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Research Article

On trees attaining the five largest ABS spectral radii

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Abstract

The atom-bond sum-connectivity (ABS) matrix of a graph G of order n is the square matrix of order n, whose (i,j)-entry is equal to $\sqrt{(d_i+d_j-2)/(d_i+d_j)}$ if the i-th vertex and the j-th vertex of G are adjacent, and 0 otherwise, where d_i is the degree of the i-th vertex of G. The ABS spectral radius of G is the largest eigenvalue of the ABS matrix of G. In this paper, the trees of order n with the first five largest ABS spectral radii are characterized.

Keywords: ABS matrix; ABS eigenvalue; ABS spectral radius; tree.

2020 Mathematics Subject Classification: 05C05, 05C09, 05C50.

1. Introduction

Let $G=(V(G),E(G))$ be a simple connected graph with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)$. The degree of a vertex v_i in G, denoted by d_{v_i} (or d_i), is the number of its neighbors. As usual, let P_n and S_n denote the path and the star on n vertices, respectively. The double star, denoted by $S_{p,q}$, is the graph consisting of the union of two stars S_{p+1} and S_{q+1} together with an edge joining their centers (see Figure 1.1). The adjacency matrix of G, denoted by $A(G)$, is a real symmetric matrix of order n whose (i,j)-th entry is 1 when $v_iv_j\in E(G)$, and 0 otherwise. The spectral radius of G, denoted by $\lambda_A(G)$, is the largest eigenvalue of $A(G)$.

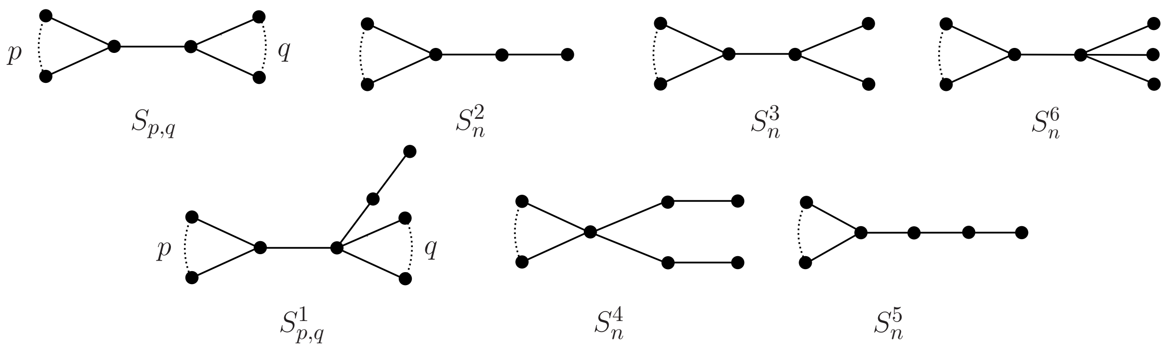

Figure 1.1: The trees $S_{p,q}, S^1_{p,q}, S^2_n, S^3_n, S^4_n, S^5_n$ and S^6_n.

In 2022, Ali et al. [2] proposed a novel degree-based topological index, called the atom-bond sum-connectivity index (ABS index for short), which is defined as

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

This index has garnered widespread attention in the research community and has become an active area of research in mathematical chemistry; for example, see [1,3,4,7,9,15].

Lin et al. [12] proposed the ABS matrix of a graph G, denoted by $\Omega(G)$, whose entries are defined as

$$\omega_{ij}=\begin{cases}\sqrt{1-\dfrac{2}{d_i+d_j}}, & \text{if } v_iv_j\in E(G);\\ 0, & \text{otherwise.}\end{cases}$$

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The largest eigenvalue of the ABS matrix of G is called the ABS spectral radius and is denoted by $\lambda_{ABS}(G)$. Lin et al. [12] showed that the ABS spectral radius is useful in predicting certain physicochemical properties of molecules with an accuracy higher than the atom-bond sum-connectivity index. For details about the existing spectral properties of the ABS matrix, the reader is referred to [10–14].

Investigating the extremal behavior of the spectral radius of graph matrices constitutes a significant area of research within spectral graph theory and mathematical chemistry. Let T_n be a tree with n vertices. Lin et al. [12] proved that

$$\lambda_{ABS}(P_n) \leq \lambda_{ABS}(T_n) \leq \lambda_{ABS}(S_n)$$

with equality in the left (respectively, right) inequality if and only if $T_n \cong P_n$ (respectively, $T_n \cong S_n$).

A natural and significant research question concerns the structural characteristics of trees that possess the second-largest, third-largest, and, in general, the k-th largest ($k \geq 2$) ABS spectral radius. In this paper, this question is answered for $k = 2, 3, 4, 5$; that is, the trees with the first five largest ABS spectral radii are characterized.

2. Lemmas

Lemma 2.1 (see [5, 8]). *Suppose that $M = (m_{i,j})$ and $N = (n_{i,j})$ are two $n \times n$ nonnegative symmetric matrices. If $M \geq N$, i.e., $m_{i,j} \geq n_{i,j}$ for all i, j, then $\lambda(M) \geq \lambda(N)$. Furthermore, if N is irreducible and $M \neq N$, then $\lambda(M) > \lambda(N)$.*

Let $\mathcal{T}_n$ be the class of all trees on n vertices.

Lemma 2.2 (see [6]). *Let $n \geq 11$ and $T_n \in \mathcal{T}_n \setminus \{S_n, S_n^2, S_n^3, S_n^4, S_n^5, S_n^6\}$. Then*

$$\lambda_A(T_n) < \sqrt{\frac{n-1+\sqrt{n^2-14n+61}}{2}}.$$

Lemma 2.3. *If $p \geq q \geq 1$, then*

$$\lambda_{ABS}(S_{p+1,\,q-1}) > \lambda_{ABS}(S_{p,\,q}).$$

Proof. With a suitable permutation of vertices, the ABS matrix of $S_{p,\,q}$ can be written as

$$\Omega\left(S_{p,\,q}\right) = \begin{bmatrix} 0 & \sqrt{\frac{p+q}{p+q+2}} & \sqrt{\frac{p}{p+2}} & \cdots & \sqrt{\frac{p}{p+2}} & 0 & \cdots & 0 \\ \sqrt{\frac{p+q}{p+q+2}} & 0 & 0 & \cdots & 0 & \sqrt{\frac{q}{q+2}} & \cdots & \sqrt{\frac{q}{q+2}} \\ \sqrt{\frac{p}{p+2}} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{p}{p+2}} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{\frac{q}{q+2}} & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{\frac{q}{q+2}} & 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix}_{n\times n}.$$

The characteristic polynomial of $\Omega\left(S_{p,\,q}\right)$ is given by

$$\begin{aligned}\Phi(S_{p,\,q},x) &= \det(xI_n-\Omega\left(S_{p,\,q}\right))\\ &= x^{n-2}\left\{\left[x-\frac{p^2}{x(p+2)}\right]\left[x-\frac{q^2}{x(q+2)}\right]-\frac{p+q}{p+q+2}\right\}.\end{aligned}$$

Hence, we have

$$\Phi(S_{p+1,\,q-1},x) = x^{n-2}\left\{\left[x-\frac{(p+1)^2}{x(p+3)}\right]\left[x-\frac{(q-1)^2}{x(q+1)}\right]-\frac{p+q}{p+q+2}\right\}.$$

Let

$$\Phi(S_{p,\,q},x)-\Phi(S_{p+1,\,q-1},x)=x^{n-2}f(x).$$

Since

$$\left[\frac{(p+1)^2}{p+3}+\frac{(q-1)^2}{q+1}-\frac{p^2}{p+2}-\frac{q^2}{q+2}\right]=\frac{4(p-q)(p+q+3)+8p+16}{(p^2+5p+6)q^2+(3p^2+15p+18)q+2p^2+10p+12}>0$$

and

$$\begin{aligned}&\left[\frac{p^2q^2}{(p+2)(q+2)}-\frac{(p+1)^2(q-1)^2}{(p+3)(q+1)}\right]\\ &= \frac{q(p-q)(p^2q+pq^2+3p^2-5q^2+6pq+6p-5q+5)+4(p^2-q^2)+20p-12q-4}{(p^2+5p+6)q^2+(3p^2+15p+18)q+2p^2+10p+12}\\ &> \frac{q(p-q)(q^3+q^3+3q^2-5q^2)+4(p^2-q^2)+20p-12q-4}{(p^2+5p+6)q^2+(3p^2+15p+18)q+2p^2+10p+12}\\ &= \frac{2q^3(p-q)(q-1)+4(p-q)(p+q+3)+8p-4}{(p^2+5p+6)q^2+(3p^2+15p+18)q+2p^2+10p+12}\\ &> 0\end{aligned}$$

for $p\geq q\geq 1$, we have

$$\begin{aligned}f(x) &= \left[x-\frac{p^2}{x(p+2)}\right]\left[x-\frac{q^2}{x(q+2)}\right]-\left[x-\frac{(p+1)^2}{x(p+3)}\right]\left[x-\frac{(q-1)^2}{x(q+1)}\right]\\ &= \left[\frac{p^2q^2}{(p+2)(q+2)}-\frac{(p+1)^2(q-1)^2}{(p+3)(q+1)}\right]\frac{1}{x^2}+\frac{(p+1)^2}{p+3}+\frac{(q-1)^2}{q+1}-\frac{p^2}{p+2}-\frac{q^2}{q+2}\\ &> 0.\end{aligned}$$

Therefore, $\lambda_{ABS}(S_{p+1,\,q-1})>\lambda_{ABS}(S_{p,\,q})$. □

Lemma 2.4. *Let $p\geq 1$ and $q\geq 1$. Then the characteristic polynomial of $\Omega\left(S^1_{p,\,q}\right)$ is*

$$\Phi(S^1_{p,\,q},x)=x^{n-4}\left\{\left(x^2-\frac{1}{3}\right)\left[\left(x-\frac{p^2}{x(p+2)}\right)\left(x-\frac{q(q+1)}{x(q+3)}\right)-\frac{p+q+1}{p+q+3}\right]-\left(x^2-\frac{p^2}{p+2}\right)\frac{q+2}{q+4}\right\},$$

where $S^1_{p,q}$ is shown in Figure 1.1.

Proof. With a suitable permutation of vertices, the ABS matrix of $S^1_{p,q}$ can be written as

$$\Omega\left(S^1_{p,q}\right)=\begin{bmatrix} 0 & \sqrt{\frac{p+q+1}{p+q+3}} & \sqrt{\frac{p+2}{p+4}} & 0 & \sqrt{\frac{p+1}{p+3}} & \cdots & \sqrt{\frac{p+1}{p+3}} & 0 & \cdots & 0 \\ \sqrt{\frac{p+q+1}{p+q+3}} & 0 & 0 & 0 & 0 & \cdots & 0 & \sqrt{\frac{q}{q+2}} & \cdots & \sqrt{\frac{q}{q+2}} \\ \sqrt{\frac{p+2}{p+4}} & 0 & 0 & \sqrt{\frac{1}{3}} & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{p+1}{p+3}} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{p+1}{p+3}} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{\frac{q}{q+2}} & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{\frac{q}{q+2}} & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix}_{n\times n},$$

and the characteristic polynomial of $\Omega\left(S^1_{p,q}\right)$ is given by

$$\Phi(S^1_{p,q},x)=x^{n-4}\left\{\left(x^2-\frac{1}{3}\right)\left[\left(x-\frac{p^2}{x(p+2)}\right)\left(x-\frac{q(q+1)}{x(q+3)}\right)-\frac{p+q+1}{p+q+3}\right]-\left(x^2-\frac{p^2}{p+2}\right)\frac{q+2}{q+4}\right\}.$$

This completes the proof. □

Using the proof of Lemmas 2.3 and 2.4, we obtain the following corollary:

Corollary 2.1.

$$\lambda_{ABS}(S^2_n) = \sqrt{\frac{3n^3-14n^2+17n+6+\sqrt{(3n^3-14n^2+17n+6)^2-12n(n-1)(n^3-6n^2+9n)}}{6n(n-1)}},$$

$$\lambda_{ABS}(S^3_n) = \sqrt{\frac{n^3-6n^2+10n+4+\sqrt{(n^3-6n^2+10n+4)^2-4n^2(n-2)(n-4)^2}}{2n(n-2)}},$$

$$\lambda_{ABS}\left(S^4_n\right) = \sqrt{\frac{3n^3-23n^2+54n-22+\sqrt{(3n^3-23n^2+54n-22)^2-12(n-1)(n-2)(n^3-10n^2+29n-20)}}{6(n-1)(n-2)}},$$

$$\lambda_{ABS}(S^5_n) = \sqrt{\frac{6n^3-43n^2+99n-50+\sqrt{(6n^3-43n^2+99n-50)^2-24(n-1)(n-2)(5n^3-43n^2+110n-68)}}{12(n-1)(n-2)}},$$

$$\lambda_{ABS}(S^6_n) = \sqrt{\frac{5n^3-36n^2+73n+30+\sqrt{(5n^3-36n^2+73n+30)^2-180n^2(n-3)(n-5)^2}}{10n(n-3)}}.$$

Lemma 2.5 (see [12]). *Let T_n be a tree with $n \geq 5$ vertices. Then*

$$\lambda_{ABS}(P_n) \leq \lambda_{ABS}(T_n) \leq \lambda_{ABS}(S_n)$$

with equality in the left (respectively, right) inequality if and only if $T_n \cong P_n$ (respectively, $T_n \cong S_n$).

3. Main result

Theorem 3.1. *Let $n \geq 6$ and $T_n \in \mathcal{T}_n \setminus \{S_n, S_n^2, S_n^3, S_n^4, S_n^5\}$, where the graphs S_n^2, S_n^3, S_n^4 and S_n^5 are shown in Figure 1.1. Then*

$$\lambda_{ABS}(T_n) < \lambda_{ABS}(S_n^5) < \lambda_{ABS}(S_n^4) < \lambda_{ABS}(S_n^3) < \lambda_{ABS}(S_n^2) < \lambda_{ABS}(S_n),$$

where

$$\begin{aligned}
\lambda_{ABS}(S_n) &= \sqrt{\frac{(n-1)(n-2)}{n}}, \\
\lambda_{ABS}(S_n^2) &= \sqrt{\frac{3n^3-14n^2+17n+6+\sqrt{(3n^3-14n^2+17n+6)^2-12n(n-1)(n^3-6n^2+9n)}}{6n(n-1)}}, \\
\lambda_{ABS}(S_n^3) &= \sqrt{\frac{n^3-6n^2+10n+4+\sqrt{(n^3-6n^2+10n+4)^2-4n^2(n-2)(n-4)^2}}{2n(n-2)}}, \\
\lambda_{ABS}\left(S_n^4\right) &= \sqrt{\frac{3n^3-23n^2+54n-22+\sqrt{(3n^3-23n^2+54n-22)^2-12(n-1)(n-2)(n^3-10n^2+29n-20)}}{6(n-1)(n-2)}}, \\
\lambda_{ABS}(S_n^5) &= \sqrt{\frac{6n^3-43n^2+99n-50+\sqrt{(6n^3-43n^2+99n-50)^2-24(n-1)(n-2)(5n^3-43n^2+110n-68)}}{12(n-1)(n-2)}}.
\end{aligned}$$

Proof. Note that $f(d_i, d_j) = \sqrt{1 - \frac{2}{d_i+d_j}}$ is an increasing function on $d_i + d_j$.

If $d_i + d_j < n - 1$ for $v_iv_j \in E(T_n)$, then

$$\omega_{ij} = f(d_i, d_j) \leq \sqrt{1 - \frac{2}{n-1}} = \sqrt{\frac{n-3}{n-1}},$$

which yields

$$\Omega(T_n) \leq \sqrt{\frac{n-3}{n-1}} A(T_n).$$

By Lemma 2.1, we have

$$\lambda_{ABS}(T_n) \leq \sqrt{\frac{n-3}{n-1}} \lambda_A(T_n).$$

By Lemma 2.2, we have

$$\lambda_{ABS}(T_n) < \sqrt{\frac{n-3}{n-1}} \sqrt{\frac{n-1+\sqrt{n^2-14n+61}}{2}} = \sqrt{\frac{(n-3)(n-1+\sqrt{n^2-14n+61})}{2(n-1)}}.$$

If $d_i + d_j = n - 1$ for $v_iv_j \in E(T_n)$, then $T_n \cong S_{p,q}^1$. By Lemma 2.2 and Corollary 2.1, we have

$$\lambda_{ABS}(S_n^4) > \lambda_{ABS}(S_n^5) > \sqrt{\frac{(n-3)(n-1+\sqrt{n^2-14n+61})}{2(n-1)}} > \lambda_{ABS}(S_n^6)$$

and

$$\lambda_{ABS}(S_n^4) > \lambda_{ABS}(S_n^5) > \sqrt{\frac{(n-3)(n-1+\sqrt{n^2-14n+61})}{2(n-1)}} > \lambda_{ABS}(T_n)$$

for $T_n \cong S_{p,q}^1$ provided that $T_n \ncong S_n^4$ and $T_n \ncong S_n^5$, where $n \geq 7$.

If $d_i + d_j = n$ for $v_iv_j \in E(T_n)$, then $T_n \cong S_n$ or $T_n \cong S_{p,q}$. By Lemma 2.5, we have

$$\lambda_{ABS}(S_n) > \lambda_{ABS}(T_n)$$

for $T_n \cong S_{p,q}$. By Lemma 2.3 and Corollary 2.1, we have

$$\lambda_{ABS}(S_n^2) > \lambda_{ABS}(S_n^3) > \lambda_{ABS}(S_n^4)$$

for $n \geq 7$.

For $2 \leq n \leq 6$, all possible trees are shown in Figure 3.1. The corresponding ABS spectral radii of these trees T^i (for $1 \leq i \leq 13$) are shown in Table 1.

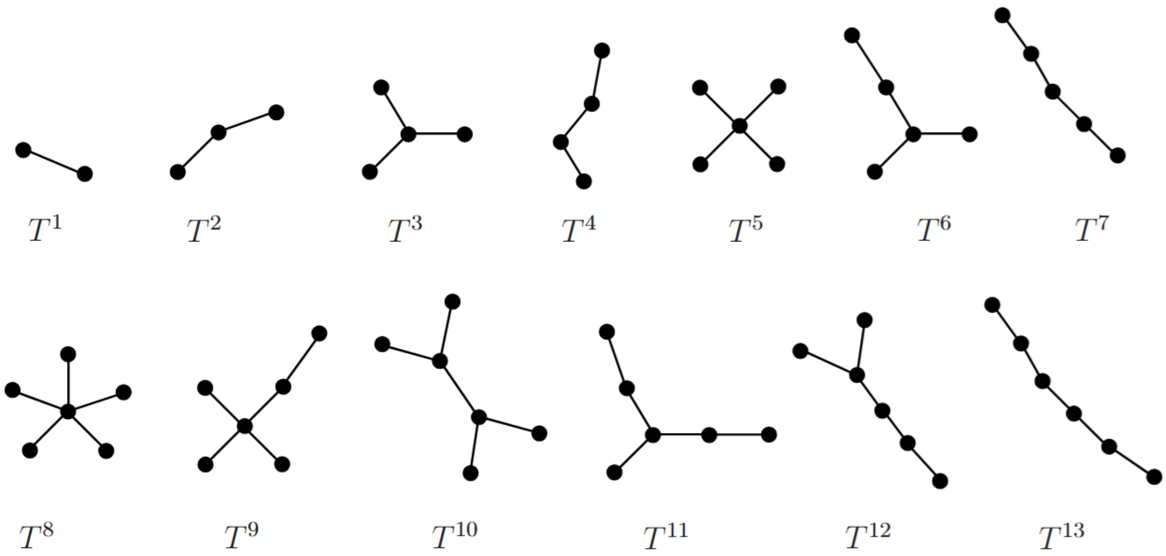

Figure 3.1: All trees with n vertices for $2 \leq n \leq 6$.

Table 3.1: The spectral radii of $\Omega(T^i)$ for the trees depicted in Figure 3.1 for $1 \leq i \leq 13$.

Trees	λ_{ABS}	Trees	λ_{ABS}	Trees	λ_{ABS}	Trees	λ_{ABS}
T^1	0	T^5	1.5492	T^9	1.5788	T^{13}	1.2291
T^2	0.8165	T^6	1.3198	T^{10}	1.4884	–	–
T^3	1.2247	T^7	1.1547	T^{11}	1.3956	–	–
T^4	1.0306	T^8	1.8257	T^{12}	1.3730	–	–

Therefore, we have

$$\lambda_{ABS}(S_n) > \lambda_{ABS}(S_n^2) > \lambda_{ABS}(S_n^3) > \lambda_{ABS}(S_n^4) > \lambda_{ABS}(S_n^5) > \lambda_{ABS}(T_n)$$

for $n \geq 6$ and $T_n \in \mathcal{T}_n \setminus \{S_n, S_n^2, S_n^3, S_n^4, S_n^5\}$. □

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