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ON THE ABC SPECTRAL RADIUS OF CACTUS GRAPHS

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Abstract. Let G be a graph with vertex set $V(G)$. Denote by d_u the degree of vertex u in G. The ABC matrix of G, proposed by Estrada, is the matrix $(ABC_{uv})_{u,v\in V(G)}$, where $ABC_{uv} = \sqrt{\frac{d_u+d_v-2}{d_ud_v}}$ if u and v are adjacent, and 0 otherwise. The ABC spectral radius of G is the largest eigenvalue of the ABC matrix of G. In this paper, we determine the unique cactus graph with the largest ABC spectral radius among all cactus graphs with fixed order and number of cycles, and the cactus graphs of order n with the first a few largest ABC spectral radii for $n \geqslant 4$.

1. Introduction

We consider simple (connected) graphs. For a graph G, denote by $V(G)$ the vertex set, and $E(G)$ the edge set of G. For $u \in V(G)$, denote by $d_G(u)$, or simply d_u when only one graph is under consideration, the degree of u in G. An edge uv of G is called a pendent edge if $d_u = 1$ or $d_v = 1$, and a vertex v is called a pendent vertex if $d_v = 1$.

The ABC matrix of G, put forward by Estrada [6] in a molecular context, is defined to be the matrix $ABC(G) = (ABC_{uv})_{u,v\in V(G)}$, where

$$ABC_{uv} = \begin{cases} \sqrt{\frac{d_u+d_v-2}{d_ud_v}} & \text{if } uv \in E(G), \\ 0 & \text{if } uv \notin E(G). \end{cases}$$

As pointed out in [6], for an edge uv of the graph G, the (u,v)-entry of the ABC matrix indicates the polarizing capacity of the bond uv in a molecular context, as it represents the probability of visiting a nearest neighbor edge from one side or the other of a given edge in a graph. Actually, Estrada [6] provided a probabilistic interpretation of a graph invariant called the generalized ABC index, which is a generalization of the much studied atom-bond connectivity index [9] (abbreviated ABC index [12]) and then introduced a matrix representation of these probabilities in the form of generalized ABC matrices.

For a graph G, the largest eigenvalue of $ABC(G)$ is called the ABC spectral radius of G, denoted by $\rho(G)$. Although initiated in 2017, the ABC spectral radius of graphs has already attracted much attention. The study of the ABC spectral radii of trees,

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unicyclic graphs and bicyclic graphs may be found in [4, 13, 15], respectively. More results on the ABC spectral radius of graphs may be found in [3, 5, 6, 11, 13, 16]. We mention that Estrada [6] also studied some other graph parameters related to the eigenvalues of the ABC matrices, such as the ABC energy and the ABC Estrada index (see [8] and [7] for a look on the ordinary energy and Estrada index, respectively). One may find some results on the ABC energy in [3, 11, 10].

A cactus graph is a connected graph in which any two cycles have at most one common vertex. Let $\mathbb{C}(n)$ be the set of cactus graphs of order n, and $\mathbb{C}(n,k)$ the set of cactus graphs of order n with k cycles, where $0 \leqslant k \leqslant \lfloor \frac{n-1}{2} \rfloor$. In this article, we determine the graph in $\mathbb{C}(n,k)$ that uniquely maximizes the ABC spectral radius for $0 \leqslant k \leqslant \lfloor \frac{n-1}{2} \rfloor$, and we further determine the graphs in $\mathbb{C}(n)$ with the first three largest ABC spectral radii for $4 \leqslant n \leqslant 23$, and with the first four largest ABC spectral radii for $n \geqslant 24$.

2. Preliminaries

For an edge subset M of a graph G, let $G-M$ denote the graph obtained from G by deleting the edges in M, and for an edge subset M^* of the complement of G, let $G+M^*$ denote the graph obtained from G by adding the edges in M^*. In particular, if $M=\{uv\}$, then we write $G-uv$ for $G-\{uv\}$, and if $M^*=\{uv\}$, then we write $G+uv$ for $G+\{uv\}$.

Note that the graphs in $\mathbb{C}(n,0)$ are trees, and graphs in $\mathbb{C}(n,1)$ are unicyclic graphs. For $n \geqslant 4$, let D_n be the tree of order n with a path of length 2 and $n-3$ edges attached at a common end vertex. Let $T_{n,1}$ be the tree of order $n \geqslant 6$ with one path of length 3 and $n-4$ edges attached at a common end vertex, and $T_{n,2}$ the tree of order $n \geqslant 6$ obtained from D_{n-1} by adding a new edge incident with the vertex of degree 2. All these trees are illustrated in Figure 1.

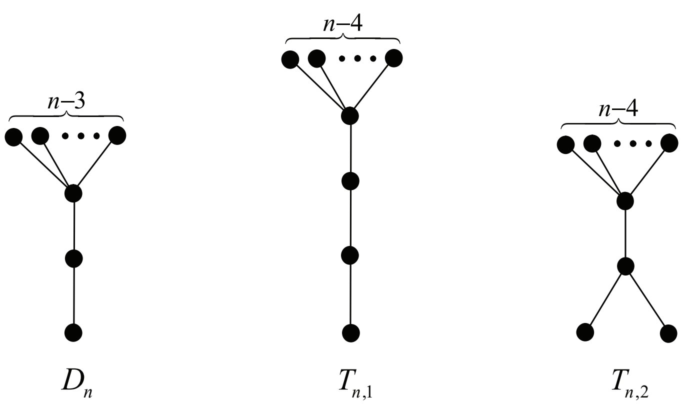

Figure 1: *The trees D_n, $T_{n,1}$ and $T_{n,2}$.*

Let $C_{n,k}$ be the cactus graph obtained from the n-vertex star S_n by adding k independent edges, where $0 \leqslant k \leqslant \lfloor \frac{n-1}{2} \rfloor$, see Figure 2.

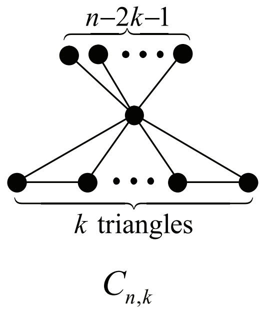

Figure 2: *The cactus graph $C_{n,k}$.*

LEMMA 1. [1, 14] *Among the trees $\mathbb{C}(n,0)$ with $n \geqslant 6$,*

(*i*) *if $n = 6,7,8$, then $C_{n,0}$, D_n, and $T_{n,2}$ are, respectively, the unique trees with the first three largest ABC spectral radii;*

(*ii*) *if $n \geqslant 9$, then $C_{n,0}$, D_n, and $T_{n,1}$ are, respectively, the unique trees with the first three largest ABC spectral radii.*

We mention that the above ordering was given in [1] for $n \geqslant 11$. As to the small n with $6 \leqslant n \leqslant 10$, one can deduce the corresponding ordering by considering maximum degree as in [14] or as what we used for unicyclic graphs in [16].

Note that $\rho(C_{n,0}) = \sqrt{n-2}$, and $\rho(D_n)$, $\rho(T_{n,1})$, and $\rho(T_{n,2})$ are, respectively, the largest roots of the equations on x:

$$2(n-2)x^4 - 2(n^2-5n+7)x^2 + (n-3)^2 = 0,$$

$$4(n-3)x^4 - 2(2n^2-13n+23)x^2 + 4n^2 - 31n + 61 = 0,$$

and

$$3(n-3)x^4 - (3n^2-19n+34)x^2 + 4(n-4)^2 = 0.$$

Let $U_{n,1}$ be the unicyclic graph of order $n \geqslant 5$ obtained from a quadrangle by adding $n-4$ edges incident with a common vertex, and $U_{n,2}$ the unicyclic graph of order $n \geqslant 5$ obtained from $C_{n-1,1}$ by adding an edge incident with a vertex of degree two, see Figure 3.

LEMMA 2. [16] *Among the graphs in $\mathbb{C}(n,1)$ with $n \geqslant 5$,*

(*i*) *if $5 \leqslant n \leqslant 18$, then $C_{n,1}$ and $U_{n,2}$ are, respectively, the unique unicyclic graphs with the first two largest ABC spectral radii;*

(*iii*) *if $n \geqslant 19$, then $C_{n,1}$ and $U_{n,1}$ are, respectively, the unique unicyclic graphs with the first two largest ABC spectral radii.*

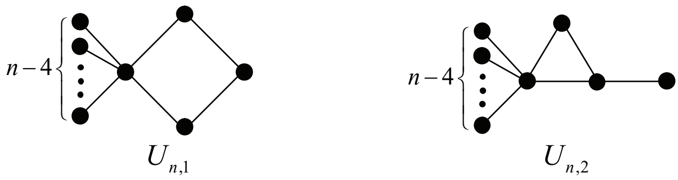

Figure 3: *The unicyclic graphs* $U_{n,1}$ *and* $U_{n,2}$.

Note that $\rho(C_{n,1})$, $\rho(U_{n,1})$, and $\rho(U_{n,2})$ are, respectively, the largest roots of the equations on x:

$$2(n-1)x^3-\sqrt{2}(n-1)x^2-2(n^2-4n+5)x+\sqrt{2}(n-2)(n-3)=0,$$

$$(n-2)x^4-(n^2-5n+8)x^2+(n-3)(n-4)=0,$$

and

$$6(n-2)x^4-2(3n^2-15n+25)x^2-2\sqrt{3(n-1)(n-2)}x+7n^2-47n+80=0.$$

3. The ABC spectral radius of cactus graphs

For an n-vertex graph G, we introduce the revised of ABC matrix of G, denoted by $\widetilde{ABC}(G)$, is the matrix $(\widetilde{ABC}_{uv})_{u,v\in V(G)}$, where

$$\widetilde{ABC}_{uv}=\begin{cases}\sqrt{\frac{n-2}{n-1}} & \text{if } uv \text{ is a pendent edge of } G,\\ \sqrt{\frac{1}{2}} & \text{if } uv \text{ is an edge of } G\text{, but not a pendent edge,}\\ 0 & \text{if } uv\notin E(G).\end{cases}$$

Let $\widetilde{\rho}(G)$ be the largest eigenvalue of $\widetilde{ABC}(G)$, which we call the revised ABC spectral radius. Note that, if $n\geqslant 3$, then $\widetilde{ABC}(G)$ has the same zero-nonzero pattern as the adjacency matrix of G, so $\widetilde{ABC}(G)$ is irreducible if and only if G is connected. In this case, by Perron-Frobenius theory (see, e.g., [2, Theorem 1.4, p. 27]), corresponding to $\widetilde{\rho}(G)$, there is a unique positive unit eigenvector, say $\mathbf{x}$. For any $v\in V(G)$, denote by x_v the entry in $\mathbf{x}$ corresponding to vertex v throughout this paper. Particularly, for any $u\in V(G)$,

$$\widetilde{\rho}(G)x_u=\sum_{v\in V(G)}\widetilde{ABC}_{uv}x_v.$$

LEMMA 3. *Let G be a graph. Then $ABC_{uv}\leqslant\widetilde{ABC}_{uv}$ for any vertices $u,v\in V(G)$.*

Proof. When uv is not an edge of G, $ABC_{uv}=\widetilde{ABC}_{uv}=0$, it is already done. Suppose that uv is an edge of G in the following. Assume that $d_u\geqslant d_v$, and set $f(d_u,d_v)=\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$.

It is easy to verify that $f(d_u,d_v)$ increases in d_u when $d_v=1$, and decreases in d_u for fixed $d_v \geqslant 2$. As a consequence, if uv is a pendent edge of G, then

$$f(d_u,d_v)=f(d_u,1)\leqslant f(n-1,1)=\sqrt{\frac{n-2}{n-1}},$$

and if uv is not a pendent edge of G, then

$$f(d_u,d_v)\leqslant f(2,2)=\sqrt{\frac{1}{2}}.$$

In either case, the corresponding inequality is equivalent to our desired result that $ABC_{uv}\leqslant \widetilde{ABC}_{uv}$. □

LEMMA 4. *Let G be a graph. Then $\rho(G)\leqslant\widetilde{\rho}(G)$ with equality when G is connected if and only if $ABC(G)=\widetilde{ABC}(G)$.*

Proof. It is a direct consequence of Lemma 3 and part of the famous Perron-Frobenius theory (see, e.g., [2, Corollary 1.5, p. 27]). □

LEMMA 5. *Let G be a connected graph of order $n\geqslant 4$, where $vw_i\in E(G)$ and $uw_i\notin E(G)$ for $1\leqslant i\leqslant r$. Assume that $d_G(v)\geqslant r+1\geqslant 2$ and $d_G(u)\geqslant 2$. Denote by $\mathbf{x}$ the unique positive unit eigenvector of $\widetilde{ABC}(G)$ corresponding to $\widetilde{\rho}(G)$. Consider $G_1=G-\{vw_1,vw_2,\dots,vw_r\}+\{uw_1,uw_2,\dots,uw_r\}$. If $x_u\geqslant x_v$, then $\widetilde{\rho}(G)<\widetilde{\rho}(G_1)$.*

Proof. Among $vw_1,vw_2,\dots,vw_r$, assume that there are s edges which are pendent in G, where $0\leqslant s\leqslant r$. Further, we may assume that vw_i is a pendent edge of G for $i=1,2,\dots,s$, and vw_i is not a pendent edge of G for $i=s+1,s+2,\dots,r$. It is easy to see that vw_i is a pendent edge of G if and only if uw_i is a pendent edge of G_1, which implies that the (v,w_i)-entry in $\widetilde{ABC}(G)$ coincides with the (u,w_i)-entry in $\widetilde{ABC}(G_1)$, for $1\leqslant i\leqslant r$.

First suppose that $d_G(v)\geqslant r+2$. Under this condition, $d_{G_1}(v)\geqslant 2$, thus wy is a pendent edge of G if and only if wy is a pendent edge of G_1, for each $wy\in E(G)\setminus\{vw_1,vw_2,\dots,vw_r\}$, that is to say, the (w,y)-entries in $\widetilde{ABC}(G)$ and $\widetilde{ABC}(G_1)$ are the same. It is standard to get by Rayleigh's principle that

$$\begin{aligned}\widetilde{\rho}(G_1)-\widetilde{\rho}(G)&\geqslant \mathbf{x}^T(\widetilde{ABC}(G_1)-\widetilde{ABC}(G))\mathbf{x}\\&=2(x_u-x_v)\left(\sqrt{\frac{n-2}{n-1}}\sum_{i=1}^{s}x_{w_i}+\sqrt{\frac{1}{2}}\sum_{i=s+1}^{r}x_{w_i}\right)\\&\geqslant 0,\end{aligned}$$

i.e., $\widetilde{\rho}(G)\leqslant\widetilde{\rho}(G_1)$. In particular, if $\widetilde{\rho}(G_1)=\widetilde{\rho}(G)$, then $\mathbf{x}$ is also an eigenvector of $\widetilde{ABC}(G_1)$ corresponding to $\widetilde{\rho}(G_1)$. However, such situation would result in

$$\widetilde{\rho}(G_1)x_u-\widetilde{\rho}(G)x_u=\sqrt{\frac{n-2}{n-1}}\sum_{i=1}^{s}x_{w_i}+\sqrt{\frac{1}{2}}\sum_{i=s+1}^{r}x_{w_i}=0,$$

which is impossible, since $x_{w_i} > 0$. Therefore, $\widetilde{\rho}(G) < \widetilde{\rho}(G_1)$ follows.

Next suppose that $d_G(v) = r+1$. At this time, $d_{G_1}(v) = 1$. Assume that z is the unique neighbor of v in G different from $w_1, w_2, \dots, w_r$. Note that vz is a pendent edge in G_1 whether $d_G(z) = 1$ or not. When $d_G(z) = 1$, the above proof (about $d_G(v) \geqslant r+2$) is still valid. But when $d_G(z) \geqslant 2$, there exists some difference, which comes from the fact that vz would be changed from a non-pendent edge in G into a pendent edge in G_1 (in the aspect of entries, the (v,z)-entry in $\widetilde{ABC}(G)$ is $\sqrt{\frac{1}{2}}$, but is $\sqrt{\frac{n-2}{n-1}}$ in $\widetilde{ABC}(G_1)$). In this case, as $\sqrt{\frac{n-2}{n-1}} > \sqrt{\frac{1}{2}}$, one has

$$
\begin{aligned}
\widetilde{\rho}(G_1) - \widetilde{\rho}(G) &\geqslant \mathbf{x}^T(\widetilde{ABC}(G_1) - \widetilde{ABC}(G))\mathbf{x} \\
&= 2(x_u - x_v)\left(\sqrt{\frac{n-2}{n-1}}\sum_{i=1}^{s} x_{w_i} + \sqrt{\frac{1}{2}}\sum_{i=s+1}^{r} x_{w_i}\right) \\
&\quad +2\left(\sqrt{\frac{n-2}{n-1}} - \sqrt{\frac{1}{2}}\right)x_v x_z \\
&> 2(x_u - x_v)\left(\sqrt{\frac{n-2}{n-1}}\sum_{i=1}^{s} x_{w_i} + \sqrt{\frac{1}{2}}\sum_{i=s+1}^{r} x_{w_i}\right) \\
&\geqslant 0,
\end{aligned}
$$

so $\widetilde{\rho}(G) < \widetilde{\rho}(G_1)$.

In conclusion, we can get $\widetilde{\rho}(G) < \widetilde{\rho}(G_1)$ in either case. □

LEMMA 6. *Let G be a graph in $\mathbb{C}(n,k)$ that maximizes the revised ABC spectral radius, where $n \geqslant 4$ and $uv \in E(G)$. If $d_G(u), d_G(v) \geqslant 2$, then uv is an edge of a triangle, and at least one of u, v is of degree 2.*

Proof. Let $\mathbf{x}$ be an eigenvector of $\widetilde{ABC}(G)$ corresponding to $\widetilde{\rho}(G)$. We always assume that $x_u \geqslant x_v$.

First suppose that uv is a cut edge of G. Then uv lies outside any cycle of G and in particular, u and v have no common neighbor. Denote by $w_1, w_2, \dots, w_r$ the neighbors of v in G different from u, where $r = d_G(v) - 1 \geqslant 1$. Let $G_1 = G - \{vw_1, vw_2, \dots, vw_r\} + \{uw_1, uw_2, \dots, uw_r\}$. As $G \in \mathbb{C}(n,k)$, we have $G_1 \in \mathbb{C}(n,k)$. By Lemma 5, we get $\widetilde{\rho}(G) < \widetilde{\rho}(G_1)$, which is a contradiction to the maximality of $\widetilde{\rho}(G)$. This shows that uv is not a cut edge.

As uv is not a cut edge of G, we may assume that u and v lie on some cycle, say C, of G. Denote by w the other neighbor of v lying on C different from u. If C is of length at least 4, then clearly u and w are not adjacent. Let $G_2 = G - vw + uw$. Clearly, G_2 is still in $\mathbb{C}(n,k)$. By Lemma 5, $\widetilde{\rho}(G) < \widetilde{\rho}(G_2)$ follows, which is a contradiction to the maximality of $\widetilde{\rho}(G)$ again. Thus C is of length 3, i.e., vu is an edge of some triangle.

We are remaining to show that at least one of u, v is of degree 2. Suppose to the contrary that $d_G(u), d_G(v) \geqslant 3$. Denote by $z_1, z_2, \dots, z_t$ the neighbors of v in G but outside C, where $t = d_G(v) - 2 \geqslant 1$. Let $G_3 = G - \{vz_1, vz_2, \dots, vz_t\} + \{uz_1, uz_2, \dots, uz_t\} \in$

$\mathbb{C}(n,k)$. It follows from Lemma 5 that $\widetilde{\rho}(G) < \widetilde{\rho}(G_3)$, which is a contradiction to the maximality of $\widetilde{\rho}(G)$. □

THEOREM 1. *Let $G \in \mathbb{C}(n,k)$, where $n \geqslant 4$. Then $\rho(G) \leqslant \rho(C_{n,k})$ with equality if and only if $G \cong C_{n,k}$, where $\rho(C_{n,k})$ is equal to the largest root of $f_{n,k}(x) = 0$ with*

$$f_{n,k}(x) = 2(n-1)x^3 - \sqrt{2}(n-1)x^2 - 2(n^2-(k+3)n+3k+2)x + \sqrt{2}(n-2)(n-2k-1).$$

Proof. By a direct calculation of the characteristic polynomial of $ABC(C_{n,k})$, it is not hard to verify that $\rho(C_{n,k})$ is the largest root of $f_{n,k}(x) = 0$.

It is easy to see that $ABC(C_{n,k}) = \widetilde{ABC}(C_{n,k})$. By Lemma 4, we have $\rho(G) \leqslant \widetilde{\rho}(G)$ with equality if and only if $ABC(G) = \widetilde{ABC}(G)$. So it suffices to show that $\widetilde{\rho}(G) \leqslant \widetilde{\rho}(C_{n,k})$ with equality if and only if $G \cong C_{n,k}$. Suppose that G is a graph in $\mathbb{C}(n,k)$ that maximizes the revised ABC spectral radius. It suffices to show that $G \cong C_{n,k}$.

Some forbidden structures are revealed in Lemma 6. Assume that uv is an edge of G, where $d_G(u), d_G(v) \geqslant 2$. Lemma 6 asserts two properties related to uv: (i) uv is an edge of a triangle; (ii) at least one of u, v is of degree 2.

If $k = 0$, then there is no cycle in G, so property (i) forces every edge of G to be a pendent edge, i.e., $G \cong C_{n,0}$. Next we assume that $k \geqslant 1$, and analyze the structures related to cycles in G.

From (i), it is known that each cycle of G is a triangle, and from (ii), exactly one vertex of each triangle in G is of degree at least 3, thus all the triangles of G converge at a common vertex, say v. As to the remaining vertices outside the cycles, they can be only pendent vertices adjacent to v, which is guaranteed by (i). So G is actually $C_{n,k}$. □

As a consequence of Theorem 1, we conclude that $C_{n,0}$ is the unique n-vertex tree that maximizes the ABC spectral radius of trees (see [4]), while $C_{n,1}$ is the unique n-vertex unicyclic graph that maximizes the ABC spectral radius of unicyclic graphs (see [13]).

In what follows we determine the graphs in $\mathbb{C}(n)$ for $n \geqslant 4$ with the first a few largest ABC spectral radii.

LEMMA 7. *For $n \geqslant 6$ and $k \geqslant 1$, we have $\rho(C_{n,k}) < \rho(C_{n,k-1})$.*

Proof. Recall that $\rho(C_{n,k})$ is the largest root of $f_{n,k}(x) = 0$, where

$$f_{n,k}(x) = 2(n-1)x^3 - \sqrt{2}(n-1)x^2 - 2(n^2-(k+3)n+3k+2)x + \sqrt{2}(n-2)(n-2k-1).$$

As

$$f_{n,k}\left(\frac{\sqrt{2}(n-2)}{n-3}\right) = -\frac{\sqrt{2}(n-2)(n-1)^2(n^2-8n+13)}{(n-3)^3} < 0,$$

we have $\rho(C_{n,k}) > \frac{\sqrt{2}(n-2)}{n-3}$.

On the other hand, it is easy to see that

$$f_{n,k}(x) - f_{n,k-1}(x) = 2(n-3)\left(x - \frac{\sqrt{2}(n-2)}{n-3}\right),$$

which is positive if $x > \frac{\sqrt{2}(n-2)}{n-3}$. As $\rho(C_{n,k}) > \frac{\sqrt{2}(n-2)}{n-3}$, we have

$$0 = f_{n,k}(\rho(C_{n,k})) > f_{n,k-1}(\rho(C_{n,k})),$$

so $\rho(C_{n,k}) < \rho(C_{n,k-1})$. $\square$

LEMMA 8. *For* $6 \leqslant n \leqslant 23$, $\rho(D_n) < \rho(C_{n,2})$, *and for* $n \geqslant 24$, $\rho(D_n) > \rho(C_{n,2})$.

Proof. Recall that $\rho(D_n)$ is the largest root of $f(x) = 0$, and $\rho(C_{n,2})$ is the largest root of $g(x) = 0$, where

$$f(x) = 2(n-2)x^4 - 2(n^2-5n+7)x^2 + (n-3)^2$$

and

$$g(x) = 2(n-1)x^3 - \sqrt{2}(n-1)x^2 - 2(n^2-5n+8)x + \sqrt{2}(n-2)(n-5).$$

For $6 \leqslant n \leqslant 23$, $\rho(D_n) < \rho(C_{n,2})$ follows from direct calculations. Suppose that $n \geqslant 24$. It is easy to verify that

$$\begin{aligned}&(n-1)f(x) - (n-2)g(x)\left(x + \frac{1}{\sqrt{2}}\right)\\ &= -(n^2-9n+16)x^2 + 2\sqrt{2}(n-2)(n-1)x + 2n^2 - 9n + 11,\end{aligned}$$

in which the larger root of the right-hand side polynomial on x is

$$x = x_0 := \frac{\sqrt{2}(n-1)(n-2) + \sqrt{(n^2-5n+8)(4n^2-19n+23)}}{n^2-9n+16},$$

so

$$(n-1)f(x) - (n-2)g(x)\left(x + \frac{1}{\sqrt{2}}\right) < 0 \text{ if } x > x_0.$$

On the other hand, we have by a tedious but straightforward calculation that $g(x_0) < 0$ (for $n \geqslant 24$), which implies that $\rho(C_{n,2}) > x_0$. It thus follows that

$$(n-1)f(\rho(C_{n,2})) = (n-1)f(\rho(C_{n,2})) - (n-2)g(\rho(C_{n,2}))\left(\rho(C_{n,2}) + \frac{1}{\sqrt{2}}\right) < 0,$$

so $f(\rho(C_{n,2})) < 0$, implying that $\rho(D_n) > \rho(C_{n,2})$. $\square$

LEMMA 9. *For* $n \geqslant 6$,

$$\rho(C_{n,1}) > \rho(D_n)$$

and

$$\rho(C_{n,2}) > \max\{\rho(T_{n,1}), \rho(T_{n,2}), \rho(U_{n,1}), \rho(U_{n,2})\}.$$

Proof. Note that $\rho(C_{n,1})$ and $\rho(D_n)$ are, respectively, the largest roots of $h(x) = 0$ and $f(x) = 0$, where

$$h(x) = 2(n-1)x^3 - \sqrt{2}(n-1)x^2 - 2(n^2-4n+5)x + \sqrt{2}(n-2)(n-3)$$

and

$$f(x) = 2(n-2)x^4 - 2(n^2-5n+7)x^2 + (n-3)^2.$$

It is easy to see that

$$(n-2)h(x)\left(x+\frac{1}{\sqrt{2}}\right) - (n-1)f(x) = -(n^2-n-4)x^2 - \sqrt{2}(n-1)(n-2)x + n - 3,$$

in which, for $x \geqslant 1$, the right-hand side decreases, so

$$\begin{aligned}(n-2)h(x)\left(x+\frac{1}{\sqrt{2}}\right) - (n-1)f(x) &\leqslant (n-2)h(1)\left(1+\frac{1}{\sqrt{2}}\right) - (n-1)f(1) \\ &= -(\sqrt{2}+1)n^2 + (3\sqrt{2}+2)n - 2\sqrt{2} + 1 \\ &< 0.\end{aligned}$$

Clearly, $\rho(D_n) \geqslant 1$. Thus

$$\begin{aligned}&(n-2)h(\rho(D_n))\left(\rho(D_n)+\frac{1}{\sqrt{2}}\right) \\ &= (n-2)h(\rho(D_n))\left(\rho(D_n)+\frac{1}{\sqrt{2}}\right) - (n-1)f(\rho(D_n)) \\ &< 0,\end{aligned}$$

which implies that $\rho(C_{n,1}) > \rho(D_n)$.

Note that $\rho(C_{n,2})$, $\rho(T_{n,i})$ and $\rho(U_{n,i})$ for $i = 1,2$ are, respectively, the largest roots of $f_{n,2}(x) = 0$, $f_i(x) = 0$ and $g_i(x) = 0$, where

$$f_{n,2}(x) = 2(n-1)x^3 - \sqrt{2}(n-1)x^2 - 2(n^2-5n+8)x + \sqrt{2}(n-2)(n-5),$$

$$\begin{aligned}f_1(x) &= 4(n-3)x^4 - 2(2n^2-13n+23)x^2 + 4n^2 - 31n + 61, \\ f_2(x) &= 3(n-3)x^4 - (3n^2-19n+34)x^2 + 4(n-4)^2, \\ g_1(x) &= (n-2)x^4 - (n^2-5n+8)x^2 + (n-3)(n-4),\end{aligned}$$

and

$$g_2(x) = 6(n-2)x^4 - 2(3n^2-15n+25)x^2 - 2\sqrt{3(n-1)(n-2)}x + 7n^2 - 47n + 80.$$

By direct calculations, we have

$$\begin{aligned} &2(n-3)f_{n,2}(x)\left(x+\frac{1}{\sqrt{2}}\right)-(n-1)f_1(x)\\ &=-4(3n-11)x^2-4\sqrt{2}(n-1)(n-3)x-2n^3+15n^2-30n+1, \end{aligned} \tag{1}$$

$$\begin{aligned} &3(n-3)f_{n,2}(x)\left(x+\frac{1}{\sqrt{2}}\right)-2(n-1)f_2(x)\\ &=(n^2-20n+67)x^2-6\sqrt{2}(n-1)(n-3)x-5n^3+42n^2-99n+38, \end{aligned} \tag{2}$$

$$\begin{aligned} &(n-2)f_{n,2}(x)\left(x+\frac{1}{\sqrt{2}}\right)-2(n-1)g_1(x)\\ &=(n^2-7n+14)x^2-2\sqrt{2}(n-1)(n-2)x-n^3+7n^2-14n+4, \end{aligned} \tag{3}$$

and

$$\begin{aligned} &3(n-2)f_{n,2}(x)\left(x+\frac{1}{\sqrt{2}}\right)-(n-1)g_2(x)\\ &=(3n^2-19n+40)x^2-2(n-1)\left(3\sqrt{2}(n-2)-\sqrt{3(n-1)(n-2)}\right)x\\ &\quad-4n^3+27n^2-55n+20. \end{aligned} \tag{4}$$

Further, one can check that as a quadric function on x, the right-hand side of (1) is always negative for $n \geqslant 6$ by noting that its discriminant is negative. As quadric functions on x, the right-hand sides of (2), (3), and (4) are negative if $x = 0, \sqrt{n}$, so they are always negative for $0 < x < \sqrt{n}$. As $f_2(x)$ increases if $x \geqslant \sqrt{n}$, we have $f_2(x) \geqslant f_2(\sqrt{n}) > 0$ if $x \geqslant \sqrt{n}$, implying that $\rho(T_{n,2}) < \sqrt{n}$. Similarly, $\rho(U_{n,1}), \rho(U_{n,2}) < \sqrt{n}$. From (1)–(4), we have $f_{n,2}(x) < 0$ for $x = \rho(T_{n,1}), \rho(T_{n,2}), \rho(U_{n,1}), \rho(U_{n,2})$. Therefore, $\rho(C_{n,2}) > \max\{\rho(T_{n,1}), \rho(T_{n,2}), \rho(U_{n,1}), \rho(U_{n,2})\}$. □

Now we can present an ordering of cactus graphs by large ABC spectral radii. If $n = 3$, then $\mathbb{C}(n) = \{C_{3,0}, C_{3,1}\}$, where $\rho(C_{3,0}) = 1$ and $\rho(C_{3,1}) = \sqrt{2}$.

THEOREM 2. *Let $G \in \mathbb{C}(n)$, where $n \geqslant 4$.*

(*i*) *If $n = 4$, then $C_{4,1}$, $C_{4,0}$ and the 4-vertex cycle C_4, and the 4-vertex path P_4 are, respectively, the unique graphs with the first three largest ABC spectral radii.*

(*ii*) *If $n = 5$, then $C_{5,2}$, $C_{5,1}$, and $C_{5,0}$ are, respectively, the unique graphs with the first three largest ABC spectral radii.*

(*iii*) *If $6 \leqslant n \leqslant 23$, then $C_{n,0}$, $C_{n,1}$, and $C_{n,2}$ are, respectively, the unique graphs with the first three largest ABC spectral radii.*

(*iii*) *If $n \geqslant 24$, then $C_{n,0}$, $C_{n,1}$, D_n, and $C_{n,2}$ are, respectively, the unique graphs with the first four largest ABC spectral radii.*

Proof. When $n = 4,5$, the result follows trivially, since there are exactly 4 and 9 graphs in $\mathbb{C}(n)$, respectively. Assume that $n \geqslant 6$ and $G \in \mathbb{C}(n,k)$ in the following.

If $k \geqslant 2$, then we have Theorem 1 and Lemma 7 that $\rho(G) \leqslant \rho(C_{n,2})$ with equality if and only if $G \cong C_{n,2}$. By Lemma 7 again,

$$\rho(C_{n,2}) < \rho(C_{n,1}) < \rho(C_{n,0}).$$

If $k = 1$, then G is a unicyclic graph, and by Lemma 2,

$$\rho(G) \leqslant \max\{\rho(U_{n,1}), \rho(U_{n,2})\} < \rho(C_{n,1})$$

when $G \ncong C_{n,1}$.

If $k = 0$, then G is a tree, and by Lemma 1,

$$\rho(G) \leqslant \max\{\rho(T_{n,1}), \rho(T_{n,2})\} < \rho(D_n) < \rho(C_{n,0})$$

when $G \ncong C_{n,0}, D_n$.

Finally, the result follows from Lemmas 8 and 9. □

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