:

Proposition 5.1. *Let $\alpha \in [0,1]$ and $S_\alpha(G) = S_\alpha$. Then*

$$\lambda_1(G) = \max_{\|\boldsymbol{x}\|_2=1} \langle S_\alpha \boldsymbol{x}, \boldsymbol{x}\rangle \quad \text{and} \quad \lambda_n(G) = \min_{\|\boldsymbol{x}\|_2=1} \langle S_\alpha \boldsymbol{x}, \boldsymbol{x}\rangle\,.$$

Also, if $\boldsymbol{x} := (x_1, x_2, \dots, x_n)$ is a unit n-vector, then $\lambda_1(G) = \langle S_\alpha \boldsymbol{x}, \boldsymbol{x}\rangle$ if and only if $\boldsymbol{x}$ is an eigenvector corresponding to $\lambda_1(G)$, and $\lambda_n(G) = \langle S_\alpha \boldsymbol{x}, \boldsymbol{x}\rangle$ if and only if $\boldsymbol{x}$ is an eigenvector corresponding to $\lambda_n(G)$.

Proposition 5.2. *Let $\alpha \in [0,1)$ and $S_\alpha(G) = S_\alpha$. Then*

$$\lambda_1(G) = \max\{\lambda_1(H)\} \quad \text{and} \quad \lambda_n(G) = \min\{\lambda_n(H)\},$$

where H is a component of G.

Before proving the next proposition, we need the following fact:

$$S_\alpha(G) - S_\beta(G) = (\alpha-\beta)\tilde{L}(G). \tag{8}$$

Proposition 5.3. *Assume that $1 \ge \alpha > \beta \ge 0$. Let $\lambda_k(G)$ and $\lambda'_k(G)$ be the k-th largest eigenvalues of $S_\alpha(G)$ and $S_\beta(G)$, respectively. Then*

$$\lambda_k(G) - \lambda'_k(G) \ge 0, \tag{9}$$

for any $k \in [n]$, where $[n] := \{1,2,\dots n\}$. If G is connected, then the equality in (9) holds if and only if $k=1$ and G is regular.

Proof. From Theorem 2.1, Proposition 4.4, and (8), it follows that

$$\lambda_k(G) - \lambda'_k(G) \ge (\alpha-\beta)\,\mu_n(G) = 0.$$

If G is a connected graph and the equality in (9) holds, then Theorem 2.1 implies that $\lambda_k(G)$, $\lambda'_k(G)$, and $\mu_n(G)$ share an eigenvector, which by Proposition 4.4 must be constant. Now, $k=1$ is implied by Proposition 5.7, and (7) implies that G is regular. □

Proposition 5.4. *If $\alpha > \frac{1}{2}$, then $S_\alpha(G)$ is positive semidefinite. If the order of G is $n \ge 3$ and G has no isolated vertices, then $S_\alpha(G)$ is positive definite.*

Proof. Note that

$$\langle S_\alpha \mathbf{x}, \mathbf{x}\rangle = (2\alpha-1)\sum_{v_i\in V(G)}(x_i^2 \sum_{v_iv_j\in E(G)} a_{ij}) + (1-\alpha)\sum_{v_iv_j\in E(G)} a_{ij}(x_i+x_j)^2,$$

where $\mathbf{x} := (x_1, x_2, \dots, x_n)$ is a nonzero vector. Recall that $a_{ij} = \sqrt{\frac{d_i+d_j-2}{d_i+d_j}} \ge 0$. If $\alpha > \frac{1}{2}$, then we have

$$\langle S_\alpha \mathbf{x}, \mathbf{x}\rangle \ge (1-\alpha)a_{ij}(x_i+x_j)^2 + (2\alpha-1)a_{ij}x_i^2 + (2\alpha-1)a_{ij}x_j^2 \ge 0,$$

for $v_iv_j \in E(G)$. Hence, $S_\alpha(G)$ is a positive semidefinite matrix.

Now, assume that the order of G is $n \ge 3$ and G has no isolated vertices. We have a vertex v_j with $x_j \ne 0$ and $v_iv_j \in E(G)$. Thus, $S_\alpha(G)$ is positive definite. □

For a graph G, if an automorphism $f: G \to G$ exists and $f(v_i) = v_j$, then v_i and v_j are called equivalent.

Proposition 5.5. *Let v_i and v_j be equivalent vertices in a connected graph G. If $(x_1, \dots, x_n)$ is an eigenvector corresponding to $\lambda_1(G)$, then $x_i = x_j$.*

Proof. Let $\mathbf{x} := (x_1, \dots, x_n)$ be the unit nonnegative eigenvector corresponding to $\lambda_1(G)$. Assume that $f : G \to G$ such that $f(v_i) = v_j$. Let F be the permutation matrix corresponding to f. Observe that f is a permutation of $V(G)$. Since f is an automorphism, we have $F^{-1}S_\alpha F = S_\alpha$. Hence, $F^{-1}S_\alpha F\mathbf{x} = S_\alpha \mathbf{x}$, and then $F\mathbf{x}$ is an eigenvector to S_α. As $\mathbf{x}$ is unique and S_α is irreducible, we have $Fx = x$; that is, $x_i = x_j$. □

Proposition 5.6. *Let $S(G) = S$, $\tilde{D}(G) = \tilde{D}$, and $S_\alpha(G) = S_\alpha$. Then*

$$\lambda_1(G) \geq \xi_1(G). \tag{10}$$

If the equality holds in (10), then G has a $\xi_1(G)$-regular component. Also, if $a_\Delta = \sqrt{\frac{\Delta-1}{\Delta}} \geq 0$, then

$$\lambda_1(G) \leq \alpha\Delta a_\Delta + (1-\alpha)\xi_1(G). \tag{11}$$

The equality holds in (11) if and only if G has a Δ-regular component.

Proof. Although Proposition 5.3 dictates (10), we present another proof to support the equality argument. We assume that H is a component of G such that $\xi_1(G) = \xi_1(H)$. Let h be the order of H, and $(x_1, x_2, \dots, x_h)$ be a positive unit vector corresponding to $\xi_1(H)$. For every $v_iv_j \in E(H)$, we have

$$a_{ij} = \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}} \geq 0,$$

and hence

$$\begin{aligned} 2a_{ij}x_ix_j &= a_{ij}(2\alpha x_ix_j + 2(1-\alpha)x_ix_j) \\ &\leq a_{ij}\left(\alpha x_i^2 + 2(1-\alpha)x_ix_j + \alpha x_j^2\right). \end{aligned}$$

Adding up all the edges $v_iv_j \in E(H)$ in this inequality, and using

$$\langle S_\alpha \mathbf{x}, \mathbf{x}\rangle = \sum_{v_iv_j \in E(G)} a_{ij}(\alpha x_i^2 + \alpha x_j^2 + 2(1-\alpha)x_ix_j),$$

we have

$$\xi_1(G) = \xi_1(H) = \langle S(H)\mathbf{x}, \mathbf{x}\rangle \leq \langle S_\alpha(H)\mathbf{x}, \mathbf{x}\rangle \leq \lambda_1(G),$$

which proves (10). If the equality holds in (10), then $x_1 = x_2 = \cdots = x_h$. Thus, H is a $\xi_1(G)$-regular graph.

We observe that (11) follows from Theorem 2.1 because

$$\lambda_1(G) \leq \alpha\Delta + (1-\alpha)\xi_1(G).$$

Next, we provide a proof, based on the following, for the equality in (11):

$$\langle S_\alpha \mathbf{x}, \mathbf{x}\rangle = \alpha \sum_{v_i \in V(G)} (x_i^2 \sum_{v_iv_j \in E(G)} a_{ij}) + 2(1-\alpha) \sum_{v_iv_j \in E(G)} a_{ij}x_ix_j.$$

Let H is a component of graph G and $\lambda_1(G) = \lambda_1(H)$. For $\lambda_1(H)$, let $\mathbf{x} := (x_1, x_2, \dots, x_h)$ be a positive unit eigenvector, then

$$\begin{aligned} \lambda_1(G) &= \alpha \sum_{v_i \in V(H)} \left[x_i^2 \left(\sum_{v_iv_j \in E(G)} a_{ij}\right)\right] + 2(1-\alpha)\left(\sum_{v_iv_j \in E(G)} x_ix_ja_{ij}\right) \\ &\leq \alpha\Delta a_\Delta \sum_{v_i \in V(H)} x_i^2 + (1-\alpha)\xi_1(H) \\ &\leq \alpha\Delta a_\Delta + (1-\alpha)\xi_1(G). \end{aligned}$$

If the equality holds in (11), then H is Δ-regular. If G contains a Δ-regular component, then $\xi_1(G) = \Delta a_\Delta = \lambda_1(G)$. Thus, the equality holds in (11). □

The Perron-Frobenius theory of nonnegative matrices can be used to obtain the following characteristics of $S_\alpha(G)$:

Proposition 5.7. *Let $\alpha \in [0,1)$ and $\boldsymbol{x}$ be a nonnegative eigenvector corresponding to $\lambda_1(G)$.*

(i). *The eigenvector $\boldsymbol{x}$ is positive and distinctive up to scale if G is a connected graph.*

(ii). *If G is not connected and P is the set of vertices in $\boldsymbol{x}$ with positive entries, then the resulting subgraph induced by P is a union of components H of G with $\lambda_1(G) = \lambda_1(H)$.*

(iii). *If G is a connected graph and λ is an eigenvalue of $S_\alpha(G)$ with a nonnegative eigenvector, then $\lambda = \lambda_1(G)$.*

(iv). *If H is a proper subgraph of a connected graph G, then $\lambda_1(H) < \lambda_1(G)$ for every $\alpha \in [0,1)$.*

Let $T_r(n)$ be an r-partite Turán graph with n vertices. Recall that $T_r(n)$ has the largest number of edges among all r-partite graphs with n vertices.

Proposition 5.8. *Let G be an r-chromatic graph of order n such that $r \geq 2$. If $\alpha < 1 - \frac{1}{r}$, then $\lambda_1(G) < \lambda_1(T_r(n))$, unless $G = T_r(n)$. If $\alpha > 1 - \frac{1}{r}$, then $\lambda_1(G) < \lambda_1(S_{n,r-1})$, unless $G = S_{n,r-1}$. If $\alpha = 1 - \frac{1}{r}$, then $\lambda_1(G) \leq (1 - \frac{1}{r})n$ with equality if and only if G is a complete r-partite graph.*

Proof. Assume that G is an r-partite graph of order n with maximum $\lambda_1(G)$ among all r-partite graph of order n. Proposition 5.7 implies that G is a complete r-partite graph. Let the partition sets of G be $V_1, \dots, V_r$. If these sets have sizes of $n_1, \dots, n_r$, respectively, then $n_1 + \cdots + n_r = n$. Let $\lambda_1 = \lambda_1(G)$ and $\mathbf{x} := (x_1, \dots, x_n)$ be a positive eigenvector corresponding to λ_1. According to Proposition 5.5, the values of the entries in $\mathbf{x}$ that belong to vertices in the same partition set are equal, say z_i for V_i, $i = 1, \dots, r$. Hence, we have

$$\lambda_1 z_k = \alpha \left(\sum_{i \in [r] \setminus \{k\}} n_i a_{ki} \right) z_k + (1-\alpha) \sum_{i \in [r] \setminus \{k\}} n_i a_{ki} z_i, \ 1 \leq k \leq r. \tag{12}$$

If $\alpha = 1 - \frac{1}{r}$, then

$$\lambda_1 = \left(1 - \frac{1}{r}\right) \sum_{i \in [r]} n_i a_{ki}$$

is an eigenvalue with an eigenvector defined by

$$z_i = \frac{1}{r a_{ki} n_i}, \quad i = 1, \dots, r.$$

Take $S = n_1 a_{k1} z_1 + \cdots + n_r a_{kr} z_r$. From (12), we have

$$\left[\lambda_1 - \alpha \left(\sum_{i \in [r]} n_i a_{ki} - n_k a_{kk} \right) + (1-\alpha) n_k a_{kk} \right] n_k z_k = (1-\alpha) n_k S,$$

for $1 \leq k \leq r$, where $a_{kk} = \sqrt{\frac{d_k - 1}{d_k}}$. Next, we note that λ_1 satisfies the following equation:

$$\sum_{j \in [r]} \frac{n_j a_{kj}}{\lambda_1 - \alpha \sum_{i \in [r]} n_i a_{ki} + n_j a_{kj}} = \frac{1}{1-\alpha}. \tag{13}$$

If $\alpha < 1 - \frac{1}{r}$, then $\frac{1}{1-\alpha} < r$. Hence, by (13), we have

$$\lambda_1 - \alpha \sum_{i \in [r]} n_i a_{ki} > 0.$$

Letting

$$f(z) = \frac{z}{\lambda_1 - \alpha \sum_{i \in [r]} n_i a_{ki} + z} = 1 - \frac{\lambda_1 - \alpha \sum_{i \in [r]} n_i a_{ki}}{\lambda_1 - \alpha \sum_{i \in [r]} n_i a_{ki} - z}, \ z > 0,$$

we have

$$f''(z) = \frac{-2(\lambda_1 - \alpha \sum_{i \in [r]} n_i a_{ki})}{(\lambda_1 - \alpha \sum_{i \in [r]} n_i a_{ki} + z)^3} < 0.$$

Let $\lambda_T = \lambda_1(T_r(n))$ and $t_1, \dots, t_r$ be the sizes of the partition sets of $T_r(n)$; in other words, $t_i = \lfloor \frac{n}{r} \rfloor$ or $t_i = \lceil \frac{n}{r} \rceil$ and $t_1 + \cdots + t_r = n$. From (13), we have

$$\sum_{j \in [r]} \frac{t_j a_{kj}}{\lambda_T - \alpha \sum_{i \in [r]} t_i a_{ki} + t_j a_{kj}} = \frac{1}{1-\alpha}.$$

Thus, we have

$$\begin{aligned}\sum_{j\in[r]} \frac{t_j a_{kj}}{\lambda_T - \alpha \sum_{i\in[r]} n_i a_{ki} + t_j a_{kj}} &= \frac{1}{1-\alpha} \\ &= \sum_{j\in[r]} \frac{n_j a_{kj}}{\lambda_1 - \alpha \sum_{i\in[r]} n_i a_{ki} + n_j a_{kj}} \\ &\le \sum_{j\in[r]} \frac{t_j a_{kj}}{\lambda_1 - \alpha \sum_{i\in[r]} n_i a_{ki} + t_j a_{kj}}.\end{aligned}$$

Consequently, we have $\lambda_T \ge \lambda_1$ with equality if and only if $n_i = \lfloor \frac{n}{r} \rfloor$ or $n_i = \lceil \frac{n}{r} \rceil$. Similarly, if $\alpha > 1 - \frac{1}{r}$, then $\frac{1}{1-\alpha} > r$. As a result, by (13), we have $\lambda_1 - \alpha \sum_{i\in[r]} n_i a_{ki} < 0$. If

$$f(z) = \frac{z}{\lambda_1 - \alpha \sum_{i\in[r]} n_i a_{ki} + z},$$

for $z > 0$, then $f''(z) > 0$. Let $s_1, \ldots, s_r$ be the sizes of the partition sets of $S_{n,r-1}$, which means that $s_1 = s_2 = \cdots = s_{r-1} = 1$ and $s_r = n - r + 1$. Assume that $\lambda_s = \lambda_1(S_\alpha(S_{n,r-1}))$. Considering (13), we obtain

$$\sum_{j\in[r]} \frac{s_j a_{kj}}{\lambda_s - \alpha \sum_{i\in[r]} s_i a_{ki} + s_j a_{kj}} = \frac{1}{1-\alpha}.$$

Then,

$$\begin{aligned}\sum_{j\in[r]} \frac{s_j a_{kj}}{\lambda_s - \alpha \sum_{i\in[r]} n_i a_{ki} + s_j a_{kj}} &= \frac{1}{1-\alpha} \\ &= \sum_{j\in[r]} \frac{n_j a_{kj}}{\lambda_1 - \alpha \sum_{i\in[r]} n_i a_{ki} + n_j a_{kj}} \\ &\le \sum_{j\in[r]} \frac{s_j a_{kj}}{\lambda_1 - \alpha \sum_{i\in[r]} n_i a_{ki} + s_j a_{kj}},\end{aligned}$$

and hence $\lambda_s \ge \lambda_1$. Note that the equation $\lambda_s = \lambda_1$ holds if and only if $G = S_{n,r-1}$. □

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