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# Bounds on the $ABC$ spectral radius of a tree

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**Abstract**

Let $G$ be a simple connected graph with vertex set $\{1, 2, \ldots, n\}$ and $d_i$ denote the degree of vertex $i$ in $G$. The $ABC$ matrix of $G$, recently introduced by Estrada, is the square matrix whose $ij$th entry is $\sqrt{\frac{d_i+d_j-2}{d_i d_j}}$; if $i$ and $j$ are adjacent, and zero; otherwise. The entries in $ABC$ matrix represent the probability of visiting a nearest neighbor edge from one side or the other of a given edge in a graph. In this article, we provide bounds on $ABC$ spectral radius of $G$ in terms of the number of vertices in $G$. The trees with maximum and minimum $ABC$ spectral radius are characterized. Also, in the class of trees on $n$ vertices, we obtain the trees having first four values of $ABC$ spectral radius and subsequently derive a better upper bound.

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## 1. Introduction

We consider simple, finite and connected graphs only. Let $G = (V(G), E(G))$ be a graph on vertex set $V(G) = \{1, 2, \ldots, n\}$. For $i = 1, 2, \ldots, n$, let $d_i$ be the degree of vertex $i$ in $G$. The adjacency matrix of $G$, $A(G)$, is a real symmetric matrix of order $n$ whose $ij$th entry is 1, if $i$ and $j$ are adjacent($i \sim j$); and 0 otherwise. The spectrum of $G$, $\sigma(G) = \{\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)\}$, where $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ is the multiset of eigenvalues of $A(G)$. The largest eigenvalue, $\lambda_1(G)$, is called the spectral radius of $G$ and is studied extensively by many researchers (see for example in [4]). Recently, in [6], Estrada provided a probabilistic interpretation of the term $\frac{d_i+d_j-2}{d_i d_j}$ and showed that it represents the probability of visiting a nearest neighbor edge from one

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side or the other of a given edge in a graph. In context of molecular graphs, this interpretation can be related to the polarizing capacity of the bond considered. He introduced a matrix representation of these probabilities in the form of generalized $ABC$ matrix which is a square matrix of order $n$, defined as $\Omega_\alpha(G) = (w_{ij}^{\alpha})_{n\times n}$, where

$$w_{ij}^{\alpha} = \begin{cases} \left(\frac{d_i+d_j-2}{d_i d_j}\right)^{\alpha}, & \text{if } i \sim j; \\ 0, & \text{otherwise.} \end{cases}$$

Following Chen [2], when $\alpha = 1/2$, we will hereafter call it the $ABC$ matrix and denote it by $\Omega(G)$. The eigenvalues of $\Omega(G)$ are called as the $ABC$ eigenvalues of $G$. Note that $\Omega(G)$ is a real symmetric matrix with real eigenvalues. Let $\vartheta_1(G) \geq \vartheta_2(G) \geq \cdots \geq \vartheta_n(G)$ are the $ABC$ eigenvalues of $G$ in nonincreasing order. The largest $ABC$ eigenvalue, $\vartheta_1(G)$, is known as $ABC$ spectral radius.

The $ABC$ matrix of $G$ can be viewed as a certain type of weighted adjacency matrix of $G$ and can be expressed as [6]

$$\Omega(G) = (AD^{-1} + D^{-1}A - 2D^{-1}AD^{-1})^{\circ\frac{1}{2}},$$

where $A$ is the adjacency matrix of $G$, $D$ is the degree diagonal matrix of $G$, and $\circ$ is the entrywise operation (also known as Hadamard or Schur-operation). Note that the matrices $AD^{-1}$ and $D^{-1}A$ are the transition probability matrices for random walkers on graph [18].

The atom-bond connectivity index (in short $ABC$ index) [7] of $G$ is defined as

$$ABC(G) = \sum_{[i,j]\in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

It is worthy to point out that the $ABC$ index is directly related to the $ABC$ matrix, namely, sum of all entries of $\Omega(G)$ is equal to $2ABC(G)$. Also, when $G$ is regular, the $ABC$ matrix is a constant multiple of the adjacency matrix, namely, $\Omega(G) = \frac{\sqrt{2(r-1)}}{r}A(G)$, where $r$ is the regularity of graph $G$ .

The $ABC$ index is a valuable predictive index in the study of the heat of formation in alkanes [7]. Gutman et al. [14] proved that the $ABC$ index reproduces the heat of formation with an accuracy comparable to that of high-level ab initio and $DFT(MP2, B3LYP)$ quantum chemical calculations. For more work on $ABC$ index, one can see [3, 5, 8, 9, 10, 11, 12, 13, 17, 19, 20]. Here, we consider the problem of studying the eigenvalues of $\Omega(G)$. Apart from the various applications of $ABC$ matrix, our motivation came from some results on the $ABC$ eigenvalues of $G$ discussed in [2]. Chen [2] has supplied a bound on $ABC$ spectral radius, namely, for a graph of order $n \geq 3$ with no isolated vertices, $\vartheta_1(G) \geq \sqrt{\frac{2}{n}(n - 2R_{-1}(G))}$, where $R_{-1}(G) = \sum_{[i,j]} \frac{1}{d_i d_j}$ is the general Randić index of graph $G$. Estrada [6] proved that for any graph $G$ on $n$ vetrices,

$$\frac{2}{n}\sum_{i=1}^{n} \Omega(i) \leq \vartheta_1(G) \leq \max_i \Omega(i),$$

where $\Omega(i)$ is the $i$th row sum of $\Omega(G)$.

In [2], the author posed the problem: *For a given class of graphs, characterize the graphs with minimum or maximum $ABC$ spectral radius $\vartheta_1(G)$.* In this article, we consider the class of trees on $n$ vertices and characterize the trees with the maximum and minimum $ABC$ spectral radius. We are able to provide the lower and upper bounds on $\vartheta_1(G)$ in terms of number of vertices in $G$. By successively removing a tree at each step from our consideration, we are able to obtain the trees with first four largest values of the $ABC$ spectral radius, in the class of trees on $n$ vertices. Subsequently, we are able to provide a better upper bound on the $ABC$ spectral radius of trees.

## 2. Main results

Let $A$ and $B$ be two square matrices of same size. We say, $A$ dominates $B$, write it as $A \geq B$ or $B \leq A$ if $A - B$ is a nonnegative matrix. If $G$ is a connected graph then $\Omega(G)$ is an irreducible matrix. If $A$ and $B$ are two nonnegative irreducible matrices such that $A \geq B$, then by a well known result of Perron Frobenius, it follows that $\lambda_1(A) \geq \lambda_1(B)$. For a reference, see [16]. Next is a well known result concerning the characteristic polynomial of a matrix, which we shall use frequently without any mention.

**Theorem 2.1.** [16] *Let $P$ be a square matrix of order $n$. Then the characteristic polynomial of $P$ is*

$$x^n - E_1 x^{n-1} + E_2 x^{n-2} + \cdots + (-1)^n E_n,$$

*where $E_k$ denotes the sum of principal minors of $P$ of size $k$ for $1 \leq k \leq n$.*

Note that the entries in $\Omega(G)$ are of the form $\sqrt{\frac{x+y-2}{xy}}$, where $x, y \in \{1, 2, \ldots, n\}$. The following result will be helpful which describes some properties of the function $f(x, y) = \frac{x+y-2}{xy}$.

**Lemma 2.1.** *Let $n \geq 3$ and $f(x, y) = \frac{x+y-2}{xy}$, where $x, y \in \{1, 2, \ldots, n\}$ and $(x, y) \neq (1, 1)$. Then*

$$\frac{1}{n} \leq f(x, y) \leq 1 - \frac{1}{n}$$

*and equality holds in the upper bound if and only if $(x, y) = (1, n)$ or $(n, 1)$.*

*Proof.* Since $(x, y) \neq (1, 1)$, at least one of $x, y$, say $x$, is greater than one. Then

$$f(x, y) = \frac{1}{x} + \frac{1}{y} - \frac{2}{xy} = \frac{1}{x} + \frac{1}{y}\left(1 - \frac{2}{x}\right) \geq \frac{1}{x} \geq \frac{1}{n}.$$

Also, if $x = 1$, then

$$f(x, y) = 1 - \frac{1}{y} \leq 1 - \frac{1}{n}$$

with equality if and only if $y = n$. Otherwise $x \geq 2$ and

$$f(x, y) = \frac{1}{x}\left(1 + \frac{x-2}{y}\right) \leq \frac{1}{x}\left(1 + \frac{x-2}{1}\right) = 1 - \frac{1}{x} \leq 1 - \frac{1}{n}$$

with equality if and only if $y = 1$ and $x = n$. Hence the result. □

The class of trees on $n$ vertices is denoted by $\mathcal{T}_n$. By $P_n, S_n$, and $K_n$, we denote the path graph, star graph, and complete graph on $n$ vertices, respectively. The trees $S_n^2, S_n^3, S_n^4, S_n^5, S_n^6$, wherever mentioned, are meant for graphs as given in Figure 1.

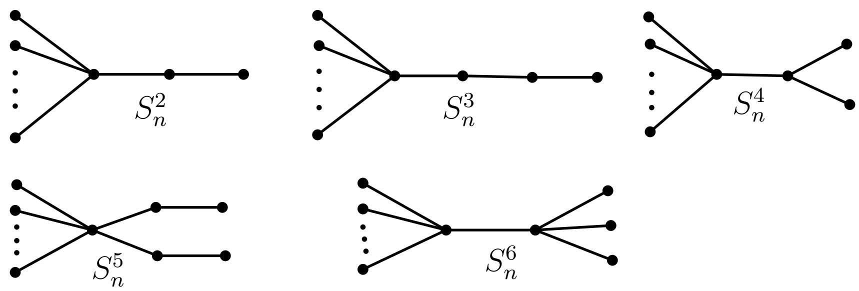


Figure 1. The trees $S_n^2, S_n^3, S_n^4, S_n^5, S_n^6$

Let us recall the following classical result concerning bounds on the spectral radius of trees.

**Lemma 2.2.** *Let $T$ be a tree in $\mathcal{T}_n$. Then $2\cos\frac{\pi}{n+1} \le \lambda_1(T) \le \sqrt{n-1}$ and the equality occurs in upper bound if and only if $T = S_n$.*

Hofmeister[15] has refined the above result and obtained the following.

**Lemma 2.3.** [15] *Let $T$ be a tree in $\mathcal{T}_n \setminus \{S_n, S_n^2\}$ and $n \ge 4$. Then*

$$\lambda_1(T) \le \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-10n+33})}$$

*and the equality holds if and only if $T = S_n^4$.*

**Lemma 2.4.** [1] *Let $T$ be a tree in $\mathcal{T}_n \setminus \{S_n, S_n^2, S_n^3, S_n^4, S_n^5\}$ and $n \ge 11$. Then $\lambda_1(T) \le \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-14n+61})}$ and the equality holds if and only if $T = S_n^6$.*

Our results are on the $ABC$ spectral radius of trees. Removing one tree from our consideration at each step, we have obtained bounds on the $ABC$ spectral radius of trees on $n$ vertices. The following result is a simple observation which provides the unique trees in $\mathcal{T}_n$ with the maximum and minimum $ABC$ spectral radius.

**Proposition 2.1.** *Let $T$ be a tree on $n \ge 3$ vertices. Then*

$$\frac{2}{\sqrt{n-1}}\cos\frac{\pi}{n+1} \le \vartheta_1(T) \le \sqrt{n-2}$$

*and the equality holds in upper bound if and only if $T = S_n$.*

*Proof.* By Lemma 2.1, it follows that an entry in $ABC$ matrix of $T$ is bounded below by $\frac{1}{\sqrt{n-1}}$ and is bounded above by $\sqrt{\frac{n-2}{n-1}}$. Moreover the $(ij)$-th entry is equal to $\sqrt{\frac{n-2}{n-1}}$ if and only if $(i,j)=(1,n-1)$ or $(n-1,1)$. This implies that $\frac{1}{\sqrt{n-1}}A(T)\leq \Omega(T)\leq \sqrt{\frac{n-2}{n-1}}A(T)$ and the equality occurs in upper bound if and only if $T=S_n$. Since both the matrices $\Omega(T)$ and $A(T)$ are nonnegative irreducible, we have $\frac{1}{\sqrt{n-1}}\lambda_1(T)\leq \vartheta_1(T)\leq \sqrt{\frac{n-2}{n-1}}\lambda_1(T)$. Now using Lemma 2.2,

$$\frac{2}{\sqrt{n-1}}\cos\frac{\pi}{n+1}\leq \vartheta_1(T)\leq \sqrt{n-2}$$

and the equality occurs in upper bound if and only if $T=S_n$. Hence the result. □

**Theorem 2.2.** *Let $n\geq 9$ and $T\in \mathcal{T}_n\setminus\{S_n\}$. Then*

$$\vartheta_1(T)\leq \sqrt{\frac{n^2-5n+7+\sqrt{(n-2)^2+(n-3)^4}}{2(n-2)}}$$

*and the equality holds if and only if $T=S_n^2$.*

*Proof.* With a suitable permutation of vertices, the $ABC$ matrix of $S_n^2$ can be written as

$$\Omega(S_n^2)=\begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & \sqrt{\frac{n-3}{n-2}} & \cdots & \sqrt{\frac{n-3}{n-2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{n-3}{n-2}} & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & & & & \\ \sqrt{\frac{n-3}{n-2}} & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Note that a nonzero principal minor in $\Omega(S_n^2)$ is of size at most $4$ and the sum of principal minors of size $2$ and $4$ are $-\left(1+\frac{(n-3)^2}{n-2}\right)$ and $\frac{(n-3)^2}{2(n-2)}$, respectively. Moreover, rest of the principal minors in $\Omega(S_n^2)$ are zero. Thus, the $ABC$ characteristic polynomial of $S_n^2$ is

$$x^{n-4}\left(x^4-\left(1+\frac{(n-3)^2}{n-2}\right)x^2+\frac{(n-3)^2}{2(n-2)}\right).$$

This implies that $\vartheta_1(S_n^2)=\sqrt{\frac{n^2-5n+7+\sqrt{(n-2)^2+(n-3)^4}}{2(n-2)}}$. Observe that if $T\neq S_n, S_n^2$, then maximum possible value of any entry in $\Omega(T)$ is $\sqrt{\frac{n-4}{n-3}}$, which implies

$$\Omega(T)\leq \sqrt{\frac{n-4}{n-3}}A(T).$$

Further, since both of $\Omega(T)$ and $A(T)$ are nonnegative irreducible matrices, we have $\vartheta_1(T) \leq \sqrt{\frac{n-4}{n-3}}\lambda_1(T)$, where $T \neq S_n, S_n^2$. Then using Lemma 2.3,

$$\vartheta_1(T) \leq \sqrt{\frac{n-4}{n-3}}\sqrt{\frac{n-1+\sqrt{n^2-10n+33}}{2}}.$$

Now we claim that

$$\sqrt{\frac{n-4}{n-3}}\sqrt{\frac{n-1+\sqrt{n^2-10n+33}}{2}} < \sqrt{\frac{n^2-5n+7+\sqrt{(n-2)^2+(n-3)^4}}{2(n-2)}}.$$

Squaring both sides and simplifying, we get

$$(n-4)(n-2)(n-1+\sqrt{n^2-10n+33}) < (n-3)(n^2-5n+7+\sqrt{(n-2)^2+(n-3)^4}),$$

that is,

$$n^2-8n+13+(n-2)(n-4)\sqrt{n^2-10n+33} < (n-3)\sqrt{(n-2)^2+(n-3)^4}.$$

For $n \geq 9$, $n^2-10n+33 < (n-4)^2$ and $(n-3)^4 < (n-2)^2+(n-3)^4$. Therefore it is sufficient to show that

$$n^2-8n+13+(n-2)(n-4)^2 < (n-3)^3.$$

Equivalently, $n^3-9n^2+24n-19 < n^3-9n^2+27n-27$, which is true. Hence, the result. $\square$

**Theorem 2.3.** *Let $n \geq 11$ and $T \in \mathcal{T}_n \setminus \{S_n, S_n^2, S_n^3, S_n^5\}$. Then*

$$\vartheta_1(T) \leq \sqrt{\frac{3n^2-19n+34+\sqrt{(3n^2-19n+34)^2-48(n-3)(n-4)^2}}{6(n-3)}}$$

*and the equality holds if and only if $T = S_n^4$.*

*Proof.* With a suitable permutation of vertices, the $ABC$ matrix of $S_n^4$ can be written as $\Omega(S_n^4) = W + W^T$ where $W = [w_{ij}]$ is a matrix with only nonzero entries $w_{12} = \sqrt{\frac{n-2}{3(n-3)}}$, $w_{15} = w_{16} = \cdots = w_{1n} = \sqrt{\frac{n-4}{n-3}}$ and $w_{23} = w_{24} = \sqrt{\frac{2}{3}}$. Note that the sum of principal minors of size 2 and 4 in $\Omega(S_n^4)$ are $-\left(\frac{3n^2-19n+34}{3(n-3)}\right)$ and $\frac{4(n-4)^2}{3(n-3)}$, respectively and rest of the principal minors are zero. Thus the $ABC$ characteristic polynomial of $S_n^4$ is

$$x^{n-4}\left(x^4 - \left(\frac{3n^2-19n+34}{3(n-3)}\right)x^2 + \frac{4(n-4)^2}{3(n-3)}\right).$$

This implies that $\vartheta_1(S_n^4) = \sqrt{\frac{3n^2-19n+34+\sqrt{(3n^2-19n+34)^2-48(n-3)(n-4)^2}}{6(n-3)}}$.

Observe that if $T \neq S_n, S_n^2, S_n^3, S_n^4, S_n^5$, then maximum possible value of any entry in $\Omega(T)$ is $\sqrt{\frac{n-5}{n-4}}$ which means $\Omega(T) \leq \sqrt{\frac{n-5}{n-4}} A(T)$. Further since both of $\Omega(T)$ and $A(T)$ are nonnegative irreducible matrices, we obtain $\vartheta_1(T) \leq \sqrt{\frac{n-5}{n-4}} \lambda_1(T)$. Using Lemma 2.4,

$$\vartheta_1(T) \leq \sqrt{\frac{n-5}{n-4}} \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-14n+61})}.$$

Next, we claim that

$$\sqrt{\frac{n-5}{n-4}} \sqrt{\frac{(n-1+\sqrt{n^2-14n+61})}{2}} < \vartheta_1(S_n^4).$$

Squaring both sides, we get

$\frac{n-5}{2(n-4)}(n-1+\sqrt{n^2-14n+61}) < \frac{3n^2-19n+34+\sqrt{(3n^2-19n+34)^2-48(n-3)(n-4)^2}}{6(n-3)}$. That is, we need to show that $f(n) < g(n)$, where

$f(n) = 3(n-3)(n-5)(n-1+\sqrt{n^2-14n+61})$ and

$g(n) = (n-4)(3n^2-19n+34+\sqrt{(3n^2-19n+34)^2-48(n-3)(n-4)^2})$. For $n = 11, 12, 13, 14, 15$, the inequality can be verified manually. Suppose $n \geq 16$. Then $n^2-14n+61 < \left(n-\frac{19}{3}\right)^2$ which implies that

$$f(n) < 3(n-3)(n-5)\left(n-1+n-\frac{19}{3}\right) = 6n^3-70n^2+266n-330. \tag{1}$$

Also, $(3n^2-19n+34)^2-48(n-3)(n-4)^2$

$$= \left(3n^2-27n+\frac{182}{3}\right)^2 + 64n - \frac{1984}{9} > \left(3n^2-27n+\frac{182}{3}\right)^2.$$

Therefore,

$$\begin{aligned} g(n) &= (n-4)\left(3n^2-19n+34+\sqrt{(3n^2-19n+34)^2-48(n-3)(n-4)^2}\right) \\ &> (n-4)\left(3n^2-19n+34+3n^2-27n+\frac{182}{3}\right) \\ &= (n-4)\left(6n^2-46n+\frac{284}{3}\right) = 6n^3-70n^2+\frac{836}{3}n-\frac{1136}{3}. \end{aligned}$$

That is,

$$g(n) > 6n^3-70n^2+\frac{836}{3}n-\frac{1136}{3}. \tag{2}$$

From equation (1) and (2), we obtain $f(n)-g(n) < -\frac{38}{3}n+\frac{146}{3} < 0$. Hence, our claim is justified. $\square$

The following two lemmas are needed to obtain the third and fourth tree in $\mathcal{T}_n$.

**Lemma 2.5.** *Let $n \geq 10$, then*

$$\vartheta_1(S_n^3) = \sqrt{\frac{2n^2-13n+23+\sqrt{(2n^2-13n+23)^2-4(n-3)(4n^2-31n+61)}}{4(n-3)}},$$

*and $\vartheta_1(S_n^3) > \vartheta_1(S_n^4)$.*

*Proof.* With a suitable permutation of vertices, the $ABC$ matrix of $S_n^3$ can be written as

$$\Omega(S_n^3) = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \sqrt{\frac{n-4}{n-3}} & \cdots & \sqrt{\frac{n-4}{n-3}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & & & & & \\ \sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Note that the sum of principal minors of size 2 and 4 in $\Omega(S_n^3)$ is $-\frac{(n-4)^2}{n-3} - \frac{3}{2} = \frac{2n^2-13n+23}{-2(n-3)}$ and $\frac{(n-4)^2}{n-3} + \frac{1}{4} = \frac{4n^2-31n+61}{4(n-3)}$, respectively, and rest of the principal minors are zero. Therefore, the $ABC$ characteristic polynomial of $S_n^3$ is

$$x^{n-4}\left(x^4 - \left(\frac{2n^2-13n+23}{2(n-3)}\right)x^2 + \frac{4n^2-31n+61}{4(n-3)}\right).$$

This implies that $\vartheta_1(S_n^3) = \sqrt{\frac{2n^2-13n+23+\sqrt{(2n^2-13n+23)^2-4(n-3)(4n^2-31n+61)}}{4(n-3)}}$.

We claim that $\vartheta_1(S_n^3) > \vartheta_1(S_n^4)$, where the expression for $\vartheta_1(S_n^4)$ is given in Theorem 2.3. Squaring both sides and then cross-multiplying, we get

$$\begin{aligned} &3\left(2n^2-13n+23+\sqrt{(2n^2-13n+23)^2-4(n-3)(4n^2-31n+61)}\right) \\ &> 2\left(3n^2-19n+34+\sqrt{(3n^2-19n+34)^2-48(n-3)(n-4)^2}\right), \end{aligned}$$

which means

$$\begin{aligned} &3\sqrt{(2n^2-13n+23)^2-4(n-3)(4n^2-31n+61)} \\ &> n-1+2\sqrt{(3n^2-19n+34)^2-48(n-3)(n-4)^2}. \end{aligned}$$

It can be seen that

$$\begin{aligned} &(3n^2-19n+34)^2-48(n-3)(n-4)^2 \\ &= (3n^2-27n+65)^2-(26n^2-298n+765) < (3n^2-27n+65)^2. \end{aligned}$$

Therefore, it suffices to show that

$$3\sqrt{(2n^2-13n+23)^2-4(n-3)(4n^2-31n+61)} > n-1+2(3n^2-27n+65).$$

Again squaring both sides and simplifying, we have $24n^3-460n^2+2748n-5292>0$, which is true for $n \geq 10$. Hence, the result. $\square$

**Lemma 2.6.** *Let $n \geq 7$, then*

$$\vartheta_1(S_n^5) = \sqrt{\frac{2n^2-15n+31+\sqrt{(2n^2-15n+31)^2-8(n-3)(n^2-9n+20)}}{4(n-3)}},$$

*and $\vartheta_1(S_n^5) < \vartheta_1(S_n^4)$.*

*Proof.* With a suitable permutation of vertices, the $ABC$ matrix of $S_n^5$ can be written as

$$\Omega(S_n^5) = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \sqrt{\frac{n-4}{n-3}} & \cdots & \sqrt{\frac{n-4}{n-3}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & \cdots & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & & & & & & \\ \sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Note that the sum of principal minors of size $2,4,6$ in $\Omega(S_n^5)$ is $-2-\frac{(n-4)(n-5)}{n-3}$, $\frac{3}{4}+\frac{(n-4)(n-5)}{n-3}$ and $-\frac{(n-4)(n-5)}{4(n-3)}$, respectively. The rest of principal minors are zero. Therefore, the $ABC$ characteristic polynomial of $S_n^5$ is

$$x^{n-6}\left(x^6-\left(2+\frac{(n-4)(n-5)}{n-3}\right)x^4+\left(\frac{3}{4}+\frac{(n-4)(n-5)}{n-3}\right)x^2-\frac{(n-4)(n-5)}{4(n-3)}\right).$$

Thus, $\vartheta_1(S_n^5)$ is the square-root of the largest root of following polynomial

$$\begin{aligned} f(x) &= x^3-\left(2+\frac{(n-4)(n-5)}{n-3}\right)x^2+\left(\frac{3}{4}+\frac{(n-4)(n-5)}{n-3}\right)x-\frac{(n-4)(n-5)}{4(n-3)} \\ &= \frac{(2x-1)\left(2(n-3)x^2-(2n^2-15n+31)x+(n^2-9n+20)\right)}{4(n-3)}. \end{aligned}$$

Now, $f(x)=0$ if and only if $x=\frac{1}{2}$ or $\frac{2n^2-15n+31\pm\sqrt{(2n^2-15n+31)^2-8(n-3)(n^2-9n+20)}}{4(n-3)}$. Since

$$\frac{1}{2} < \frac{2n^2-15n+31+\sqrt{(2n^2-15n+31)^2-8(n-3)(n^2-9n+20)}}{4(n-3)},$$

it follows that

$$\vartheta_1(S_n^5) = \sqrt{\frac{2n^2 - 15n + 31 + \sqrt{(2n^2 - 15n + 31)^2 - 8(n-3)(n^2 - 9n + 20)}}{4(n-3)}}.$$

Now to show that $\vartheta_1(S_n^5) < \vartheta_1(S_n^4)$, it suffices to show

$$\begin{aligned} &3\left(2n^2 - 15n + 31 + \sqrt{(2n^2 - 15n + 31)^2 - 8(n-3)(n^2 - 9n + 20)}\right) \\ &\quad < 2\left(3n^2 - 19n + 34 + \sqrt{(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2}\right). \end{aligned}$$

Equivalently, it suffices to show that

$$\begin{aligned} &3\sqrt{(2n^2 - 15n + 31)^2 - 8(n-3)(n^2 - 9n + 20)} \\ &\quad < 7n + 5 + 2\sqrt{(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2}. \end{aligned} \tag{3}$$

It can be easily verified that for $n \geq 7$,

$$(2n^2 - 15n + 31)^2 - 8(n-3)(n^2 - 9n + 20) < (2n^2 - 16n + 38)^2$$

and

$$(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2 > (3n^2 - 27n + 60)^2.$$

Therefore, the left side of (3) is less than $3(2n^2 - 16n + 38)$ and the right side of (3) is greater than $7n + 5 + 2(3n^2 - 27n + 60)$. Further,

$$3(2n^2 - 16n + 38) < 7n + 5 + 2(3n^2 - 27n + 60)$$

is true for $n \geq 7$, which proves the inequality (3). Hence, the result. □

The following two theorems provide us the trees with the third and fourth largest $ABC$ spectral radius. The results are immediate from Theorem 2.3, Lemma 2.5 and Lemma 2.6.

**Theorem 2.4.** *Let $n \geq 11$ and $T \in \mathcal{T}_n \setminus \{S_n, S_n^2\}$. Then*

$$\vartheta_1(T) \leq \sqrt{\frac{2n^2 - 13n + 23 + \sqrt{(2n^2 - 13n + 23)^2 - 4(n-3)(4n^2 - 31n + 61)}}{4(n-3)}},$$

*and the equality holds if and only if $T = S_n^3$.*

**Theorem 2.5.** *Let $n \geq 11$ and $T \in \mathcal{T}_n \setminus \{S_n, S_n^2, S_n^3\}$. Then*

$$\vartheta_1(T) \leq \sqrt{\frac{3n^2 - 19n + 34 + \sqrt{(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2}}{6(n-3)}},$$

*and the equality holds if and only if $T = S_n^4$.*

## Conclusion

We prove that for any tree on $n$ vertices, $2\cos\frac{\pi}{n+1} \leq \vartheta_1(T) \leq \sqrt{n-2}$. Then refining this upper bound on $\vartheta_1(T)$ at each step, we have obtained that $S_n, S_n^2, S_n^3, S_n^4$ are the trees with first four values of $\vartheta_1(T)$ in $\mathcal{T}_n$. As expected, we notice that ordering of trees according the $ABC$ spectral radius is different than the ordering of trees according the spectral radius as given in Hofmeister [15].

It is easy to see that, when $G$ is a regular graph of regularity $r$, $\Omega(G) = \frac{\sqrt{2(r-1)}}{r}A(G)$. So, in some sense spectrum of both the matrices contain the same information about the graph. For example, the graph with largest spectral radius is $n-1$ regular graph $K_n$ which is also the graph with largest $\vartheta_1(G)$. However, in case of nonregular graphs, $\Omega(G)$ would contain more information than $A(G)$. It seems that $ABC$ spectrum may lead to some new and nontrivial results on graph structure.

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