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Character of Trees with Extreme Balaban Index *

Hawei Dong [a,b] **and** **Xiaofeng Guo** [a]

[a] *School of Mathematical Sciences, Xiamen University, Xiamen Fujian 361005, China*

[b] *Department of Mathematics, Minjiang University, Fuzhou Fujian 350108, China*

e-mail: donghawei@126.com , xfguo@xmu.edu.cn

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Abstract

The Balaban index (also called J index) of a connected graph G is defined as $J = J(G) = \frac{|E(G)|}{\mu+1} \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma_G(u)\sigma_G(v)}}$,where $\sigma_G(u) = \sum_{w \in V(G)} d_G(u,w)$ and μ is the cyclomatic number. Balaban index has been used in various QSAR and QSPR studies. In this paper, we characterize the trees with the maximum Balaban index among all the trees with n vertices and either the maximum degree Δ, or a given degree sequence, or k pendent vertices. In addition, the tree with the minimum Balaban index and n vertices and the maximum degree Δ, and the tree with the maximum Balaban index and n vertices and the maximum degree Δ and k pendent vertices are also determined.

On the other hand, we find that a lemma without proof in our paper [MATCH Commu. Math. Comput. Chem. 63 (2010) 799-812] is incorrect, and so are several related theorems. In the appendix of this paper, we rework the lemma and theorems, and give a new character for the graph with maximum Balaban index among graphs with n vertices. Several open problems on graphs with extreme Balaban indices are proposed.

Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The distance between vertices u and v in G is denoted by $d_G(u,v)$. $\sigma_G(v) = \sum\limits_{u \in V(G)} d(u,v)$ is called the distance of vertex v. The Balaban index was proposed by Balaban [1, 2]. It was defined as:

$$J = J(G) = \frac{|E(G)|}{\mu + 1} \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma_G(u)\sigma_G(v)}} ,$$

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where $\mu = |E(G)| - |V(G)| + 1$ is the cyclomatic number.

Balaban index was used subsequently in various QSAR and QSPR studies [3]-[10]. It has been shown that Balaban index has a strong correlation with the chemical properties of the chemical compound.

The effect of a restricted branching pattern on the Balaban index is discussed in [11]. In [12], Balaban et al compared the ordering of constitutional isomers of alkanes with 6 through 9 carbon atoms. It was shown that the ordering induced by Balaban index parallels the ordering induced by Wiener index, but reduces the degeneracy of the latter index and provides a much higher discriminating ability. Therefore Balaban index also is called 'sharpened Wiener index' sometimes. Also there are results about tight lower and upper bounds of Balaban indices of some graphs, see [13] and [14]. In [15], we determine the graphs with some parameters (such as the number of vertices, connectivity, diameter) and extreme Balaban indices. In the present paper, we characterize the trees with extreme Balaban index among all the trees with n vertices and either the maximum degree Δ, or a given degree sequence, or k pendent vertices. In addition, the tree with the minimum Balaban index and n vertices and the maximum degree Δ, and the tree with the maximum Balaban index and n vertices and the maximum degree Δ and k pendent vertices are also determined. As a corollary, the chemical tree with the maximum Balaban index and n vertices and k pendent vertices is given.

Preliminaries

Let T be a tree and $v \in V(T)$. A maximal subtree containing v as an end vertex is called a branch of T at v. The set of all branches of T at v will be denoted by $B(T; v)$. The edge set of every branch B will be denoted by $E(B)$, its cardinality by $|E(B)|$. For each $v \in V(T)$, let $bw(v) = \{max|E(B)| : B \in B(T; v)\}$. The number $bw(v)$ is called the branch weight of v in T. The set of vertices v of T in which $bw(v)$ attains its minimum is called the centroid $C(T)$ of T.

Lemma 1 *[16] If $C = C(T)$ be the centroid of a tree T with n vertices then one of the following holds:*

(1) $C = \{c\}$ and $bw(c) \leq (n-1)/2$;

(2) $C = \{c_1, c_2\}$ and $bw(c_1) = bw(c_2) = n/2$;

In both cases, if $v \in V(T) \setminus C$ then $bw(v) \geq n/2$.

For any edge $uv \in E(G)$ and any subgraph G' of G, we let $J_G(uv) = \frac{1}{\sqrt{\sigma_G(u)\sigma_G(v)}}$ and $J_G(G') = \sum_{uv \in E(G')} \frac{1}{\sqrt{\sigma_G(u)\sigma_G(v)}}$. Thus the Balaban index of G can be expressed as: $J(G) =$

$\frac{|E(G)|}{\mu+1} \sum\limits_{e \in E(G)} J_G(e) = \frac{|E(G)|}{\mu+1} \sum\limits_{i=1}^{p} J_G(G_i)$, where G_i, $i = 1, 2, \cdots, p$, are edge disjoint subgraphs of G and $\cup_{i=1}^{p} E(G_i) = E(G)$.

For any vertices u, v in tree T, the path from u to v is denoted by P_{uv}.

Lemma 2 *[15] If $a,\ a',\ b,\ b',\ w,\ x,\ y,\ z \in R^+$ such that $\frac{b}{x} \geq \frac{a}{w}$, $\frac{b'}{y} \geq \frac{a'}{z}$, $w \geq x$ and $z \geq y$, then $\frac{1}{\sqrt{(w+a)(z+a')}} + \frac{1}{\sqrt{xy}} \geq \frac{1}{\sqrt{wz}} + \frac{1}{\sqrt{(x+b)(y+b')}}$. And the equation holds if and only if $b = a$, $b' = a'$, $w = x$ and $z = y$.*

Lemma 3 *[15] If $x, y, a \in R^+$ such that $x \geq y + a$, then $\frac{1}{\sqrt{(x-a)(y+a)}} \leq \frac{1}{\sqrt{xy}}$. And the equation holds if and only if $x = y + a$.*

Lemma 4 *[15] Let $P = u_1 u_2 \cdots u_n$ be a path in a graph G with $d(u_2) = d(u_3) = \cdots = d(u_{n-1}) = 2$ and $d(u_1), d(u_n) \geq 2$, let G_1 be the component of $G - u_2$ containing u_1, and let G_2 be the component of $G - u_{n-1}$ containing u_n. Construct $G' = G - \{u_n v | v \in V(G_2) \cap N_G(u_n)\} + \{u_1 v | v \in V(G_2) \cap N_G(u_n)\}$ (See Fig. 1), then $J(G') > J(G)$. The transformation from G to G_0 is called the path-lifting transformation of G.*

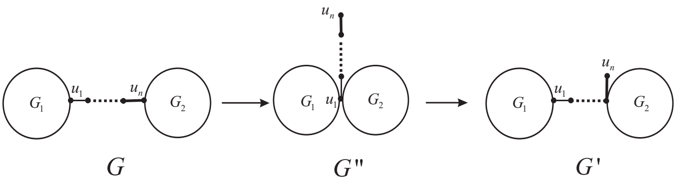

Figure 1: The path-lifting transformation from graph G to G'.

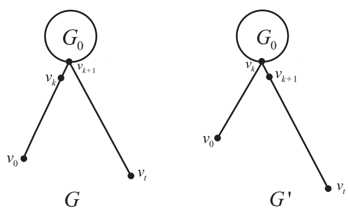

Figure 2: the path-moving transformation from G to G'.

Lemma 5 *[15] Let G_0 be a graph, and $P = v_0 v_1 \cdots v_t$ a path of length t. Let G (resp. G') be the graph obtained from G_0 and P by identifying a vertex v_{k+1} $(k < t/2)$ (v_k) to a same vertex of G_0 (See Fig. 2). Then $J(G) > J(G')$. The transformation from G to G' is called the path-moving transformation of G.*

Let T be a tree rooted at vertex r and $v \in V(T)$, $d(v,r)$ is called the depth of v. The maximum depth of vertices of T is called the height of T, denoted by $h(T)$.

Definition 6 *Let T be a tree rooted at vertex u. Label u as $u_{(0)}$. For $d = 1, 2\cdots$, a vertex in T with depth d is labeled $u_{(0,x_1,\cdots,x_d)}$ if its father has been labeled $u_{(0,x_1,\cdots,x_{d-1})}$ such that x_i is a positive real number for $i = 1, 2, \cdots, d$ and any two children $u_{(0,x_1,\cdots,x_{d-1},x_d)}$ and $u_{(0,x_1,\cdots,x_{d-1},y_d)}$ of $u_{(0,x_1,\cdots,x_{d-1})}$ satisfy that $x_d \neq y_d$. The above labeling of $V(T)$ is called a root-tree labeling of T, and the subscript set of the root-tree labeling is denoted by $\mathcal{S}(T)$.*

For trees T_u rooted at u and tree T_v rooted at v, label $V(T_u)$ and $V(T_v)$ by the root-tree labeling way to get $\mathcal{S}(T_u)$ and $\mathcal{S}(T_v)$, respectively. Clearly $\mathcal{S}(T_u)\cap\mathcal{S}(T_v) \neq \emptyset$. Let $U_0 = \{u_s|s \in \mathcal{S}(T_u)\cap\mathcal{S}(T_v)\}$ and $V_0 = \{v_s|s \in \mathcal{S}(T_u)\cap\mathcal{S}(T_v)\}$. Then both $T[U_0]$ and $T[V_0]$ are trees and $T[U_0] \cong T[V_0]$.

For any vertex u in a tree T and $V \subseteq V(T)$, let $\sigma_T(u,V) = \sum_{v\in V} d_T(u,v)$.

Lemma 7 *Let P be a path in tree T with end vertices u and v such that $d(u,v) = 1$ or 2 and let T_u and T_v be the component of $T - E(P)$ rooted at u and v, respectively. $V(T_u)$ and $V(T_v)$ are labeled by the root-tree labeling way to get $\mathcal{S}(T_u)$ and $\mathcal{S}(T_v)$, respectively. Let $T' = T - \{u_su_t|s \in \mathcal{S}(T_u)\cap\mathcal{S}(T_v), t \in \mathcal{S}(T_u)\backslash\mathcal{S}(T_v),\ u_su_t \in E(T_u)\} + \{v_su_t|s \in \mathcal{S}(T_u)\cap\mathcal{S}(T_v),\ t \in \mathcal{S}(T_u)\backslash\mathcal{S}(T_v),\ u_su_t \in E(T_u)\}$ (see an example in Fig. 3). If $T \ncong T'$, then $J(T) < J(T')$.*

Proof. Let $U_0 = \{u_s|s \in \mathcal{S}(T_u)\cap\mathcal{S}(T_v)\}$, $U_1 = V(T_u)\backslash U_0$, $V_0 = \{v_s|s \in \mathcal{S}(T_u)\cap\mathcal{S}(T_v)\}$, and $V_1 = V(T_v)\backslash V_0$. Suppose $T \ncong T'$, then $U_1 \neq \emptyset$ and $V_1 \neq \emptyset$.

For any vertex $u_s \in U_0$, there is $v_s \in V_0$ such that $\sigma_T(u_s,V_0) = \sigma_{T'}(v_s,U_0)$ and $\sigma_{T_u}(u_s) = \sigma_{T'[V_0\cup U_1]}(v_s)$, since $T'[U_0] \cong T[V_0]$ and $T_u \cong T'[V_0 \cup U_1]$. Clearly $\sigma_T(u_s,V_1) > \sigma_{T'}(v_s,V_1)$, it follows that $\sigma_T(u_s) = \sigma_T(u_s,V_0) + \sigma_{T_u}(u_s) + \sigma_T(u_s,V_1) + \sigma_T(u_s,V(T) - V(T_u) - V(T_v)) > \sigma_{T'}(v_s,U_0) + \sigma_{T'[V_0\cup U_1]}(v_s) + \sigma_{T'}(v_s,V_1) + \sigma_T(v_s,V(T) - V(T_u) - V(T_v)) = \sigma_{T'}(v_s)$. Due to $U_1 \neq \emptyset$, $\sigma_{T'}(u_s) - \sigma_T(u_s) = \sigma_T(v_s) - \sigma_{T'}(v_s) > 0$. Therefore for any edge $u_su_t \in E(T[U_0])$ and $v_sv_t \in E(T[V_0])$, $J_T(u_su_t) + J_T(v_sv_t) < J_{T'}(u_su_t) + J_{T'}(v_sv_t)$ by Lemma 2.

Obviously, $\sigma_T(w) > \sigma_{T'}(w)$ for any vertex $w \in U_1 \cup V_1$, it follows that $J_T(e) < J_{T'}(e)$ for any edge $e \in E(T[U_1]) \cup (E(T_v) - E(T[V_0]))$ and $J_T(u_su_t) < J_{T'}(v_su_t)$ for any edge u_su_t in T_u with $u_s \in U_0$ and $u_t \in U_1$.

If $d(u,v) = 1$, then $J_T(uv) < J_{T'}(uv)$ by Lemma 3. If $d(u,v) = 2$, then $\sigma_T(w) = \sigma_{T'}(w)$ for any $w \in V(T) - V(T_u) - V(T_v)$. Hence $J_T(e) = J_{T'}(e)$ for any $e \in E(T - V(T_u) - V(T_v))$, and $J_T(P) < J_{T'}(P)$ by Lemma 2.

So $J(T) < J(T')$. ■

Definition 8 *The transformation from T to T' in Lemma 7 is called a (T_u, T_v)-transformation.*

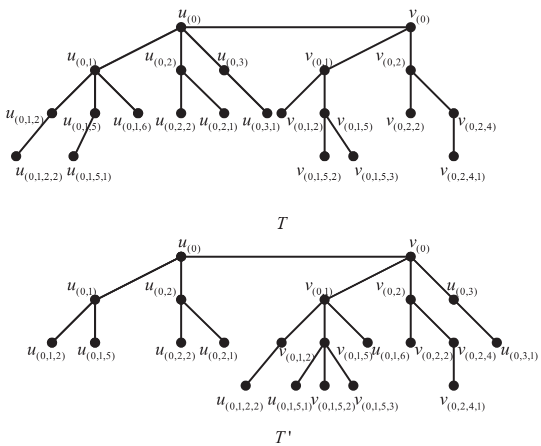

Figure 3: A tree T is transformed to a new tree T' by a (T_u, T_v)-transformation.

Trees with the maximum Balaban indices and n vertices and either a given degree sequence, or the maximum degree, or the number of pendent vertices

Definition 9 [17] *Suppose that the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following 'greedy algorithm' (see Fig. 4):*

(1) *Label the vertex with the largest degree as v (the root);*

(2) *Label the neighbors of v as $v_1, v_2, \cdots$, assign the largest degrees available to them such that $d(v_1) \geq d(v_2) \geq \cdots$;*

(3) *Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \cdots$ such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \cdots$, then do the same for $v_2, v_3, \cdots$;*

(4) *Repeat (3) for all the newly labeled vertices, always stars with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.*

From the definition of the greedy tree, we immediately get:

Lemma 10 *A tree T rooted at r with a given degree sequence is a greedy tree if :*
(1) *For $h(T) > i \geq 0$, the degree of any vertex with depth i is greater or equal to the degree of any vertex with depth $i+1$.*

(2) *For distinct vertices w, x of the same depth with $d(x) > d(w) \geq 2$, the minimum degree of the children of x is greater or equal to the maximum degree of the children of w.*

(3) *For distinct vertices w, x of the same depth with $d(x) = d(w) \geq 2$, the minimum degree of*

the children of x is greater or equal to the maximum degree of the children of w or the same statement holds with the roles of x and w reversed.

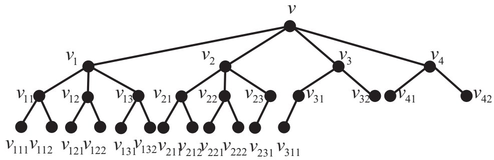

Figure 4: A greedy tree with degree sequence $\{4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 3, 2, 2, 1, \cdots, 1\}$.

Theorem 11 *Given a degree sequence $\pi = (d_1, d_2, \cdots, d_n)$, the greedy tree maximizes the Balaban index among all the trees with degree sequence π.*

Proof. Let T be a tree rooted at $r \in C(T)$ with degree sequence π. For finishing our proof, it is enough to prove that if T is not isomorphic to a greedy tree then T can be transformed to another tree T' with the same degree sequence π such that $J(T) < J(T')$.

Suppose that T is not isomorphic to a greedy tree. According to Lemma 10, one of the following three statements holds:

(1) There are $x, y \in V(T)$ such that $d(x, r) > d(y, r)$ and $d(x) > d(y)$.

(2) There are $x', y' \in V(T)$ with the same depth and $d(y') > d(x') \geq 2$ such that a child x of x' and a child y of y' satisfy that $d(x) > d(y)$.

(3) There are $x', y' \in V(T)$ with the same depth and $d(x') = d(y') \geq 2$ such that the minimum degree of the children of x' is less than the maximum degree of the children of y' and a child y of y' with the minimum degree and a child x of x' with the maximum degree satisfy that $d(x) > d(y)$.

For anyone of the above three cases, let $u, v \in V(P_{xy})$ such that $d(u, x) = d(v, y)$ and $d(x, v) - d(x, u) = 1$ or 2. Let T_u and T_v be the component of $T - E(P_{uv})$ rooted at u and v, respectively. Give a special root-tree labeling of $V(T_u)$ (resp. $V(T_v)$) such that

(1) for $d \geq 0$ and any vertex w labeled $u_{(0,x_1,\cdots,x_d)}$ (resp. $v_{(0,x_1,\cdots,x_d)}$) with $d(w) > 1$, children of w are labeled $u_{(0,x_1,\cdots,x_d,1)}$, $u_{(0,x_1,\cdots,x_d,2)}$, $\cdots$, $u_{(0,x_1,\cdots,x_d,d(w)-1)}$ (resp. $v_{(0,x_1,\cdots,x_d,1)}$, $v_{(0,x_1,\cdots,x_d,2)}$, $\cdots$, $v_{(0,x_1,\cdots,x_d,d(w)-1)}$), and

(2) label x as $u_{(0,1,\cdots,1)}$ and y as $v_{(0,1,\cdots,1)}$.

Then T can be transformed to a new tree T' by a (T_u, T_v)-transformation. Note that the transformation from T to T' would less the number of pairs of vertices satisfying above three statements. If $T \ncong T'$, then $J(T) < J(T')$ by Lemma 7 and we have done; Otherwise, we repeat the transformation as above and T can be transformed into a new tree, say T'', which is isomorphic to the greedy tree with degree sequence π. Since $T \ncong T''$, $J(T) < J(T'')$ by Lemma 7. ■

Lemma 12 *Let T and T' be greedy trees with degree sequences $(d_1, \cdots, d_i, \cdots, d_j, \cdots d_n)$ and $(d_1, \cdots, d_i + 1, \cdots, d_j - 1, \cdots d_n)$, respectively, where $d_1 \geq \cdots \geq d_i \geq \cdots \geq d_j \geq \cdots \geq d_n$ and $d_j > 1$. Then $J(T) < J(T')$.*

Proof. Let x and y be the vertices with degree d_j and d_i in T, respectively. Let $u, v \in V(P_{xy})$ such that $d(u, x) = d(v, y)$ and $d(x, v) - d(x, u) = 1$ or 2. And let T_u and T_v be the component of $T - E(P_{uv})$ rooted at u and v, respectively. Give a special root-tree labeling of $V(T_u)$ (resp. $V(T_v)$) such that

(1) for $d \geq 0$ and any vertex $w(\neq x)$ labeled $u_{(0,x_1,\cdots,x_d)}$ (resp. $v_{(0,x_1,\cdots,x_d)}$) with $d(w) > 1$, children of w are labeled $u_{(0,x_1,\cdots,x_d,1)}$, $u_{(0,x_1,\cdots,x_d,2)}$, $\cdots$, $u_{(0,x_1,\cdots,x_d,d(w)-1)}$ (resp. $v_{(0,x_1,\cdots,x_d,1)}$, $v_{(0,x_1,\cdots,x_d,2)}$, $\cdots$, $v_{(0,x_1,\cdots,x_d,d(w)-1)}$), and

(2) label x as $u_{(0,1,\cdots,1)}$ and y as $v_{(0,1,\cdots,1)}$, and

(3) label children of x as $u_{(0,1,\cdots,1,1)}$, $u_{(0,1,\cdots,1,2)}$, $\cdots$, $u_{(0,1,\cdots,1,d_j-2)}$,$u_{(0,1,\cdots,1,d_i)}$.

(4) for the vertex z labeled $u_{(0,1,\cdots,1,d_i)}$, and the subtree T_z induced by z and all its successors, $V(T_z) = V(T_u) \setminus U_0$ where $U_0 = \{u_s | s \in \mathcal{S}(T_u) \cap \mathcal{S}(T_v)\}$ (note that the depth of u is greater than or equal to the depth of v in the greedy tree T, so in T_v there is a subtree rooted at v isomorphic to T_u).

Then T can be transformed to a new tree T'' by a (T_u, T_v)-transformation. It is not difficult to see that T'' has the degree sequence $(d_1, \cdots, d_i + 1, d_j - 1, \cdots d_n)$ and $T \ncong T''$. By Lemma 7 and Theorem 11, $J(T) < J(T'') \leq J(T')$. ■

Recall that a partition of n is a sequence $\lambda = (\lambda_1, \lambda_2, \cdots, \lambda_l)$ where the λ_i are weakly decreasing and $\sum_{i=1}^{l} \lambda_i = n$. Suppose $\lambda = (\lambda_1, \lambda_2, \cdots, \lambda_l)$ and $\mu = (\mu_1, \mu_2, \cdots, \mu_l)$ are partitions of n. Then λ dominates μ, if $\lambda_1 + \lambda_2 + \cdots + \lambda_i \geq \mu_1 + \mu_2 + \cdots + \mu_i$ for all $1 \leq i \leq l$ and $\sum_{i=1}^{l} \lambda_i = \sum_{i=1}^{l} \mu_i$. For degree sequence $(d_1, \cdots, d_n)$ of any tree with n vertices, we always let $d_1 \geq \cdots \geq d_n$ and it can be seen as a partition of $2(n-1)$. Then a degree sequence is called the dominate degree sequence in a tree set S, if it dominates the degree sequence of any tree in S.

Corollary 13 *Let T and T' be greedy trees with degree sequences π and π', respectively, where π dominates π'. Then $J(T) \geq J(T')$ and the equation holds if and only if $T \cong T'$.*

From Theorem 11 and Corollary 13, we have the following.

Theorem 14 *Let $\mathcal{S}$ be a set of some trees with n vertices, and T a greedy tree in $\mathcal{S}$ with a dominate degree sequence. Then T has the maximum Balaban index in $\mathcal{S}$.*

Based on Theorem 14, a series of theorems can be deduced.

Definition 15 *Let $n, \Delta \in Z^+$, $\Delta \geq 3$. Let $T(n, \Delta)$ be a tree rooted at v_0 and defined inductively as follows: $T(1, \Delta)$ consists of a single vertex labeled v_0. The tree $T(n, \Delta)$ has vertex set $\{v_0, \cdots, v_{n-1}\}$. For $2 \leq n \leq \Delta + 1$, the edge set of $T(n, \Delta)$ is $\{v_0v_1, \cdots, v_0v_{n-1}\}$. For $n > \Delta + 1$, $T(n, \Delta)$ is obtained by attaching a leaf v_{n-1} to the vertex in $\{v_1, \cdots, v_{n-2}\}$ which has degree $< \Delta$ in $T(n-1, \Delta)$ and has subscript as small as possible.*

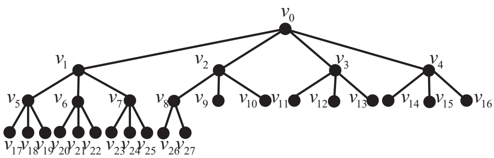

Figure 5: T(28,4).

For example, $T(28, 4)$ is shown in Fig. 5.

Note that $T(n, \Delta)$ is a greedy tree with a dominate degree sequence in the set of trees with n vertices and the maximum degree Δ.

Theorem 16 *Let T be a tree with n vertices and the maximum degree Δ. Then $J(T) \leq J(T(n, \Delta))$ and the equation holds if and only if $T \cong T(n, \Delta)$.*

A vertex u of a tree T is said to be a branching vertex of T if $d_T(u) \geq 3$. Let's denote $T(n; n_1, \cdots, n_k)$ the starlike tree with n vertices and just one branching vertex, say u, such that k components of $T-u$ are paths of lengths $n_1-1, \cdots, n_k-1$, respectively, where $n_1+\cdots+n_k = n-1$. A starlike tree $T(n; n_1, \cdots, n_k)$ with $n_i = \lfloor \frac{n-1}{k} \rfloor$ or $\lceil \frac{n-1}{k} \rceil$ for $1 \leq i \leq k$ is denoted by $S(n, k)$. Note that $S(n, k)$ is a greedy tree with a dominate degree sequence in the set of trees with n vertices and k pendent vertices.

Theorem 17 *If T is a starlike tree $T(n; n_1, \cdots, n_k)$, then $J(T) \leq J(S(n, k))$ and the equation holds if and only if $T \cong S(n, k)$.*

Denote by $\mathcal{T}(k, n, \Delta)$ the set of all the trees with n vertices, the maximum degree Δ, and k ($> \Delta$) pendent vertices. Let m be the minimum integer such that $T(m, \Delta)$ (defined in Definition 15) has exactly k pendent vertices. Let $i < k$, $i \equiv n-m \pmod{k}$, and let $T(k, n, \Delta) \in \mathcal{T}(k, n, \Delta)$ be constructed from $T(m, \Delta)$ by attaching an end vertex of a path of length $\lceil \frac{n-m}{k} \rceil$ to each of the i pendent vertices of $T(m, \Delta)$ with subscripts as small as possible, and an end vertex of a path of length $\lfloor \frac{n-m}{k} \rfloor$ to each of the other pendent vertices of $T(m, \Delta)$. For example, $T(19, 69, 4)$

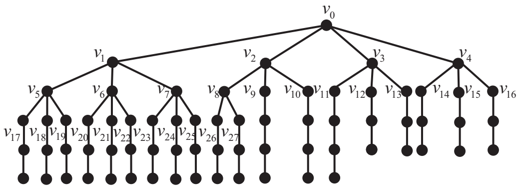

Figure 6: T(19,69,4).

is constructed by $T(28, 4)$ attaching 3 paths of length 3 and 16 paths of length 2 to pendent vertices of $T(28, 4)$ respectively (see Fig. 6).

Note that the tree $T(k, n, \Delta)$ is a greedy tree with a dominate degree sequence in $\mathcal{T}(k, n, \Delta)$.

Theorem 18 *Let T be a tree in $\mathcal{T}(k, n, \Delta)$. Then $J(T) \leq J(T(k, n, \Delta))$, and the equation holds if and only if $T \cong T(k, n, \Delta)$.*

Corollary 19 *The tree with the maximum Balaban index among all chemical trees with n vertices and k pendent vertices is isomorphic to $T(k, n, 4)$ for $k > 4$ and isomorphic to $S(n, k)$ for $k \leq 4$.*

The tree with the minimum Balaban index and n vertices and the maximum degree Δ

Theorem 20 *Let T be a tree with n vertices and the maximum degree Δ. Then $J(T) \geq J(T(n; 1, \cdots, 1, n - \Delta))$ and the equation holds if and only if $T \cong T(n; 1, \cdots, 1, n - \Delta)$.*

Proof. Let $u \in V(T)$ with $d(u) = \Delta$, and Δ components of $T - u$ have $n_1, \cdots, n_\Delta$ vertices, respectively. If $T \ncong T(n; n_1, \cdots, n_\Delta)$, then T can be transformed into $T(n; n_1, \cdots, n_\Delta)$ by carrying out repeatedly inverse path-lifting transformations. If $T(n; n_1, \cdots, n_\Delta) \ncong T(n; 1, \cdots, 1, n - \Delta)$, $T(n; n_1, \cdots, n_\Delta)$ can be transformed into $T(n; 1, \cdots, 1, n - \Delta)$ by carrying out repeatedly path-moving transformations. By Lemmas 4, 5, $J(T) \geq J(T(n; n_1, \cdots, n_\Delta)) \geq J(T(n; 1, \cdots, 1, n - \Delta))$, and $J(T) = J(T(n; 1, \cdots, 1, n - \Delta))$ if and only if $T \cong T(n; 1, \cdots, 1, n - \Delta)$. ■

Appendix

This part is for correcting some errors in the paper [15] (Hawei Dong, Xiaofeng Guo, Character of Graphs with Extremal Balaban Index, MATCH - Commun. Math. Comput. Chem. 63 (2010) 799-812).

In [15], we gave the following lemma without proof.

Lemma [15, Lemma 3] Let G be a graph. Then $J(G-e) < J(G)$ for any $e \in E(G)$.

However, the conclusion of the lemma is incorrect, because we neglect the effect of the coefficient $\frac{|E(G)|}{\mu+1}$ in $J(G)$.

Let $J^*(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma_G(u)\sigma_G(v)}}$. Then $J(G) = \frac{|E(G)|}{\mu+1} J^*(G)$.

It is easy to see that, for any edge e of G, $J^*(G) > J^*(G-e)$, but $\frac{|E(G)|}{\mu(G)+1} = \frac{|E(G)|}{|E(G)|-|V(G)|+2} \leq \frac{|E(G-e)|}{|E(G-e)|-|V(G-e)|+2} = \frac{|E(G-e)|}{\mu(G-e)+1}$. So, it can not be claimed that $J(G-e) < J(G)$ for any $e \in E(G)$.

Due to the above inaccurate Lemma, some related theorems in [15] (Theorem 13, Theorem 14, Theorem 16, Theorem 18) are also incorrect. The other results in [15] not related to the inaccurate lemma are still valid.

Now we rework the inaccurate lemma and theorems (Lemma 3, Theorem 13, Theorem 14, Theorem 16, Theorem 18) in [15] as follows (the proofs in [15] for the theorems are valid for the following theorems).

Lemma 21 *Let G be a graph. Then $J^*(G-e) < J^*(G)$ for any $e \in E(G)$.*

Theorem 22 *If G is a connected graph with n vertices, then $J^*(K_n) \geq J^*(G) \geq J^*(P_n)$. The lower bound is realized if and only if $G \cong P_n$ and the upper bound is realized if and only if $G \cong K_n$.*

Theorem 23 *If G is a k-connected (k-edge-connected) graph with n vertices, then $J^*(G) \leq J^*(K_k + (K_1 \cup K_{n-k-1}))$. The bound is realized if and only if $G \cong K_k + (K_1 \cup K_{n-k-1})$.*

Theorem 24 *If G is a 2-connected graph with n vertices, then $J^*(G) \geq J^*(C_n)$. The bound is realized if and only if $G \cong C_n$.*

Theorem 25 *Let G be a graph with n vertices and diameter d, then $J^*(G) \leq J^*(G_d)$ and the bound is achieved if and only if $G \cong G_d$.*

Now we give a new character for the graph with the maximum Balaban index and n vertices.

Theorem 26 *If G is a connected graph with n vertices, then $J(G) \leq J(S_n)$. The bound is realized if and only if $G \cong S_n$.*

Proof. Let $|E(G)| = m$.

If $m = n-1$, $J(S_n) \geq J(G)$ by [15, Theorem 12], and equation holds if and only if $G \cong S_n$. So we can suppose $n \leq m \leq \frac{n(n-1)}{2}$.

$$J(G) = \frac{m}{m-n+2} \sum_{e \in E(G)} J(e) \leq \frac{m}{m-n+2} \sum_{e \in E(G)} \frac{1}{n-1} \leq \frac{m^2}{(m-n+2)(n-1)}.$$

$J(S_n) = \frac{(n-1)^2}{\sqrt{(n-1)(2n-3)}} > \frac{(n-1)^2}{\sqrt{(n-1)(2n-2)}} = \frac{(n-1)^2}{\sqrt{2}(n-1)}$.

To show $J(S_n) > J(G)$, we just need to prove $\frac{m^2}{m-n+2} < \frac{(n-1)^2}{\sqrt{2}}$, that is, $(n-1)^2(m-n+2) - \sqrt{2}m^2 > 0$.

Let $f(m) = (n-1)^2(m-n+2) - \sqrt{2}m^2$. When $m < \frac{(n-1)^2}{2\sqrt{2}}$, $f(m)$ increases with m; when $m > \frac{(n-1)^2}{2\sqrt{2}}$, $f(m)$ decreases with m.

When $n \geq 9$, $f(\frac{n(n-1)}{2}) = (n-1)^2(\frac{n(n-1)}{2} - n + 2) - \sqrt{2}(\frac{n(n-1)}{2})^2 = (\frac{2-\sqrt{2}}{4}n^2 - \frac{3}{2}n + 2)(n-1)^2 > 0$, $f(n) = (n-1)^2(n-n+2) - \sqrt{2}n^2 = (2-\sqrt{2})n^2 - 4n + 2 > 0$. Hence $f(m) = (n-1)^2(m-n+2) - \sqrt{2}m^2 > 0$. ■

We also try to give the other new characters for Theorems 13,14,16,18 in [15], however, the problems are more difficult. Here we propose the following open problems.

Problem 1. Under what conditions $J(G-e) \leq J(G)$ (resp. $J(G-e) \geq J(G)$) for an edge e of a graph G.

Problem 2. Characterize graphs with the minimum Balaban index and n vertices.

Problem 3. Characterize graphs with the maximum (the minimum) Balaban index among k-connected (k-edge-connected) graphs with n vertices.

Problem 4. Characterize graphs with the maximum (the minimum) Balaban index among graphs with n vertices and diameter d.

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