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Two Degree Distance Based Topological Indices of Chemical Trees

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ABSTRACT Let $\mathcal{G} = (V_{\mathcal{G}}, E_{\mathcal{G}})$ be a simple and connected graph. The eccentric connectivity index of $\mathcal{G}$ is represented as $\xi^c(\mathcal{G}) = \sum_{x\in V_{\mathcal{G}}} \deg_{\mathcal{G}}(x) ec_{\mathcal{G}}(x)$, where $\deg_{\mathcal{G}}(x)$ and $ec_{\mathcal{G}}(x)$ represent the degree and the eccentricity of x, respectively. The eccentric adjacency index of $\mathcal{G}$ is represented as $\xi^{ad}(\mathcal{G}) = \sum_{x\in V_{\mathcal{G}}} \frac{S_{\mathcal{G}}(x)}{ec_{\mathcal{G}}(x)}$, where $S_{\mathcal{G}}(x)$ is the sum of degrees of neighbors of x. In this paper, we determine the trees with the smallest eccentric connectivity index when bipartition size, independence number, and domination number are given. Furthermore, we discuss the trees with the largest eccentric adjacency index when bipartition size, matching number, and independence number are given.

INDEX TERMS Eccentric connectivity index, eccentric adjacency index, bipartition, matching number, independence number, domination number.

I. INTRODUCTION

Let $\mathcal{G} = (V_{\mathcal{G}}, E_{\mathcal{G}})$ be a simple and connected graph where $V_{\mathcal{G}}$ and $E_{\mathcal{G}}$ represent the vertex and edge set respectively. The degree of a vertex x in $\mathcal{G}$, symbolized by $\deg_{\mathcal{G}}(x)$, is the number of vertices linked to x. A vertex x is labeled as a leaf or a pendent vertex if $\deg_{\mathcal{G}}(x) = 1$. Let $P_{\mathcal{G}}$ represents the set of all pendent vertices of $\mathcal{G}$ and $P_{\mathcal{G}}(x)$ represents the set of all pendent vertices adjacent at $x \in V_{\mathcal{G}}$. The neighborhood $\Gamma_{\mathcal{G}}(x)$ of $x \in V_{\mathcal{G}}$ is the set of vertices linked to x in $\mathcal{G}$. The length of a smallest path between two vertices x, y in $\mathcal{G}$ is said to be the distance among x and y and is represented by $d_{\mathcal{G}}(x, y)$. The eccentricity $ec_{\mathcal{G}}(x)$ of $x \in V_{\mathcal{G}}$ is characterized by $ec_{\mathcal{G}}(x) = \max_{y\in V_{\mathcal{G}}} d_{\mathcal{G}}(x, y)$. The radius $r(\mathcal{G})$ and the diameter $d(\mathcal{G})$ of $\mathcal{G}$ are represented by $r(\mathcal{G}) = \min_{x\in V_{\mathcal{G}}} ec_{\mathcal{G}}(x)$ and $d(\mathcal{G}) = \max_{x\in V_{\mathcal{G}}} ec_{\mathcal{G}}(x)$, respectively. Let $S_{\mathcal{G}}(x)$ be the sum of degrees of linked vertices of the vertex x in $\mathcal{G}$. A path P_n is an arrangement of n distinct vertices such that two vertices are linked if they are sequent in this arrangement. A path consisting of vertices $x_1, x_2, \ldots, x_n$ such that x_i is linked to x_{i+1} is written by $x_1x_2\ldots x_n$ and is called x_1, x_n-path. The vertices x_1 and x_n are the end vertices and $x_2, x_3, \ldots, x_{n-1}$ are the internal vertices of the path $x_1x_2\ldots x_n$. Two paths are said to be internally disjoint paths if they do not contain any common internal vertex. Also, two paths are edge-disjoint if they do not contain a common edge. The diametrical path of $\mathcal{G}$ is the path of length $d(\mathcal{G})$. A chemical tree is a graph-theoretical representation of acyclic chemical structures. A tree with $n-1$ pendent vertices and a vertex with $n-1$ degree is said to be a star and is symbolized by S_n.

Let $\mathcal{G}$ be a bipartite graph. Then $V_{\mathcal{G}}$ has two unique partitioned subsets V_1 and V_2 such that every individual edge has one end vertex in V_1 and other end vertex in V_2. If $|V_1| = r$ and $|V_2| = s$ then (r, s) is the bipartition size of $\mathcal{G}$, where $r \leq s$ and $r + s = n$.

A matching M in $\mathcal{G}$ is the subset of edge set of $\mathcal{G}$ as long as any two edges of M do not have a same vertex in $\mathcal{G}$. A matching M is called a maximum matching if $|M| \geq |M_1|$ for any other matching M_1 in $\mathcal{G}$. The matching number of $\mathcal{G}$ is the cardinality of the largest matching in $\mathcal{G}$ and is represented by $m_{\mathcal{G}}$. If $w \in V_{\mathcal{G}}$ is an end vertex of an edge in M, then w is recognized as M-saturated. A matching M is recognized as a perfect matching in $\mathcal{G}$ if every single vertex of $\mathcal{G}$ is M-saturated and $\mathcal{G}$ is said to be a conjugated graph if it has a perfect matching.

A subset $I \subseteq V_{\mathcal{G}}$ is represented as an independent set of $\mathcal{G}$ if vertices of I are pairwise not linked. The independence number of $\mathcal{G}$ is the maximum number of vertices in I and is denoted by $\alpha_{\mathcal{G}}$.

A subset $A \subseteq V_{\mathcal{G}}$ is a dominating set of $\mathcal{G}$ if for every single vertex $u_1 \in V_{\mathcal{G}} \setminus A$, there is a vertex $u_2 \in A$ such that

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$u_1u_2 \in E_{\mathcal{G}}$. The domination number is the number of vertices in the smallest dominating set of $\mathcal{G}$ and is denoted by $\gamma_{\mathcal{G}}$.

Chemical graph theory is the part of mathematical chemistry and this theory plays a major role in the field of chemical science. A molecular graph $\mathcal{G}$ is an illustration of the structural formula of a chemical compound in respects to graph theory. The vertices and edges of $\mathcal{G}$ be equivalent to atoms and chemical bonds, respectively. A single quantity that can be given to distinguish some property of $\mathcal{G}$ of a molecule is recognized to be a topological index. Recently, there has been developing attraction in the area of computational chemistry in topological indices. The topological indices are mainly used in nonempirical QSPR and QSAR. There are many classes of topological indices; some of them are distance based, degree based, distance degree based and eccentricity based indices of graphs.

Recently, many eccentricity based topological indices have been interpreted; one of them is the eccentric connectivity index, which was proposed by Sharma *et al.* [15]. The eccentric-connectivity index is interpreted as:

$$\xi^c(\mathcal{G}) = \sum_{x \in V_{\mathcal{G}}} \deg_{\mathcal{G}}(x) ec_{\mathcal{G}}(x). \tag{1}$$

The eccentric connectivity index has been exhibited to give an upper ranking of characterization of pharmaceutical properties and furnish leads to the growth of safe and useful anti-HIV compounds [4].

The eccentric adjacency index [5] is the variation of eccentric connectivity index. It is interpreted as:

$$\xi^{ad}(\mathcal{G}) = \sum_{x \in V_{\mathcal{G}}} \frac{S_{\mathcal{G}}(x)}{ec_{\mathcal{G}}(x)}.$$

Morgan *et al.* [13] computed sharp bounds of ξ^c of graphs with respect to order and also bounds for trees. In 2012, Zhang *et al.* [19] gave lower bounds of eccentric connectivity index in the form of size of graphs with a given diameter. Later on, Zahng *et al.* [20] determined the largest eccentric connectivity index of n-vertex graphs with m links, where $(n \leq m \leq n+4)$. Zhou *et al.* [21] derived bounds for eccentric connectivity index in order of graph parameters. Relationship of eccentric connectivity index and eccentric adjacency index has been researched by Gupta *et al.* [9]. Ilić *et al.* [12] derived ξ^c of trees with a fixed largest vertex degree. For additional studies on topological indices with given parameters (bipartition, domination number, independence number, etc) we refer [2], [3], [6]–[8], [10], [14], [16], [17] to the readers.

Motivated by the above statements, it is quite natural for us to carry on the investigation on the eccentric connectivity index and the eccentric adjacency index with some given parameters. This article is structured as: In Section II, we derive the trees with the smallest eccentric connectivity index and the largest eccentric adjacency index among the n-vertex trees with a given bipartition. In Section III, we find the trees with the smallest eccentric adjacency index and the largest eccentric adjacency index among n-vertex trees with fixed matching number and independence number. In Section IV, we derive the trees with the smallest eccentric connectivity index among n-vertex trees with domination number.

FIGURE 1. **The graph $T(n, r, s)$.**

II. ECCENTRIC CONNECTIVITY INDEX AND THE ECCENTRIC ADJACENCY INDEX OF TREES WITH A (r, s)-BIPARTITION

Let $\mathcal{T}(n; r, s)$ be the set of all n-vertex trees, every one of which has a (r, s)-bipartition, where $r \leq s$ and $r + s = n$. Note that $\mathcal{T}(n; 1, n-1) = \{S_n\}$. Let $T(n, r, s)$ be the n-vertex tree acquired by connecting $r-1$ and $s-1$ pendent vertices to the two vertices of P_2, respectively, where $2 \leq r \leq s$ and $r+s = n$. The graph $T(n, r, s)$ is depicted in Figure 1. In this section, we find the tree with smallest eccentric connectivity index in $\mathcal{T}(n; r, s)$ and also determine the tree with largest eccentric adjacency index in $\mathcal{T}(n; r, s)$.

In Lemma 1, we establish a new tree in $\mathcal{T}(n; r, s)$ from a given tree in $\mathcal{T}(n; r, s)$ such that the new tree has smaller eccentric connectivity index and larger eccentric adjacency index.

Lemma 1: Let $T \in \mathcal{T}(n; r, s)$ with $uv, vw \in E_T$, $\deg_T(u) \geq 2$ and $\Gamma_T(w) = \{v, w_1, w_2, \ldots, w_t\}$, where $w_1, w_2, \ldots, w_t \in P_T(w)$, $t \geq 1$ and also $w_1, w_2, \ldots, w_t$ be the end vertices of a diametrical path in T. Construct a new tree T_1 from T as $T_1 = (T - \{ww_1, \ldots, ww_t\}) \cup \{uw_1, \ldots, uw_t\}$. Then $\xi^c(T_1) \leq \xi^c(T)$ and $\xi^{ad}(T_1) \geq \xi^{ad}(T)$.

Proof: By the construction of T_1, it is obvious that $T_1 \in \mathcal{T}(n; r, s)$. Let T_v be the component of $T - \{u, w\}$ which includes the vertex v and take $x \in P_T(w)$, define $\mathcal{A} = \{y \in V_T \mid d_T(x, y) = ec_T(y)\}$. It is natural to see that for any $x \in V_T \setminus (\mathcal{A} \cup P_T(w))$, we have

$$ec_{T_1}(x) = ec_T(x). \tag{2}$$

- If $ec_{T_v}(v) = 2$ then for any $y \in \mathcal{A}$, we have $ec_{T_1}(y) = ec_T(y)$.
- If $ec_{T_v}(v) \in \{0, 1\}$ then there are some vertex $z \in V_T$ such that $d_{T_1}(y, z) = ec_{T_1}(y)$, for any $y \in \mathcal{A}$. There are two possibilities: either $z = w$ or $z \in V_T \setminus \{w\}$. If $z = w$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, w) = d_T(y, w) = ec_T(y) - 1. \tag{3}$$

Now if $z \in V_T \setminus \{w\}$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, z) = d_T(y, z) \leq ec_T(y). \tag{4}$$

Note that $ec_T(x) = ec_T(w) + 1$ for any $x \in P_T(w)$. Therefore from (2)-(4), we get

$$ec_{T_1}(x) = ec_{T_1}(u) + 1 \leq ec_T(u) + 1. \tag{5}$$

Case I: By the construction of T_1, it is easily seen that

$$\deg_{T_1}(y) = \deg_T(y),\ \forall\, y \in V_T \setminus \{u, w\}. \tag{6}$$

Also, the degrees of vertices u and w are given by

$$\deg_{T_1}(w) = \deg_T(w) - t = 1, \quad \deg_{T_1}(u) = \deg_T(u) + t. \tag{7}$$

Thus from (2)-(7), we obtain

$$\begin{aligned}
\xi^c(T_1) - \xi^c(T) &= ec_{T_1}(u)\deg_{T_1}(u) - ec_T(u)\deg_T(u) \\
&\quad + ec_{T_1}(w)\deg_{T_1}(w) - ec_T(w)\deg_T(w) \\
&\quad + \sum_{x\in P_T(w)} ec_{T_1}(x)\deg_{T_1}(x) \\
&\quad - \sum_{x\in P_T(w)} ec_T(x)\deg_T(x) \\
&\le ec_T(u)(\deg_T(u)+t) - ec_T(u)\deg_T(u) \\
&\quad + ec_T(w)(\deg_T(w)-t) - ec_T(w)\deg_T(w) \\
&\quad + \sum_{x\in P_T(w)} (ec_T(u)+1)\deg_T(x) \\
&\quad - \sum_{x\in P_T(w)} (ec_T(w)+1)\deg_T(x) \\
&= t\, ec_T(u) - t\, ec_T(w) + t\, ec_T(u) - t\, ec_T(w) \\
&= 2t(ec_T(u) - ec_T(w)).
\end{aligned}$$

Note that $ec_T(u) \le ec_T(w)$, equality holds if $d(T) = 4$. Therefore $\xi^c(T_1) \le \xi^c(T)$.

Case II: By the construction of T_1, we have

$$S_{T_1}(y) = S_T(y),\ \forall\, y \in V_T \setminus \{u, w\}. \tag{8}$$

Also, the sum of the degrees of neighbor vertices of v in T_1 is given by

$$\begin{aligned}
S_{T_1}(v) &= \sum_{x\in\Gamma_T(v)\setminus\{u,w\}} \deg_{T_1}(x) + \deg_{T_1}(w) + \deg_{T_1}(u) \\
&= \sum_{x\in\Gamma_T(v)\setminus\{u,w\}} \deg_T(x) + (\deg_T(w) - t) \\
&\quad + (\deg_T(u) + t) \\
&= S_T(v).
\end{aligned} \tag{9}$$

Also

$$\begin{aligned}
S_{T_1}(u) &= S_T(u) + t, \quad S_{T_1}(w) = S_T(w) - t \\
S_{T_1}(x) &= S_T(x) + t, \quad \forall\, x \in \Gamma_T(u) \setminus \{v\}.
\end{aligned} \tag{10}$$

Note that $S_T(x) = \deg_T(w) = t + 1$ and given that $\deg_T(u) \ge 2$, for any $x \in P_T(w)$. Therefore we have

$$\begin{aligned}
S_{T_1}(x) &= \deg_{T_1}(u) = \deg_T(u) + t \ge 2 + t \\
&> \deg_T(w) = S_T(x).
\end{aligned} \tag{11}$$

Thus from (2)-(5) and (8)-(9), we obtain

$$\begin{aligned}
&\xi^{ad}(T_1) - \xi^{ad}(T) \\
&= \frac{S_{T_1}(v)}{ec_{T_1}(v)} - \frac{S_T(v)}{ec_T(v)} + \frac{S_{T_1}(w)}{ec_{T_1}(w)} - \frac{S_T(w)}{ec_T(w)} \\
&\quad + \sum_{x\in P_T(w)} \frac{S_{T_1}(x)}{ec_{T_1}(x)} - \sum_{x\in P_T(w)} \frac{S_T(x)}{ec_T(x)} \\
&\quad + \sum_{x\in\Gamma_T(u)\setminus\{v\}} \frac{S_{T_1}(x)}{ec_{T_1}(x)} - \sum_{x\in\Gamma_T(u)\setminus\{v\}} \frac{S_T(x)}{ec_T(x)} \\
&\ge \frac{S_T(v)}{ec_{T_1}(v)} - \frac{S_T(v)}{ec_T(v)} + \frac{S_T(w)-t}{ec_T(w)} - \frac{S_T(w)}{ec_T(w)} \\
&\quad + \sum_{x\in P_T(w)} \frac{S_T(x)}{ec_T(x)} - \sum_{x\in P_T(w)} \frac{S_T(x)}{ec_T(x)} \\
&\quad + \sum_{x\in\Gamma_T(u)\setminus\{v\}} \frac{S_T(x)+t}{ec_T(x)} - \sum_{x\in\Gamma_T(u)\setminus\{v\}} \frac{S_T(x)}{ec_T(x)} \\
&= \frac{t}{ec_T(u)} - \frac{t}{ec_T(w)} + \sum_{x\in\Gamma_T(u)\setminus\{v\}} \frac{t}{ec_T(x)}.
\end{aligned}$$

Note that $ec_T(u) \le ec_T(w)$, equality holds if $d(T) = 4$. Therefore $\xi^{ad}(T_1) \ge \xi^{ad}(T)$. □

Applying Lemma 1 repeatedly yields the following theorem.

Theorem 1: The tree $T(n, r, s)$ is the unique tree in $\mathcal{T}(n; r, s)$ which has the smallest eccentric connectivity index among trees in $\mathcal{T}(n; r, s)$, where $n \ge 3$ and $2 \le r \le s$.

Proof: Let $T \in \mathcal{T}(n; r, s)$ be an n-vertex tree. If $T \ncong T(n, r, s)$ then there is a path uvw in T with $\deg_T(u) \ge 2$ and $\Gamma_T(w) = \{v, w_1, w_2, \ldots, w_t\}$, where $w_1, w_2, \ldots, w_t \in P_T(w)$, $t \ge 1$ and also $w_1, w_2, \ldots, w_t$ be the end vertices of a diametrical path in T. By using Lemma 1, we construct a tree form T as $T_1 = (T - \{ww_1, \ldots, ww_t\}$ that satisfies $\xi^c(T_1) \le \xi^c(T)$. Now if $T_1 \ncong T(n, r, s)$ then there is a path $u'v'w'$ in T_1 with $\deg_{T_1}(u') \ge 2$ and $\Gamma_{T_1}(w') = \{v', w'_1, w'_2, \ldots, w'_t\}$, where $w'_1, w'_2, \ldots, w'_t \in P_{T_1}(w')$, $t \ge 1$ and also $w'_1, w'_2, \ldots, w'_t$ be the end vertices of a diametrical path in T_1. By applying Lemma 1, we construct a tree from T_1 as $T_2 = (T_1 - \{w'w'_1, \ldots, w'w'_t\}$ that satisfies $\xi^c(T_2) \le \xi^c(T_1)$. Therefore by using repeatedly Lemma 1 on diametrical paths in T we obtain a sequence of trees in $\mathcal{T}(n, r, s)$ with smaller eccentric connectivity index such that $\xi^c(T) \ge \xi^c(T_1) \ge \cdots \ge \xi^c(T_k)$, where $T_k \cong T(n, r, s)$. This shows that $T(n, r, s)$ has the smallest eccentric connectivity index among trees in $T(n, r, s)$. □

By simple determining and using Theorem 1, we acquire following result.

Corollary 1: Let $T \in \mathcal{T}(n; r, s)$ with $2 \le r \le s$ and $r + s = n$. Then $\xi^c(T) \le 5n - 6$ with equality if and only if $T \cong T(n, r, s)$.

By the definition of eccentric adjacency index and a similar interpretation given in Theorem 1, we can find the extremal tree with largest eccentric adjacency index in $\mathcal{T}(n; r, s)$ in the next theorem.

Theorem 2: The tree $T(n, r, s)$ is the unique tree in $\mathcal{T}(n; r, s)$ that has the largest eccentric adjacency index among trees in $\mathcal{T}(n; r, s)$, where $n \ge 3$ and $2 \le r \le s$.

By simple assessment and using Theorem 2, we acquire next result.

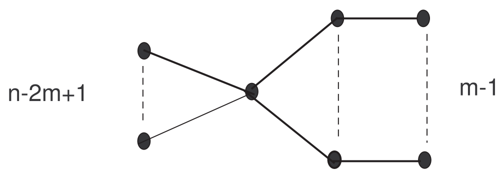

FIGURE 2. The graph $S_{n,m}$.

Corollary 2: Let $T \in \mathcal{T}(n; r, s)$ be an n-vertex tree with $2 \le r \le s$ and $r + s = n$. Then $\xi^{ad}(T) \le \frac{1}{3}((r+1)^2 + (s+1)^2 - 5)$ with equality if and only if $T \cong T(n, r, s)$.

III. ECCENTRIC CONNECTIVITY INDEX AND ECCENTRIC ADJACENCY INDEX OF TREES WITH FIXED MATCHING NUMBER AND INDEPENDENCE NUMBER

Let $\mathcal{T}(n, m)$ be the set of all n-vertex trees with a fixed matching number m and $\mathcal{T}(n, \alpha)$ be the set of all the n-vertex trees with independence number α. If $m = 1$, then T is a star S_n with $\xi^c(S_n) = 3(n-1)$ and $\xi^{ad}(S_n) = \frac{n^2-1}{2}$ for $n \ge 3$. Let $S_{n,m} \in \mathcal{T}(n, m)$ be a tree acquired from star S_{n-m+1} by attaching a pendent edge to each $m-1$ pendent vertices in S_{n-m+1}. The graph $S_{n,m}$ is shown in Figure 2.

In this section, we derive the smallest eccentric connectivity index of trees in $\mathcal{T}(n, m)$ and $\mathcal{T}(n, \alpha)$. Also we find the largest eccentric adjacency index of trees in $\mathcal{T}(n, m)$ and $\mathcal{T}(n, \alpha)$.

The following lemmas present the classic properties of a tree with maximum matching m and these lemmas are beneficial in the proofs of main results.

Lemma 2 Hou and Li [11]: Let $T \in \mathcal{T}(2m, m)$ be a tree with $m \ge 3$. Then T contains at least two pendent vertices such that they are linked to the degree 2 vertices, respectively.

Lemma 3 Hou and Li [11]: Let $T \in \mathcal{T}(n, m)$ be a tree with $m \ge 3$ and $n = 2m + 1$. Then T contains a pendent vertex linked to a degree 2 vertex.

Lemma 4 Hou and Li [11]: Let $T \in \mathcal{T}(n, m)$ be a tree with $n > 2m$ and $m \ge 3$. Then there exists a m-matching M and $u \in P_T$ such that u does not M-saturated.

Theorem 3 Xu et al. [18]: Let $T \in \mathcal{T}(n, m)$ be a tree with $n \ge 2m$ and $m \ge 3$. Then we have $\xi^c(T) \ge 5n + 2m - 7$ with equality if and only if $T \cong S_{n,m}$.

For an n-vertex tree T, it is widely known that $\alpha + m = n$. By Theorem 3, it results that

Theorem 4: Let $T \in \mathcal{T}(n, \alpha)$ be an n-vertex tree with $\alpha \le n - 3$. Then we have $\xi^c(T) \ge 7n - 2\alpha - 7$ with equality if and only if $T \cong S_{n,n-\alpha}$.

Theorem 5 Akhter and Farooq [1]: Let $T \in \mathcal{T}(2m, m)$ be an n-vertex tree with $m \ge 3$. Then $\xi^{ad}(T) \le \frac{1}{6}(2m^2 + 11m - 8)$, with equality if and only if $T \cong S_{2m,m}$.

Theorem 6: Let $T \in \mathcal{T}(n, m)$ be an n-vertex tree with $n \ge 6$ and $m \ge 3$. Then we have $\xi^{ad}(T) \le \frac{1}{6}(2n^2 + 2m^2 - 4nm + 3n + 5m - 8)$ with equality if and only if $T \cong S_{n,m}$.

Proof: We establish the result using induction on n. If $n = 2m$, then the required result holds from Theorem 5. Suppose that $n > 2m$ and the outcome satisfies for trees in $T \in \mathcal{T}(n-1, m)$. Let $T \in \mathcal{T}(n, m)$ and M be a largest matching of T. By Lemma 4, there is a pendent vertex w in T such that w is not M-saturated. Let v be the unique neighbor of w in T and $T_1 = T - \{w\}$. Then $T_1 \in \mathcal{T}(n-1, m)$. Since M is a largest matching, therefore M contains one edge linked with v. There are $n - 1 - m$ edges of T outside M, therefore $\deg_T(v) \le n - m$. If $ec_T(w) = 2$, then $T \cong S_n$ with w as a pendent vertex in S_n. Therefore we take $ec_T(w) \ge 3$ and $ec_T(v) \ge 2$.

Now take $x \in P_T(v)$, define $\mathcal{A} = \{y \in V_T \mid d_T(x, y) = ec_T(y)\}$. It is casual to see that for any $x \in V_T \setminus (\mathcal{A} \cup P_T(v))$, we have

$$ec_{T_1}(x) = ec_T(x).$$

There are some vertex $z \in V_T$ such that $d_{T_1}(y, z) = ec_{T_1}(y)$, for any $y \in \mathcal{A}$. There are two possibilities: either $z = v$ or $z \in V_T \setminus \{v, w\}$. If $z = v$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, v) < d_T(y, x) = ec_T(y).$$

Now if $z \in V_T \setminus \{v, w\}$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, z) = d_T(y, z) \le ec_T(y).$$

By the construction of T_1, we acquire

$$S_{T_1}(v) = S_T(v) - 1.$$

Also. for $x \in \Gamma_T(v) \setminus \{w\}$, we have

$$\begin{aligned} S_{T_1}(x) &= \sum_{y \in \Gamma_T(x)\setminus\{v\}} \deg_{T_1}(y) + \deg_{T_1}(v) \\ &= \sum_{y \in \Gamma_T(x)\setminus\{v\}} \deg_T(y) + (\deg_T(v) - 1) \\ &= S_{T_1}(x) - 1. \end{aligned}$$

Therefore by the induction hypothesis, we have

$$\begin{aligned} &\xi^{ad}(T) \\ &= \sum_{z \in V_T\setminus(\{v\}\cup\Gamma_T(v))} \frac{S_T(z)}{ec_T(z)} + \frac{S_T(v)}{ec_T(v)} \\ &\quad + \sum_{x \in \Gamma_T(v)\setminus\{w\}} \frac{S_T(x)}{ec_T(x)} + \frac{S_T(w)}{ec_T(w)} \\ &\le \sum_{z \in V_T\setminus(\{v\}\cup\Gamma_T(v))} \frac{S_T(z)}{ec_T(z)} + \frac{S_T(v)+1}{ec_T(v)} \\ &\quad + \sum_{x \in \Gamma_T(v)\setminus\{w\}} \frac{S_T(x)+1}{ec_T(x)} + \frac{\deg_T(v)}{ec_T(w)} \\ &= \xi^{ad}(T_1) + \frac{1}{ec_T(v)} + \sum_{x \in \Gamma_T(v)\setminus\{w\}} \frac{1}{ec_T(x)} + \frac{\deg_T(v)}{ec_T(w)} \end{aligned}$$

$$\begin{aligned} &\xi^{ad}(T) \\ &\le \frac{2(n-1)^2 + 2m^2 - 4(n-1)m + 3(n-1) + 5m - 8)}{6} \\ &\quad + \frac{1}{2} + \sum_{x \in \Gamma_T(v)\setminus\{w\}} \frac{1}{3} + \frac{n-m}{3} \end{aligned}$$

$$= \frac{2n^2+2m^2-4nm+3n+5m-8)}{6} + \frac{(-4n+4m-1)}{6} + \frac{1}{2} + \frac{n-m-1}{3} + \frac{n-m}{3} = \frac{2n^2+2m^2-4nm+3n+5m-8)}{6}.$$

The first equality holds if and only if $ec_{T_1}(z) = ec_T(z)$, for all $z \in V_T$ and second equality proved if and only if $\deg_T(v) = n-2m$, $|\Gamma_T(v) \setminus \{w\}| = n-m-1$, $ec_T(v) = 2$ and $ec_T(x) = 3$ for all $x \in \Gamma_T(v) \setminus \{w\}$, that is, $T \cong S_{n,m}$. Therefore, all the equalities proved if and only if $T \cong S_{n,m}$. This finishes the proof. □

By using $\alpha+m = n$ in Theorem 6, we acquire the following result.

Theorem 7: Let $T \in \mathcal{T}(n,\alpha)$ with $\alpha \leq n-3$. Then we have $\xi^{ad}(T) \leq \frac{1}{6}(8n+2\alpha^2-5\alpha-8)$ with equality if and only if $T \cong S_{n,n-\alpha}$.

IV. ECCENTRIC CONNECTIVITY INDEX OF TREES WITH DOMINATION NUMBER

Let $\mathcal{T}(n,\gamma)$ be the set of all the n-vertex trees with domination number γ. If $\gamma = 1$, then T is a star S_n with $\xi^c(S_n) = 3(n-1)$. Let $S_{n,\gamma} \in \mathcal{T}(n,\gamma)$ be a tree acquired from star $S^*_{1,\gamma}$ by attaching a pendent edge to each $n-\gamma-1$ pendent vertices.

In this section, we find the smallest eccentric connectivity index of trees in $\mathcal{T}(n,\gamma)$ and the largest eccentric adjacency index of trees in $\mathcal{T}(n,\gamma)$.

Lemma 5: Let T be a tree with $n \geq 4$ and $u_1u_2 \in E_T$ such that $u_1, u_2 \notin P_T$. Let T' be the new tree acquired from T by deleting u_1u_2 and identifying u_1 and u_2, denoted by u_1' and introducing a pendent edge $u_1'u_2'$, where u_2' be a pendent vertex. Then we have $\xi^c(T') < \xi^c(T)$ and $\xi^{ad}(T') > \xi^{ad}(T)$.

Proof: Let T_1 and T_2 be two components of $T - \{u_1u_2\}$ such that $u_1 \in V_{T_1}$ and $u_2 \in V_{T_2}$. For each vertex $w \in V_{T_1} \setminus \{u_1\}$, we have

$$\begin{aligned} ec_T(w) &= \max\{ec_{T_1}(w), d_{T_1}(w,u_1)+1+ec_{T_2}(u_2)\},\\ ec_{T'}(w) &= \max\{ec_{T_1}(w), d_{T_1}(w,u_1)+ec_{T_2}(u_2),\\ &\quad d_{T_1}(w,u_1)+1\}. \end{aligned} \tag{12}$$

For each vertex $w \in V_{T_2} \setminus \{u_2\}$, we have

$$\begin{aligned} ec_T(w) &= \max\{ec_{T_2}(w), d_{T_2}(w,u_2)+1+ec_{T_1}(u_1)\},\\ ec_{T'}(w) &= \max\{ec_{T_2}(w), d_{T_2}(w,u_2)+ec_{T_1}(u_1),\\ &\quad d_{T_2}(w,u_1)+1\}. \end{aligned} \tag{13}$$

Now, it is simply seen that the eccentricities of u_1' and u_2' in T' are as follows:

$$\begin{aligned} ec_{T'}(u_1') &= \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)\},\\ ec_{T'}(u_2') &= \max\{ec_{T_1}(u_1)+1, ec_{T_2}(u_2)+1\}. \end{aligned} \tag{14}$$

By the construction of T', we have

$$\deg_{T'}(w) = \deg_T(w), \quad \forall\, w \in V_T \setminus \{u_1,u_2\}. \tag{15}$$

Also, the degrees of vertices u_1' and u_2' in T' are given by

$$\begin{aligned} \deg_{T'}(u_1') &= \deg_T(u_1)+\deg_T(u_2)-1,\\ \deg_{T'}(u_2') &= 1. \end{aligned} \tag{16}$$

Note that from (12) and (13), we get $ec_{T'}(w) \leq ec_T(w)$ for all $w \in (V_{T_1} \setminus \{u_1\}) \cup (V_{T_2} \setminus \{u_2\})$. Thus from (12)-(16), we obtain

$$\begin{aligned} &\xi^c(T) - \xi^c(T')\\ &= \sum_{w \in V_{T_1} \setminus \{u_1\}} (\deg_T(w)ec_T(w) - \deg_{T'}(w)ec_{T'}(w))\\ &\quad + \sum_{w \in V_{T_2} \setminus \{u_2\}} (\deg_T(w)ec_T(w) - \deg_{T'}(w)ec_{T'}(w))\\ &\quad + \deg_T(u_1)ec_T(u_1) + \deg_T(u_2)ec_T(u_2)\\ &\quad - \deg_{T'}(u_1')ec_{T'}(u_1') - \deg_{T'}(u_2')ec_{T_2}(u_2')\\ &\geq \sum_{w \in V_{T_1} \setminus \{u_1\}} (\deg_T(w)ec_T(w) - \deg_T(w)ec_T(w))\\ &\quad + \sum_{w \in V_{T_2} \setminus \{u_2\}} (\deg_T(w)ec_T(w) - \deg_T(w)ec_T(w))\\ &\quad + \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)+1\}\deg_T(u_1)\\ &\quad + \max\{ec_{T_1}(u_1)+1, ec_{T_2}(u_2)\}\deg_T(u_2)\\ &\quad - \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)\}(\deg_T(u_1)+\deg_T(u_2)\\ &\quad -1) - \max\{ec_{T_1}(u_1)+1, ec_{T_2}(u_2)+1\}(1)\\ &= \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)+1\}\deg_T(u_1)\\ &\quad + \max\{ec_{T_1}(u_1)+1, ec_{T_2}(u_2)\}\deg_T(u_2)\\ &\quad - \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)\}(\deg_T(u_1)+\deg_T(u_2)\\ &\quad -1) - \max\{ec_{T_1}(u_1)+1, ec_{T_2}(u_2)+1\} \end{aligned} \tag{17}$$

Case I: If $ec_{T_1}(u_1) \geq ec_{T_2}(u_2)+1$, then

$$\begin{aligned} &\xi^c(T) - \xi^c(T')\\ &\quad = ec_{T_1}(u_1)\deg_T(u_1) + (ec_{T_1}(u_1)+1)\deg_T(u_2)\\ &\qquad - ec_{T_1}(u_1)(\deg_T(u_1)+\deg_T(u_2)-1)\\ &\qquad - (ec_{T_1}(u_1)+1)\\ &\quad = \deg_T(u_2) - 1 > 0. \end{aligned} \tag{18}$$

Case II: If $ec_{T_2}(u_2) \geq ec_{T_1}(u_1)+1$, then

$$\begin{aligned} &\xi^c(T) - \xi^c(T')\\ &\quad = (ec_{T_2}(u_2)+1)\deg_T(u_1) + ec_{T_2}(u_2)\deg_T(u_2)\\ &\qquad - ec_{T_2}(u_2)(\deg_T(u_1)+\deg_T(u_2)-1)\\ &\qquad - (ec_{T_2}(u_2)+1)\\ &\quad = \deg_T(u_1) - 1 > 0. \end{aligned} \tag{19}$$

Case III: If $ec_{T_1}(u_1) = ec_{T_2}(u_2)$, then

$$\begin{aligned} &\xi^c(T) - \xi^c(T')\\ &= (ec_{T_2}(u_2)+1)\deg_T(u_1) + (ec_{T_2}(u_2)+1)\\ &\quad \times \deg_T(u_2) - ec_{T_2}(u_2)(\deg_T(u_1)+\deg_T(u_2)-1)\\ &\quad - (ec_{T_2}(u_2)+1)\\ &= \deg_T(u_1) + \deg_T(u_2) - 1 > 0. \end{aligned} \tag{20}$$

The proof is complete. □

Xu *et al.* [18] determined that any graph $\mathcal{G}$ without isolated vertices has a subset A of $V_{\mathcal{G}}$ of cardinality $\gamma_{\mathcal{G}}$ such that for each $u \in A$, there is a vertex in $V_{\mathcal{G}} \setminus A$ that is only linked to u. Therefore we acquire the following lemma.

Lemma 6 Xu et al. [18]: For any graph $\mathcal{G}$, we have $\gamma_{\mathcal{G}} \leq m_{\mathcal{G}}$.

Lemma 7: If $T_1 \in \mathcal{T}(n, \gamma)$ has the smallest eccentric connectivity index, then $\gamma_{T_1} = m_{T_1} = \gamma$.

Proof: By Lemma 6, we have $\gamma = \gamma_{T_1} \leq m_{T_1}$. Now it suffices to prove that $\gamma_{T_1} \geq m_{T_1}$. Let $A = \{u_1, u_2, \ldots, u_\gamma\}$ be a dominating set of T_1 with cardinality γ. Then there exists γ edges $u_1u_1', u_2u_2', \ldots, u_\gamma u_\gamma' \in E_{T_1}$, where $u_1', u_2', \ldots, u_\gamma' \in V_{T_1} \setminus A$. Note that if $\gamma = \gamma_{T_1} < m_{T_1}$, there exists another edge x_1x_1', that is independent of each edge $u_1u_1', u_2u_2', \ldots, u_\gamma u_\gamma'$.

If $u_i \in A$ dominate both the vertices x_1 and x_2, then a triangle $x_1x_2u_i$ occurs, where $i = 1, 2, \ldots, \gamma$. But we know that T_1 is a tree therefore it is impossible. Thus x_1 and x_2 are dominated by two quite different vertices of A. Without loss of generality we suppose that x_i is dominated by u_i, for $i = 1, 2$, with $\deg_{T_1}(x_1), \deg_{T_1}(x_2) \geq 2$ and $\deg_{T_1}(u_1), \deg_{T_1}(u_2) \geq 2$. Now we can construct a new tree $T_1' \in \mathcal{T}(n, \gamma)$ from T_1 by applying transformation described in Lemma 5 on the edge x_1u_1 or x_2u_2 and we get $\xi^c(T_1) > \xi^c(T_1')$. This is the contradiction of our assumption. Therefore $\gamma_{T_1} \geq m_{T_1}$. □

By using Lemma 7, Theorem 3 and a simple calculation, we have following result.

Theorem 8: Let $T \in \mathcal{T}(n, \gamma)$ with $2 \leq \gamma \leq \left\lfloor \frac{n}{2} \right\rfloor$. Then we have $\xi^c(T) \geq 5n + 2\gamma - 7$ with equality if and only if $T \cong S_{n,\gamma}$.

V. CONCLUSION

In this paper, we focuss on determining the trees with the smallest eccentric connectivity index and the largest eccentric adjacency index among the n-vertex trees with a given bipartition size. Also we discuss the smallest eccentric adjacency index and the largest eccentric adjacency index of trees among n-vertex trees with fixed matching number and independence number. Finally, we characterize the smallest trees among all n-vertex trees with domination number with respect to eccentric connectivity index. Finding extremal graphs with different parameters in general classes of graphs with respect to distance based indices will be an interesting and a challenging problem.

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