Extremal trees of the eccentric connectivity index

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Abstract

Chemical indices are introduced to correlate chemical compounds' physical properties with their structures. Among recently introduced such indices, the eccentric connectivity index of a graph G is defined as $\xi^C(G) = \sum_{v \in V(G)} deg(v)ec(v)$, where $deg(v)$ is the degree of a vertex v and $ec(v)$ is its eccentricity. The extremal values of $\xi^C(G)$ have been studied among graphs with various given parameters. In this note we study trees with extremal values of the eccentric connectivity index with a given degree sequence. The extremal structures are identified, however they are not unique.

Keyword: tree, eccentric connectivity index, distance
2000 Mathematics Subject Classification: 05C05, 05C07, 05C90

1 Terminology and introduction

A *tree* $T = (V, E)$ is a connected, acyclic graph. $V(T)$ denotes the vertex set of a tree T. *Leaves* are vertices of degree 1. The unique path connecting two vertices v, u in T will be denoted by $P_T(v, u)$. The *distance* $d_T(v, u)$ between them is the number of edges on the path (or shortest path for general graphs) $P_T(v, u)$.

The *eccentricity* $ec_G(v)$ of a vertex v in a graph G is the maximum distance between v and any other vertex in G. The *radius* of G is the minimum value of the eccentricities of the vertices in G. A *central vertex* of G is a vertex with eccentricity equal to the radius. The *center* is the set consisting of the central vertices.

For any vertex $v \in V(T)$, $deg(v)$ denote the *degree* of v. The *degree sequence* of a tree is the sequence of the degrees (in descending order) of the internal vertices.

We call a tree (T, r) *rooted at the vertex* r (or just T if it is clear what the root is) by specifying a vertex $r \in V(T)$. The *height* of a vertex v of a rooted tree (T, r) is $h_T(v) = d_T(r, v)$.

For any two different vertices u, v in a rooted tree (T, r), we say that v is a *descendant* of u and u is an *ancestor* of v if $P_T(r, u) \subset P_T(r, v)$. Furthermore, if u and v are adjacent to each other and $d_T(r, u) = d_T(r, v) - 1$, we say that u is the *parent* of v and v is a *child* of u. For a vertex v in a rooted tree (T, r), we use T_v or $T(v)$ to denote the subtree induced by v and all its descendants.

The structure of a chemical compound is usually modeled as a polygonal shape, often called the *molecular graph* of this compound. Topological indices have been used to correlate a compound's molecular graph with experimentally gathered data regarding the compound's characteristics.

Through the past years, numerous indices have been introduced. Among them the adjacency-sum-distance based *eccentric connectivity index* has been considered in many literatures. Denoted by $\xi^C(G)$, the eccentric connectivity index is defined as

$$\xi^C(G) = \sum_{v \in V(G)} deg(v) ec(v).$$

It was pointed out that "these topological models have been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds". Other generalizations of this index have also been found useful.

Since ample applications of chemical indices deal with chemical compounds that have acyclic organic molecules, whose molecular graphs are trees, mathematical properties of various indices of trees have been extensively studied over past years, see, for example, [2, 4, 10] and the references there.

The eccentric connectivity index was discussed in many chemical related literatures [3, 5, 8, 11]. Since the degrees of vertices in a molecular graph correspond to the valences of the atoms in a compound, tree structures with various restrictions on their degrees have been of practical interests. Most recently Ilic and Gutman [6] studied this index for chemical trees (trees with maximum degree 4) and trees with bounded degrees in general. Similar questions for other chemical indices (the Wiener index for instance) among trees with bounded degrees or a given degree sequence are studied in [4, 7, 10]. In this note, we aim to fill the gap by characterizing the extremal trees with respect to the eccentric connectivity index among trees with a given degree sequence.

We examine extremal trees with a given degree sequence in Sections 2.1 and 2.2; we identify the structure of such trees in Section 2.3, with examples showing that they are not unique; in Section 2.4 we examine the value of $\xi^C(T)$ of these extremal trees.

2 Trees with a given degree sequence

In this section we consider the extremal trees with respect to the eccentric connectivity index for trees with a given degree sequence. For convenience, we call an extremal tree T optimal (minimizing $\xi^C(T)$ in section 2.1 and maximizing $\xi^C(T)$ in section 2.2). First note the following known observation, see for instance [1].

Lemma 2.1. *The center (containing one or two vertices) lies in the middle of a diametral path.*

To introduce our results, we define the *greedy type trees* (with a given degree sequence) as a generalization of the *greedy trees* in [10]:

Definition 2.2. *Suppose the degrees of the non-leaf vertices are given, a greedy type tree is achieved by the following 'greedy algorithm':*

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

ii) Label the neighbors of v as $v_1, v_2, \ldots$, assign the largest degrees available to them. In particular, v_1 gets the second largest degree in the degree sequence;

iii) Label the neighbors of v_i (except v) and let them take all the largest degrees available, the children of v_1 takes the remaining largest degrees;

iv) Repeat (iii) for all the newly labeled vertices, with the largest available degrees assigned to the descendants of v_1.

Fig. 1 shows a greedy type tree with degree sequence {4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2}, note that such trees are not necessarily unique with a given degree sequence. Intuitively speaking, one just fill the levels (the root first, then the vertices with height one, etc.) with largest degrees available. v_1 and its descendants always get assigned the largest degrees in each level, while the order of the other degrees in each level can be random.

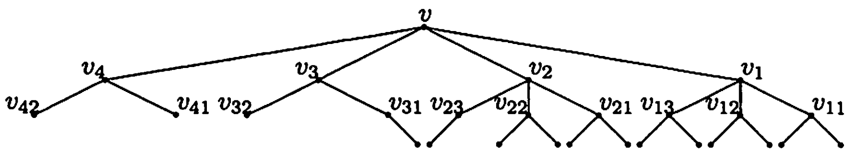

Figure 1: A greedy type tree

Also, a *caterpillar* tree is a tree which has a path (the 'backbone' of the caterpillar) and every vertex not on the path is adjacent to some vertex on the backbone. The *greedy type caterpillar* is a tree T with given degree sequence $\{d_1 \geq d_2 \geq \ldots \geq d_k \geq 2\}$, formed by attaching pendant edges to a path $v_1 v_2 \ldots v_k$ of length $k-1$ such that

$$\min\{d(v_1), d(v_k)\} \geq \max\{d(v_2), d(v_{k-1})\} \geq \min\{d(v_2), d(v_{k-1})\} \geq \ldots$$

$$\ldots \geq \max\{d(v_{\lceil \frac{k}{2} \rceil}), d(v_{\lceil \frac{k+1}{2} \rceil})\} \geq \min\{d(v_{\lceil \frac{k}{2} \rceil}), d(v_{\lceil \frac{k+1}{2} \rceil})\}.$$

Note that $v_{\lceil \frac{k}{2} \rceil}$ and $v_{\lceil \frac{k+1}{2} \rceil}$ can be identical if k is odd.

Fig. 2 shows a greedy type caterpillar with degree sequence {6, 5, 5, 5, 5, 5 ,4 ,3 , 3}. Similar to the greedy type trees, the greedy type caterpillars are not necessarily unique with a given degree sequence.

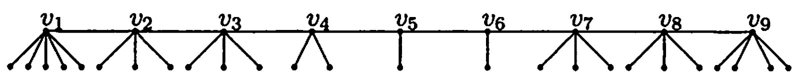

Figure 2: A greedy type caterpillar

2.1 Minimization

Take a central vertex v with eccentricity k (lying on a diametral path of length $2k$ or $2k-1$), partition the vertex set into $L_0, L_1, \ldots, L_k$ while L_i consists of vertices at distance i from v. In particular, $L_0 = \{v\}$ and L_k contains only leaves. Let $v_i \in L_i$ and $v_j \in L_j$, $i < j$, then we have the following lemma, which claims that larger degrees lie closer to the central vertex in an optimal tree.

Lemma 2.3. *In an optimal tree T that minimizes $\xi^C(T)$, we can assume $deg(v_i) \geq deg(v_j)$.*

Proof. Let a diametral path start from u, passing through v and end at w.

Suppose that $deg(v_i) = a < b = deg(v_j)$, then $b \geq 2$ and $j \leq k-1$ since $ec(v) = k$. Also, $v_i \neq u$ or w since $i \leq j-1 \leq k-2$.

Consider T as rooted at v, let $B := \{B_1, B_2, \dots, B_{b-1}\}$ denote the set of components/branches (each considered as a rooted subtree) in $T_{v_j}/\{v_j\}$.

If $a \geq 2$, let T' be the tree obtained from T by removing $b-a$ branches in B and reattaching them to v_i. Obviously T' has the same degree sequence. Since $b-(b-a) = a \geq 2$, we can choose these branches such that u and w are not contained in any of them. Note that in this process, $deg(x)$ stays the same for any vertex x other than v_i, v_j while $ec(x)$ stays the same or decreases. v_i and v_j switched degrees and the larger degree is associated with the vertex with smaller or same eccentricity in T'. Thus $\xi^C(T') \leq \xi^C(T)$.

If $a = 1$, further assume that B does not contain u or w. Let T' be the tree obtained from T by removing all the branches in B and reattaching them to v_i. Note that after this operation the path $P_T(u,w)$ is still a diametral path. Similar to above, we have $\xi^C(T') \leq \xi^C(T)$.

This leaves us with the case $a = 1$ and every diametral path has an end in B. Construct T' as above, since the eccentricity of any vertex is achieved between itself and one end of a diametral path, the eccentricity of any vertex will only decrease (if not the same as before). In particular, $ec(v)$ decreases. Then again $\xi^C(T') \leq \xi^C(T)$.

□

Remark: One can also display the proof in a straightforward manner without the different cases.

Now we are ready to prove our first main result:

Theorem 2.4. *Among trees of given degree sequence, the 'greedy type trees' minimize $\xi^C(T)$.*

Proof. From Lemma 2.3, the structure of the optimal tree is already close to the 'greedy type trees'. Let the resulted optimal tree be of height k, the eccentricity of the root (a central vertex) v. Then a vertex $v_i \in L_i$ is of height i in this tree.

Note that the eccentricity of v_i is:

(i) $i+k$ if there is a vertex $v_k \in L_k$ whose only common ancestor with v_i is the root v;

(ii) $i+k-1$ if every v_k shares some common ancestor (other than the root v) with v_i.

In order to minimize $\xi^C(T)$, case (ii) is desired, which applies only when all vertices of height k are descendants of the same child of v (otherwise one always end up with case (i)). In this situation, it is obviously our interest to get as many vertices as possible to be the descendants of v_1 and consequently as large degrees as possible for these vertices. It is easy to see that the greedy type trees, with the restriction of having v_1 and its descendants taking the largest degrees in each level, achieve this goal. □

Remark: By no means do we claim that the optimal tree has to be a greedy type tree. As discussed in the proof, in the situations when case (i) always holds, one do not need the restriction of associating largest degrees with the descendants of v_1 in each level. This will be further explained in section 2.3.

2.2 Maximization

In this case, we first present the following simple observation similar to the case for the Wiener index [9].

Lemma 2.5. *The optimal tree has to be a caterpillar tree.*

Proof. Let T be an optimal tree that maximizes the eccentric connectivity index with a given degree sequence. Consider a diametral path $v_1v_2\ldots v_m$ with v_1 and v_m being leaves.

Suppose for contradiction that there exists some non leaf vertex not on this path. Let x be such a vertex which is also a neighbor of v_i, we must have $3 \leq i \leq m-2$ since $v_1v_2\ldots v_m$ is a diametral path. Let T_x denote the subtree rooted at x, resulted from the component containing x in $T/\{v_ix\}$.

Now consider a tree T' obtained from T by removing T_x from x and reattaching to v_1. T' shares the same degree sequence as T. After this operation, the eccentricity of the vertices in T_x increased while the eccentricities for other vertices either increase or stay the same. Therefore $\xi^C(T') > \xi^C(T)$, contradicting to the optimality of T.

Thus every vertex not on the diametral path has to be a leaf, consequently T is a caterpillar tree. □

With this lemma, the next result immediately follows.

Theorem 2.6. *Among trees of given degree sequence, the 'greedy type caterpillars' maximizes $\xi^C(T)$.*

Proof. Since the optimal tree has to be a caterpillar tree, it is only a matter of arranging the degrees for the internal vertices on the diametral path (backbone) of this caterpillar. Indeed, we want the largest degrees to be assigned to the vertices as far from the middle as possible (so that these degrees are associated with large eccentricities) and the smallest degrees to be assigned to the vertices in the middle.

From this we get a greedy type caterpillar. □

2.3 The extremal trees

Here we discuss the possible extremal trees. With a given degree sequence, one can always construct a greedy type tree according to Definition 2.2 (Fig. 1). Such trees minimize $\xi^C(T)$ as shown in section 2.1. However they are not unique, as one can permute the degrees within the descendants of v_1 and within the other vertices at each level. For instance Fig. 3 shows another greedy type tree with the same degree sequence, the degrees of v_{22} and v_{31} are switched compared to Fig. 1.

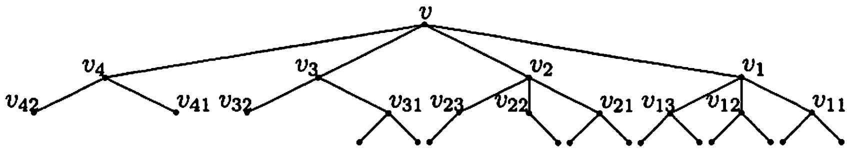

Figure 3: Another greedy type tree

Further more, if there exists some vertex that is not a descendant of v_1 and is of the greatest height (as is the case with the trees in Fig. 1 and Fig. 3). Case (i) in the proof of Theorem 2.4 will always occur and it is not necessary to follow the 'descendants of v_1 taking largest degrees in each level' restriction. In this case, the degrees of the vertices at each level can be randomly permuted. As a result, Fig. 4 shows an optimal tree with the same degree sequence that is not a greedy type tree. Here the degrees of v_{13} and v_{23} are switched compared to Fig. 3, for the vertices of height 2, it is no longer the case that the descendants of v_1 take the largest degrees.

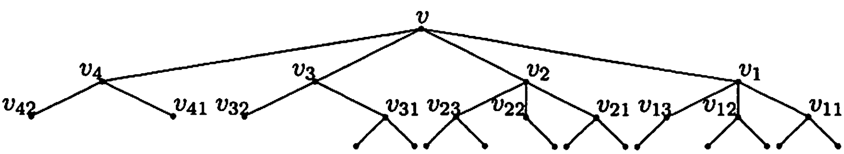

Figure 4: An optimal tree that is not 'greedy'

The reason for Definition 2.2 can be illustrated in the next example. With the degree sequence $\{4,4,3,3,3,3,3,3\}$, the greedy type tree is shown in Fig. 5, in this case all vertices of the greatest height are descendants of v_1. For all the descendants of v_1, case (ii) in the proof of Theorem 2.4 applies and the greedy type trees (still not necessarily unique) maximize the number of 'cases (ii)' (therefore minimize $\xi^C(T)$).

As for the greedy type caterpillars, it is obvious that they are not necessarily unique since one can exchange the degrees of any pair of vertices

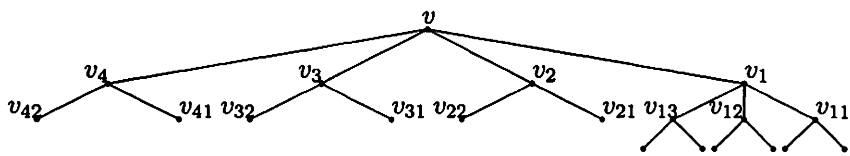

Figure 5: An optimal tree for which 'greedy' is necessary

(on the diametral path) at the same distance from the center.

2.4 Extremal values of $\xi^C(T)$

Here we briefly discuss the values of $\xi^C(T)$ with T being the extremal structures. As corollaries from the previous theorems, these rather simple conclusions can shed some light on the influence of the degree sequence on the possible extremal values of $\xi^C(T)$.

For a greedy type caterpillar T with degree sequence $\{d_1, d_2, \ldots, d_k\}$, we immediately get the following from the definition:

$$\xi^C(T) = \sum_{i=1}^{k} d_i(k - \left\lfloor \frac{i-1}{2} \right\rfloor) + \sum_{i=1}^{k}(d_i - 2)(k+1-\left\lfloor \frac{i-1}{2} \right\rfloor) + 2(k+1) \quad (1)$$

where the first sum comes from the contribution from the internal vertices and the other terms correspond to the leaves.

From (1) it is easy to see that if k (the number of internal vertices) is fixed, an 'even' distribution of the degrees will minimize the maximal value of $\xi^C(T)$, and the maximal value of $\xi^C(T)$ is maximized when we have a degree sequence of the form $\{d_1, 2, 2, \ldots, 2\}$.

In the case of a greedy type tree T with degree sequence $\{d_1, d_2, \ldots, d_k\}$, it is not as easy to get a 'nice' explicit formula as the caterpillar. However, from the proof of optimality one can think of the construction as a simple algorithm, starting with the largest degree and attach the degrees from largest to smallest such that the larger degrees are associated with smaller eccentricities.

From this argument we can come to a similar conclusion. When k is fixed, an 'even' distribution of the degrees will maximize the minimal value of $\xi^C(T)$, and the minimal value of $\xi^C(T)$ is minimized when we have a degree sequence of the form $\{d_1, 2, 2, \ldots, 2\}$.

3 Summary

To summarize, we found the extremal tree structures with a given degree sequence, which maximize or minimize the eccentric connectivity index.

We point out that these extremal structures are not unique, in particular partial restriction of 'greedy' is sometimes not necessary. We see in section 2.3 that this depends on the number of non leaf vertices of the greatest height and the largest degrees at each level. With a given degree sequence, one can easily see what is the case. A more straight forward description of this phenomenon is desired.

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