Bounds on the $ABC$ spectral radius of a tree

Sasmita Barik, Sonu Rani

School of Basic Sciences, IIT Bhubaneswar, Bhubaneswar, 752050, India
sasmita@iitbbs.ac.in, sr18@iitbbs.ac.in

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 $\sqrt{d_i + d_j - 2d_id_j}$; 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 $\frac{d_i + d_j - 2}{d_id_j}$ 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

\[
\Omega_\alpha(G) = (w^{\alpha}_{ij})_{n \times n},
\]

where

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

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]

\[
\Omega(G) = (AD^{-1} + D^{-1}A - 2D^{-1}AD^{-1})^{\circ 1/2},
\]

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

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

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 \( R_{-1}(G) = \sum_{[i,j]} \frac{1}{d_id_j} \) is the general Randić index of graph \( G \). Estrada [6] proved that for any graph \( G \) on \( n \) vertices,

\[
\frac{2}{n} \sum_{i=1}^{n} \Omega(i) \leq \vartheta_1(G) \leq \max_i \Omega(i),
\]
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 $\sqrt{x+y-2/xy}$, 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

$$f(x, y) = \frac{1}{x} \left(1 + \frac{x-2}{y}\right) \leq \frac{1}{x} \left(1 + \frac{x-2}{1}\right) = 1 - \frac{1}{x} \leq 1 - \frac{1}{n}.$$
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with equality if and only if \( y = 1 \) and \( x = n \). Hence the result.

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

![Figure 1. The trees \( S^2_n, S^3_n, S^4_n, S^5_n, S^6_n \)](image)

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

**Lemma 2.2.** Let \( T \) be a tree in \( T_n \). Then \( 2 \cos \frac{\pi}{n+1} \leq \lambda_1(T) \leq \sqrt{n-1} \) 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 \( T_n \setminus \{S_n, S^2_n\} \) and \( n \geq 4 \). Then

\[
\lambda_1(T) \leq \sqrt{\frac{1}{2}(n - 1 + \sqrt{n^2 - 10n + 33})}
\]

and the equality holds if and only if \( T = S^4_n \).

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

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 \( T_n \) with the maximum and minimum ABC spectral radius.

**Proposition 2.1.** Let \( T \) be a tree on \( n \geq 3 \) vertices. Then

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

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 $T \in T_n \setminus \{S_n\}$. 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 $T = S^2_n$.

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

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

Note that a nonzero principal minor in $\Omega(S^2_n)$ 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 $\Omega(S^2_n)$ are zero. Thus, the $ABC$ characteristic polynomial of $S^2_n$ 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 $\vartheta_1(S^2_n) = \sqrt{\frac{n^2 - 5n + 7 + \sqrt{(n-2)^2 + (n-3)^4}}{2(n-2)}}$. Observe that if $T \neq S_n, S^2_n$, 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 $T \neq S_n^1, S_n^2$. 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
\[
\sqrt{\frac{n-4}{n-3}}\sqrt{\frac{n-1 + \sqrt{n^2 - 10n + 33}}{2}} \leq \sqrt{\frac{n^2 - 5n + 7 + \sqrt{(n-2)^2 + (n-3)^4}}{2(n-2)}}.
\]

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. \qed

**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 $w_{23} = w_{24} = \sqrt{\frac{1}{2}}$. 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 $\vartheta_1(S_n^4) = \sqrt{\frac{3n^2 - 19n + 34 + \sqrt{(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2}}{6(n-3)}}$.  

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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 \( \sqrt{\frac{n-2}{n-4}} \) 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 \( \varphi_1(T) \leq \sqrt{\frac{n-5}{n-4}} \lambda_1(T) \). Using Lemma 2.4,

\[
\varphi_1(T) \leq \sqrt{\frac{n-5}{n-4}} \sqrt{\frac{1}{2}(n - 1 + \sqrt{n^2 - 14n + 61})}.
\]

Next, we claim that

\[
\sqrt{\frac{n-5}{n-4}} \sqrt{\frac{1}{2}(n - 1 + \sqrt{n^2 - 14n + 61})} < \varphi_1(S^4_n).
\]

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 \( n^2 - 14n + 61 < (n - \frac{19}{3})^2 \) 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,

\[
g(n) = (n-4) \left( 3n^2 - 19n + 34 + \sqrt{(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2} \right)
\]

\[
> (n-4) \left( 3n^2 - 19n + 34 + 3n^2 - 27n + \frac{182}{3} \right)
\]

\[
= (n-4) \left( 6n^2 - 46n + \frac{284}{3} \right) = 6n^3 - 70n^2 + \frac{836}{3}n - \frac{1136}{3}.
\]

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.

The following two lemmas are needed to obtain the third and fourth tree in \( T_n \).
Lemma 2.5. Let \( n \geq 10 \), then
\[
\vartheta_1(S^3_n) = \sqrt{\frac{2n^2 - 13n + 23 + \sqrt{(2n^2 - 13n + 23)^2 - 4(n-3)(4n^2 - 31n + 61)}}{4(n-3)}},
\]
and \( \vartheta_1(S^3_n) > \vartheta_1(S^4_n) \).

Proof. With a suitable permutation of vertices, the ABC matrix of \( S^3_n \) can be written as
\[
\Omega(S^3_n) = \begin{bmatrix}
0 & \frac{1}{\sqrt{2}} & 0 & 0 & \sqrt{\frac{n-4}{n-3}} & \cdots & \sqrt{\frac{n-4}{n-3}} \\
\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 \\
0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 \\
\sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & \cdots & 0 \\
\vdots & & & & & & \\
\sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & \cdots & 0 
\end{bmatrix}
\]

Note that the sum of principal minors of size 2 and 4 in \( \Omega(S^3_n) \) 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 \( S^3_n \) 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 \( \vartheta_1(S^3_n) = \sqrt{\frac{2n^2 - 13n + 23 + \sqrt{(2n^2 - 13n + 23)^2 - 4(n-3)(4n^2 - 31n + 61)}}{4(n-3)}} \).

We claim that \( \vartheta_1(S^3_n) > \vartheta_1(S^4_n) \), where the expression for \( \vartheta_1(S^4_n) \) is given in Theorem 2.3. Squaring both sides and then cross-multiplying, we get
\[
3 \left( 2n^2 - 13n + 23 + \sqrt{(2n^2 - 13n + 23)^2 - 4(n-3)(4n^2 - 31n + 61)} \right) > 2 \left( 3n^2 - 19n + 34 + \sqrt{(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2} \right),
\]
which means
\[
3 \sqrt{(2n^2 - 13n + 23)^2 - 4(n-3)(4n^2 - 31n + 61)} > n - 1 + 2 \sqrt{(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2}.
\]

It can be seen that
\[
(3n^2 - 19n + 34)^2 - 48(n-3)(n-4)^2 = (3n^2 - 27n + 65)^2 - (26n^2 - 298n + 765) < (3n^2 - 27n + 65)^2.
\]
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.

**Lemma 2.6.** Let \(n \geq 7\), then
\[
\vartheta_1(S^5_n) = \sqrt{\frac{2n^2 - 15n + 31 + \sqrt{(2n^2 - 15n + 31)^2 - 8(n - 3)(n^2 - 9n + 20)}}{4(n - 3)}},
\]
and \(\vartheta_1(S^5_n) < \vartheta_1(S^4_n)\).

**Proof.** With a suitable permutation of vertices, the ABC matrix of \(S^5_n\) can be written as
\[
\Omega(S^5_n) = \begin{bmatrix}
0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \sqrt{\frac{n-4}{n-3}} & \cdots & \sqrt{\frac{n-4}{n-3}} \\
\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \cdots & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & \cdots & 0 \\
\frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 \\
0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 \\
\sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\sqrt{\frac{n-4}{n-3}} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 
\end{bmatrix}
\]

Note that the sum of principal minors of size 2, 4, 6 in \(\Omega(S^5_n)\) is \(-2 - \frac{(n-4)(n-5)}{n-3} \cdot \frac{3}{4} + \frac{(n-4)(n-5)}{n-3}\) and \(-\frac{(n-4)(n-5)}{4(n-3)}\), respectively. The rest of principal minors are zero. Therefore, the ABC characteristic polynomial of \(S^5_n\) 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, \(\vartheta_1(S^5_n)\) is the square-root of the largest root of following polynomial
\[
f(x) = x^3 - \left( 2 + \frac{(n-4)(n-5)}{n-3} \right) x^2 + \left( \frac{3}{4} + \frac{(n-4)(n-5)}{n-3} \right) x - \frac{(n-4)(n-5)}{4(n-3)}
= \frac{(2x-1) (2(n-3)x^2 - (2n^2 - 15n + 31)x + (n^2 - 9n + 20))}{4(n-3)}.
\]

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
\[
3 \left(2n^2 - 15n + 31 + \sqrt{(2n^2 - 15n + 31)^2 - 8(n - 3)(n^2 - 9n + 20)}\right) \\
< 2 \left(3n^2 - 19n + 34 + \sqrt{(3n^2 - 19n + 34)^2 - 48(n - 3)(n - 4)^2}\right).
\]

Equivalently, it suffices to show that
\[
3\sqrt{(2n^2 - 15n + 31)^2 - 8(n - 3)(n^2 - 9n + 20)} \\
< 7n + 5 + 2\sqrt{(3n^2 - 19n + 34)^2 - 48(n - 3)(n - 4)^2}.
\] (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 \( S_n, S^2_n, S^3_n, S^4_n \) are the trees with first four values of \( \vartheta_1(T) \) in \( T_n \). 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 \( r \), \( \Omega(G) = \sqrt{2(r-1)} A(G) \). 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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