

ON THE MAXIMUM ABC SPECTRAL RADIUS OF CONNECTED GRAPHS WITH GIVEN MAXIMUM DEGREE

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The ABC spectral radius of a graph G , denoted by $\rho(G)$, has attracted more and more attentions. In this paper, we prove that $\rho(G) \leq \sqrt{\Delta + (2m - n + 1)/\Delta - 2}$, where G is a connected graph with n vertices, m edges, and maximum degree Δ . As applications, we reproduce the upper bounds of ABC spectral radius for connected graphs, trees, unicyclic graphs, and bicyclic graphs. In addition, we determine the unique tree with second largest ABC spectral radius.

1. INTRODUCTION


Let $G = (V, E)$ be a simple connected graph, where $V = \{v_1, v_2, \dots, v_n\}$. If $c = m - n + 1$ (≥ 0), then G is called a c -cyclic graph. In particular, G is called a tree, unicyclic graph, and bicyclic graph, if $c = 0, 1, 2$, respectively. As usual, S_n , P_n , C_n , and K_n will denote the star, path, cycle, and complete graph, respectively.

Let d_i denote the degree of vertex v_i , and $\Delta = \Delta(G)$ the maximum degree of G . The atom-bond connectivity index (ABC index in short) of G is defined [21] as $ABC(G) = \sum_{v_i v_j \in E} f(d_i, d_j)$, where $f(x, y) = \sqrt{(x + y - 2)/(xy)}$. Since this index can predict well the heat of formation of alkanes (see [20, 26]), it became a hot

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topic in the past few years (see [22, 7, 36, 37, 2, 6, 3, 24, 32, 33, 25, 8, 9, 18, 10, 11, 13, 29, 34, 12, 30, 14, 16, 39, 17, 27, 15]).

In 2017, Estrada [19] defined the ABC matrix of G as $M = M(G) = (m_{ij})_{n \times n}$, where $m_{ij} = f(d_i, d_j)$ if $v_i v_j \in E$, and 0 otherwise. The entry m_{ij} indicates the polarizing capacity of the bond $v_i v_j \in E$, which is considered in a molecular context, and stands for the probability of visiting a nearest neighbor edge from one side or the other of a given edge in graph G . The eigenvalues of M are called the ABC eigenvalues of G . Because M is non-negative, symmetric, and irreducible, any ABC eigenvalue of G is real. In particular, the largest ABC eigenvalue of G is called its ABC spectral radius, and denoted by $\rho(G)$. Obviously, $\rho(G)$ is positive and simple. Moreover, there exists a unique vector $x > 0$ such that $\rho(G) = \max_{\|y\|=1} y^T M y = x^T M x$, which is known as the Perron vector of M .

Estrada [19] proved that $\frac{2}{n} ABC(G) \leq \rho(G) \leq \max_{1 \leq i \leq n} M_i$, with both equalities iff M_i is the same for $1 \leq i \leq n$, where $M_i = \sum_{1 \leq j \leq n} m_{ij}$. Recently, Chen [4] presented another lower bound of $\rho(G)$ in terms of $R_{-1}(G)$, which is the sum of $\frac{1}{d_i d_j}$ over all edges $v_i v_j \in E$. Chen [4] further proposed the problem of characterizing graphs with extremal ABC spectral radius for a given graph class. Soon, this problem for trees, connected graphs, and unicyclic graphs were solved by Chen [5], Ghorbani et al. [23], and Li et al. [28], respectively.

Theorem 1. ([5]) *Let T be a tree of order $n \geq 3$. Then*

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

with the left (right) equality iff $T \cong P_n$ (resp., $T \cong S_n$).

Theorem 2. ([23]) *Let G be a connected graph of order $n \geq 3$. Then*

$$\sqrt{2} \cos \frac{\pi}{n+1} \leq \rho(G) \leq \sqrt{2n-4},$$

with the left (right) equality iff $G \cong P_n$ (resp., $G \cong K_n$).

Theorem 3. ([28]) *Let G be a unicyclic graph of order $n \geq 4$. Then*

$$\sqrt{2} = \rho(C_n) \leq \rho(G) \leq \rho(S_n + e),$$

with the left (right) equality iff $G \cong C_n$ (resp., $G \cong S_n + e$).

Recently, Yuan and Du [38] determined the first two bicyclic graphs with maximum ABC spectral radii. Their main result can be restated as follows.

Theorem 4. ([38]) *Let G be a bicyclic graph of order $n \geq 7$ other than B_1 and B_2 (shown in Figure 1). Then*

$$\rho(G) < \rho(B_2) < \rho(B_1).$$

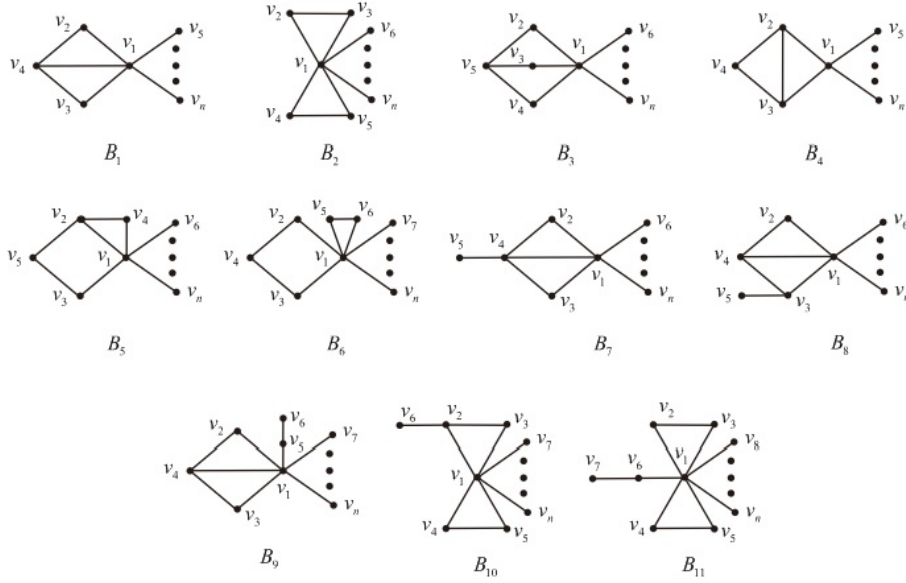


Figure 1: The 11 bicyclic graphs of order n with maximum degree $n - 1$ or $n - 2$.

In the present paper, we establish an upper bound of ρ for connected graphs in terms of maximum degree. It is shown that, if G is a connected graph with n vertices, m edges, and maximum degree Δ , then $\rho(G) \leq \sqrt{\Delta + (2m - n + 1)/\Delta} - 2$. As applications, we reproduce (the upper bound parts of) Theorems 1.1–1.4, and determine the unique tree with second largest ABC spectral radius.

2. AN UPPER BOUND IN TERMS OF MAXIMUM DEGREE

In this section, we present an upper bound of ρ for connected graphs in terms of maximum degree.

Theorem 5. *If G is a connected graph with n vertices, m edges, and maximum degree Δ , then*

$$\rho(G) \leq \sqrt{\Delta + (2m - n + 1)/\Delta} - 2.$$

Moreover, the bound is attainable.

Proof. Let $M = M(G)$, $D = 2m - n + 1$, and $x = (\sqrt{d_1}, \sqrt{d_2}, \dots, \sqrt{d_n})^T$. From the Perron-Frobenius theory, it suffices to confirm the claim: $(Mx)_i \leq \sqrt{d_i} \sqrt{\Delta + D/\Delta} - 2$ or $[(Mx)_i / \sqrt{d_i}]^2 \leq \Delta + D/\Delta - 2$ holds for $1 \leq i \leq n$.

If $d_i < D/\Delta$, then

$$(Mx)_i = \sum_{v_i v_j \in E} f(d_i, d_j) \sqrt{d_j} \leq d_i \sqrt{\frac{d_i + \Delta - 2}{d_i}} < \sqrt{d_i} \sqrt{D/\Delta + \Delta - 2}.$$

Hence assume $d_i \geq D/\Delta$. By using the Cauchy-Schwarz inequality we have

$$\begin{aligned} [(Mx)_i]^2 &= \left[\sum_{v_i v_j \in E} \sqrt{(d_i + d_j - 2)/d_i} \right]^2 \\ &\leq \sum_{v_i v_j \in E} 1^2 \cdot \sum_{v_i v_j \in E} (d_i + d_j - 2)/d_i \\ &= d_i \sum_{v_i v_j \in E} (d_i + d_j - 2)/d_i \\ &= \sum_{v_i v_j \in E} (d_i + d_j - 2) \\ &= d_i^2 - 2d_i + \sum_{v_i v_j \in E} d_j \\ &\leq d_i^2 - 2d_i + [2m - d_i - (n - d_i - 1)] \\ &= d_i^2 - 2d_i + D. \end{aligned}$$

Thus $[(Mx)_i/\sqrt{d_i}]^2 \leq d_i + D/d_i - 2$. Since $\eta(t) = t + D/t - 2$ is a Nike function and $D/\Delta \leq d_i \leq \Delta$, it follows that

$$[(Mx)_i/\sqrt{d_i}]^2 \leq \max\{\eta(D/\Delta), \eta(\Delta)\} = \Delta + D/\Delta - 2.$$

Finally, to see the bound is attainable, one can take S_n and K_n as examples. The proof is thus completed. \square

Obviously, $\theta(m, \Delta) = \sqrt{\Delta + (2m - n + 1)/\Delta - 2}$ strictly increases with m for fixed Δ . On the other hand, for fixed m , the monotonicity of $\theta(m, \Delta)$ with respect to Δ is also clear. That is, if $\Delta_1 \leq \Delta(G) \leq \Delta_2$, then $\rho(G) \leq \max\{\theta(m, \Delta_1), \theta(m, \Delta_2)\}$. In practice, one can take $\Delta_1 = 2$ or $2m/n$, the average degree of G . Note please, $\theta(m, 2m/n)$ also strictly increases with m . Thus, we can easily reproduce the upper bound part of Theorem 1.2 as follows.

Corollary 6. ([23]) *Let G be a connected graph of order $n \geq 3$. Then $\rho(G) \leq \sqrt{2n - 4}$, with equality iff $G \cong K_n$.*

Proof. Let m be the edge number of G . From Theorem 2.1 and the monotonicity of $\theta(m, \Delta)$, we have

$$\rho(G) \leq \max\{\theta(m, 2m/n), \theta(m, n - 1)\} \leq \theta(n(n - 1)/2, n - 1) = \sqrt{2n - 4},$$

with equalities only if $G \cong K_n$. Conversely, it holds $\rho(K_n) = \sqrt{2n - 4}$. \square

3. UPPER BOUNDS OF c -CYCLIC GRAPHS

Theorem 7. *Let G be a c -cyclic graph of order $n \geq 3$ with maximum degree Δ , and $c \leq (n - 1)/2$. Then*

$$\rho(G) \leq \sqrt{\Delta - 2 + (n - 1 + 2c)/\Delta} \leq \sqrt{n - 2 + 2c/(n - 1)} \leq \sqrt{n - 1}.$$

Proof. Since $m = n - 1 + c$ and $c \leq (n - 1)/2$, by direct calculations we have

$$\theta(m, 2) = \sqrt{(n - 1)/2 + c} \leq \theta(m, n - 1) = \sqrt{n - 2 + 2c/(n - 1)} \leq \sqrt{n - 1},$$

and the conclusion follows from Theorem 2.1. □

For trees ($c = 0$), we immediately reproduce the upper bound part of Theorem 1.1.

Corollary 8. ([5]) *Let T be a tree of order $n \geq 3$. Then $\rho(T) \leq \sqrt{n - 2}$, with equality iff $T \cong S_n$.*

Proof. From Theorem 3.1 we have $\rho(T) \leq \sqrt{n - 2}$, with equality only if $\Delta(T) = n - 1$ or $T \cong S_n$. Conversely, it holds $\rho(S_n) = \sqrt{n - 2}$. □

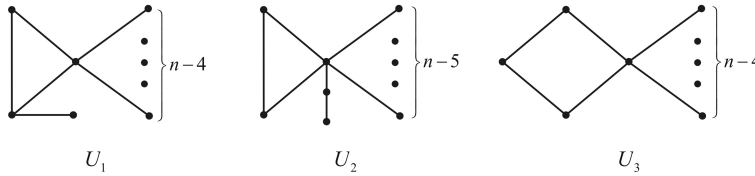


Figure 2: The 3 unicyclic graphs of order n with maximum degree $n - 2$.

For unicyclic graphs ($c = 1$), it is easily verified that $S_n + e$ (the graph formed from S_n by adding one edge between two pendent vertices) uniquely has largest ABC spectral radius if $n \leq 6$. Hence assume $n \geq 7$. If G is a unicyclic graph of order n with $\Delta(G) \leq n - 3$, then $\rho(G) \leq \sqrt{n - 5 + (n - 1 + 2)/(n - 3)} \leq \sqrt{n - 3}$ from Theorem 3.1. Hence the upper bound part of Theorem 1.3 can be easily reproduced by showing that $\rho(U_1), \rho(U_2), \rho(U_3) < \sqrt{n - 3} < \rho(S_n + e)$, where U_1, U_2 , and U_3 (shown in Figure 2) are the unicyclic graphs with maximum degree $n - 2$.

For bicyclic graphs ($c = 2$), it is easily verified that B_1 and B_2 are the unique graphs with the first two maximum ABC spectral radii for $n \leq 21$, respectively. Hence assume $n \geq 22$. It is easily seen that $\rho(B_1) > \rho(B_2) > \sqrt{n - 4 + 12/n}$. If G is a bicyclic graph of order n with $\Delta(G) \leq n - 3$, from Theorem 3.1 we have $\rho(G) \leq \sqrt{n - 5 + (n + 3)/(n - 3)} < \sqrt{n - 4 + 12/n}$. Hence, to reproduce Theorem 1.4, it remains to show that $\rho(B_i) < \sqrt{n - 4 + 12/n}$, where B_i 's ($i = 3, 4, \dots, 11$, shown in Figure 1) are the bicyclic graphs with maximum degree $n - 2$.

4. THE TREE WITH SECOND LARGEST ABC SPECTRAL RADIUS

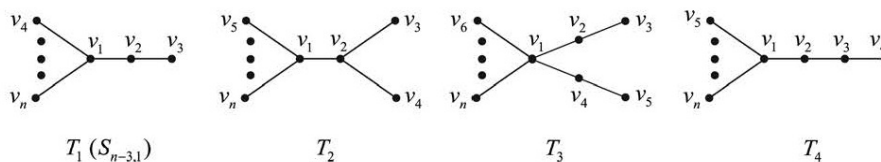


Figure 3: The trees T_i , $i=1, 2, 3, 4$.

In order to further illustrate the application of Theorem 2.1, in this section we determine the tree of order $n \geq 4$ with second largest ABC spectral radius. We would like to remark that, though the this tree has been determined in [1], the method we use here is different. In addition, in order to avoid circular citation, any results from [1] or [35] will not be used.

For convenience, let \mathcal{T}_n be the set of trees of order n . Let $T_1 (= S_{n-3,1}), T_2, T_3$, and T_4 are the trees shown in Figure 3. Our aim is to prove the following result.

Theorem 9. *If $n \geq 4$ and $T \in \mathcal{T}_n - \{S_n, S_{n-3,1}\}$, then*

$$\rho(T) < \rho(S_{n-3,1}) < \rho(S_n).$$

Obviously, $\mathcal{T}_4 = \{S_4, S_{1,1} \cong P_4\}$, $\mathcal{T}_5 = \{S_5, S_{2,1}, P_5\}$, and $\mathcal{T}_6 = \{S_6, S_{3,1}, T_2, T_3, T_4, P_6\}$. It is easily verified that, $\rho(T) < \rho(S_{n-3,1}) < \rho(S_n)$ for $n \leq 6$. Hence assume $n \geq 7$. We will complete the proof of Theorem 4.1 by the following Lemmas.

For two vertices v_i and v_j of a graph G , they are said to be equivalent, denoted by $v_i \sim v_j$, if there is an automorphism of G sending v_i to v_j . By symmetry, the following result is immediate.

Lemma 10. *Let $x = (x_1, x_2, \dots, x_n)^T$ be the Perron vector of the ABC matrix $M(G)$ of a connected graph G . If $v_i \sim v_j$, then $x_i = x_j$.*

Lemma 11. $\rho(S_{n-3,1}) > \sqrt{n-3.5}$.

Proof. Let $\rho = \rho(S_{n-3,1})$, and label the vertices of $S_{n-3,1}$ as in Figure 2. Based on Lemma 4.2, let $x = (x_1, x_2, x_3, x_4, \dots, x_n)^T$ be the Perron vector of $M = M(S_{n-3,1})$. From $\rho x = Mx$ we have

$$\begin{cases} \rho x_1 = (n-3)\sqrt{\frac{n-3}{n-2}}x_4 + \sqrt{\frac{1}{2}}x_2 \\ \rho x_2 = \sqrt{\frac{1}{2}}x_1 + \sqrt{\frac{1}{2}}x_3 > \sqrt{\frac{1}{2}}x_1 \\ \rho x_4 = \sqrt{\frac{n-3}{n-2}}x_1 \end{cases} .$$

Hence $\rho^2 x_1 = (n-3)\sqrt{\frac{n-3}{n-2}}\rho x_4 + \sqrt{\frac{1}{2}}\rho x_2 > \frac{(n-3)^2}{n-2}x_1 + \frac{1}{2}x_1$, and we arrive at

$$\rho^2 > (n-3)^2/(n-2) + 1/2 > n-4 + 0.5 = n-3.5.$$

□

Lemma 12. *If $T \in \mathcal{T}_n$ and $\Delta(T) \leq n-3$, then $\rho(T) \leq \sqrt{n-3.5}$.*

Proof. From Theorem 3.1, $\rho(T) \leq \sqrt{n-5 + (n-1)/(n-3)} \leq \sqrt{n-3.5}$. □

5. FURTHER DISCUSSIONS

In this paper, we present an upper bound of ABC spectral radius in terms of maximum degree. That is, we prove that $\rho(G) \leq \sqrt{\Delta + (2m-n+1)/\Delta - 2}$ for a connected graph G with n vertices, m edges, and maximum degree Δ . The bound is attained by S_n and K_n . Firstly, the following problem may be worth considering.

Problem 1. *Characterize connected graphs G with n vertices, m edges, and maximum degree Δ such that $\rho(G) = \sqrt{\Delta + (2m-n+1)/\Delta - 2}$.*

The main result is quite strong, hence we are able to easily reproduce the upper bounds for connected graphs and c -cyclic graphs ($c = 0, 1, 2$) which were obtained in [5, 23, 28, 38]. In addition, the double star $S_{n-3,1}$ is shown to be the unique tree having second largest ABC spectral radius if $n \geq 4$. Recall that, Lin et al. [31] ordered trees by their (adjacent) spectral radius λ_1 , and showed that, if T_1 and T_2 are two trees of order $n \geq 4$, and $\Delta(T_1) > \Delta(T_2) \geq \lceil 2n/3 \rceil - 1$, then $\lambda_1(T_1) > \lambda_1(T_2)$. Naturally, the following question is interesting.

Question 2. *Let G_1 and G_2 be two graphs with n vertices and m edges. Is there some integer $\ell(m, n)$ (depending on n and/or m), such that if $\Delta(G_1) > \Delta(G_2) \geq \ell(m, n)$, then $\rho(G_1) > \rho(G_2)$?*

This question may be difficult to answer at the present, even for trees, and the following two problems are worth investigation in advance.

Problem 3. *Order graphs in some classes of connected graphs by their ABC spectral radii.*

Problem 4. *Establish non-trivial lower bounds of $\rho(G)$ for a connected graph G in terms of maximum degree.*

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