Extremal graphs with respect to the total-eccentricity index

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Abstract

In a connected graph $G$, the distance between two vertices of $G$ is the length of a shortest path between these vertices. The eccentricity of a vertex $u$ in $G$ is the largest distance between $u$ and any other vertex of $G$. The total-eccentricity index $\tau(G)$ is the sum of eccentricities of all vertices of $G$. In this paper, we find extremal trees, unicyclic and bicyclic graphs with respect to total-eccentricity index. Moreover, we find extremal conjugated trees with respect to total-eccentricity index.

Keywords: Topological indices, total-eccentricity index, extremal graphs.

1 Introduction

A topological index can be defined as a function $T : \mathcal{G} \to \mathbb{R}$, where $\mathcal{G}$ denotes the class of all finite graphs, such that for any $G, H \in \mathcal{G}$, $T(G) = T(H)$ if $G$ and $H$ are isomorphic. It is a numerical value which is associated with the chemical structure of a certain chemical compound. The aim of such association is to correlate various physico-chemical properties or some biological activity in a chemical compound.

Let $G$ be an $n$-vertex molecular graph with vertex set $V(G)$ and edge set $E(G)$. The vertices of $G$ correspond to atoms and an edge between two vertices corresponds to the chemical bond between these vertices. An edge between two vertices $u, v \in V(G)$ is denoted by $uv$. The order and size of $G$ are respectively the cardinalities $|V(G)|$ and $|E(G)|$. The neighbourhood $N_G(v)$ of a vertex $v$ in $G$ is the set of vertices adjacent to $v$. The degree $d_G(v)$ of a vertex $v$ in $G$ is the cardinality $|N_G(v)|$. If $d_G(v) = k$ for all $v \in V(G)$, then $G$ is called a $k$-regular graph. A vertex of degree 1 is called a pendant vertex. A path $P_n$ of order $n$ and length $n - 1$ is a connected graph with exactly two pendant vertices and $n - 2$ vertices of degree 2. A $(v_1, v_n)$-path on vertices $v_1, v_2, \ldots, v_n$ with end-vertices $v_1$ and $v_n$ is denoted

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by \(v_1v_2\ldots v_n\). A graph \(G\) is said to be connected if there exists a path between every pair of vertices in \(G\). A cycle \(C_n\) of order and length \(n\) is a connected graph all of whose vertices are of degree two. A complete graph \(K_n\) of order \(n\) is a graph in which every two distinct vertices are adjacent. Let \(U\) and \(V\) be two sets of vertices with \(|U| = m\) and \(|V| = n\). Then a complete bipartite graph \(K_{m,n}\) is defined as a graph obtained by joining every vertex of \(U\) with every vertex of \(V\). A star \(S_n\) of order \(n\) is a connected graph with \(n-1\) pendant vertices and one vertex with degree \(n-1\). A tree is a connected graph containing no cycle. Thus, an \(n\)-vertex tree is a connected graph with exactly \(n-1\) edges. An \(n\)-vertex unicyclic graph is a connected graph which contains \(n\) edges. Similarly, an \(n\)-vertex bicyclic graph is a connected graph which contains \(n+1\) edges.

Now we define some basic graph operations which are required to construct some new classes of graphs used in this paper. A graph \(H\) is a subgraph of a graph \(G\) if \(V(H) \subseteq V(G)\) and \(E(H) \subseteq E(G)\). Let \(u, v\) be two non-adjacent vertices of a graph \(G\). Then the union of graph \(G\) and edge \(e = uv \notin E(G)\) is denoted as \(G \cup \{e\}\). The disjoint union of two graphs \(G\) and \(H\) with \(V(G) \cap V(H) = \emptyset\) is defined as the graph \(G \cup H\) with vertex set \(V(G \cup H) = V(G) \cup V(H)\) and edge set \(E(G \cup H) = E(G) \cup E(H)\). Let \(S \subseteq V(G)\), then the vertex deleted subgraph \(G - S\) is obtained from \(G\) by deleting all the vertices in \(S\) from \(G\) along with all the edges incident on the vertices of \(S\). If \(S = \{u\}\), we simply write \(G - u\). The subgraph \(G[S]\) of \(G\) induced by \(S \subseteq V(G)\) is the graph obtained by \(G - S^c\), where \(S^c = V(G) \setminus S\). The subdivision of an edge \(e = uv\) in \(G\) is performed by replacing the edge \(uv\) by a path \(uwv\) of length 2, where \(w \notin V(G)\).

A matching \(M\) in a graph \(G\) contains those edges of \(G\) which do not share any vertex. A vertex \(u\) in \(G\) is said to be \(M\)-saturated if an edge of \(M\) is incident with \(u\). A matching \(M\) is said to be perfect if every vertex in \(G\) is \(M\)-saturated. A conjugated graph is the one which contains a perfect matching. The distance \(d_G(u, v)\) between two vertices \(u, v \in V(G)\) is defined as the length of a shortest path between \(u\) and \(v\) in \(G\). The eccentricity \(e_G(v)\) of a vertex \(v \in V(G)\) is defined as the largest distance from \(v\) to any other vertex in \(G\). The diameter \(\text{diam}(G)\) and radius \(\text{rad}(G)\) of a graph \(G\) are respectively defined as:

\[
\text{rad}(G) = \min_{v \in V(G)} e_G(v), \quad (1.1)
\]

\[
\text{diam}(G) = \max_{v \in V(G)} e_G(v). \quad (1.2)
\]

A vertex \(v \in V(G)\) is said to be central (resp. peripheral) if \(e_G(v) = \text{rad}(G)\) (resp. \(e_G(v) = \text{diam}(G)\)). The graph induced by the central vertices of \(G\) is called the center of \(G\), denoted as \(C(G)\).

The first topological index was introduced by Wiener [13] in 1947, to calculate the boiling points of paraffins. In 1971, Hosoya [3] defined the notion of Wiener index for any graph as the half sum of distances between all pairs of vertices. The average-eccentricity of an \(n\)-vertex graph \(G\) was defined in 1988 by Skorobogatov and Dobrynin [11] as:

\[
\text{avec}(G) = \frac{1}{n} \sum_{u \in V(G)} e_G(u). \quad (1.3)
\]

In the recent literature, a minor modification of average-eccentricity index \(\text{avec}(G)\) is used
and cited as total-eccentricity index $\tau(G)$. It is defined as:

$$\tau(G) = \sum_{u \in V(G)} e_G(u). \quad (1.4)$$

Dankelmann et al. [2] studied the bounds on the average-eccentricity of a graph and the change in $\text{avec}(G)$ when $G$ is replaced by any of its spanning subgraphs. Smith et al. [12] studied the extremal values of total-eccentricity index in trees. Ilić [4] studied some extremal graphs with respect to average-eccentricity. Shi [10] studied the chemical indices namely Randić index, Harmonic index and the radius of graph and proved some conjectures for dense triangle free graphs. Qi and Du [8] studied the Zagreb eccentricity indices of trees.

For some special families of graphs of order $n \geq 4$, the total-eccentricity index is given as follows:

1. For a $k$-regular graph $G$, we have $\tau(G) = \frac{\xi(G)}{k}$.
2. $\tau(K_n) = n$,
3. $\tau(K_{m,n}) = 2(m + n)$, $m, n \geq 2$,
4. The total-eccentricity index of a star $S_n$, a cycle $C_n$ and a path $P_n$ is given by

$$\tau(S_n) = 2n - 1,$$

$$\tau(C_n) = \begin{cases} \frac{n}{2} & \text{if } n \equiv 0(\text{mod}2) \\ \frac{n-1}{2} & \text{if } n \equiv 1(\text{mod}2), \end{cases}$$

$$\tau(P_n) = \begin{cases} \frac{3n^2}{4} - \frac{n}{2} & \text{if } n \equiv 0(\text{mod}2) \\ \frac{3n^2}{4} - \frac{n}{2} - \frac{1}{4} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \quad (1.6)$$

This paper is structured as follows: In Section 2, we study extremal trees with respect to the total-eccentricity index. In Section 3, we study the extremal unicyclic and bicyclic graphs with respect to total-eccentricity index and Section 4 deals with the study of extremal conjugated trees with respect to total-eccentricity index.

## 2 Extremal trees with respect to total-eccentricity index

It is known that the star and the path respectively minimizes and maximizes the total-eccentricity index among all trees of a given order [2,4,12]. We go further and for a given tree $T$ with $n$ vertices, $n \geq 4$, we find a sequence of $n$-vertex trees $T_1, T_2, \ldots, T_k$ such that

$$\tau(T) < \tau(T_1) < \ldots < \tau(T_k) = \tau(P_n). \quad (2.1)$$

Similarly, for a given tree $T$ with $n$ vertices, $n \geq 4$, we find a sequence of $n$-vertex trees $T'_1, T'_2, \ldots, T'_l$ such that

$$\tau(T) > \tau(T'_1) > \ldots > \tau(T'_l) = \tau(S_n). \quad (2.2)$$

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Consider an $n$-vertex tree $T$ with vertex set $V(T)$ and edge set $E(T)$. The following inequalities are easy to see:

\[
\begin{align*}
\mathrm{rad}(T) & \leq \mathrm{diam}(T) \leq 2\mathrm{rad}(T), \\
\frac{1}{2} \mathrm{diam}(T) & \leq \mathrm{rad}(T) \leq e_{T}(v), \quad \forall \ v \in V(T).
\end{align*}
\] (2.3)

A vertex $v \in V(T)$ is said to be an eccentric vertex of a vertex $u \in V(T)$ if $d_{T}(u, v) = e_{T}(u)$. Let $E_{T}(u)$ denote the set of all eccentric vertices of $u$ in $T$. For any $w \in E_{T}(u)$, the shortest $(u, w)$-path is called an eccentric path for $u$. It is known that the center of a tree is $K_{1}$ if $\mathrm{diam}(T) = 2\mathrm{rad}(T)$ and is $K_{2}$ if $\mathrm{diam}(T) = 2\mathrm{rad}(T) - 1$ [5]. Moreover, every diametrical path in a tree $T$ contains $C(T)$ [1]. Clearly every diametrical path in $T$ is an eccentric path for some peripheral vertex $v$ in $T$. In the next lemma, we prove a result about the eccentric vertices in a tree.

**Lemma 2.1.** Let $T$ be an $n$-vertex tree and $P$ be a diametrical $(u, v)$-path in $T$. Then for any $x \in V(T)$, either $u \in E_{T}(x)$ or $v \in E_{T}(x)$.

**Proof.** Let $x \in V(T)$. On contrary, assume that $u \notin E_{T}(x)$ and $v \notin E_{T}(x)$. Let $v' \in E_{T}(x)$. Without loss of generality, assume that $d_{T}(x, v) \geq d_{T}(x, u)$. Then

\[
d_{T}(x, v') > d_{T}(x, v) \geq d_{T}(x, u).
\] (2.4)

Let $u', u'' \in V(P)$ such that $d_{T}(x, u') = \min\{d_{T}(x, w) \mid w \in V(P)\}$ and $d_{T}(v', u'') = \min\{d_{T}(v', w) \mid w \in V(P)\}$. Then

\[
\begin{align*}
d_{T}(x, v') &= d_{T}(x, u') + d_{T}(u', v') \quad \text{(2.5)} \\
d_{T}(x, v) &= d_{T}(x, u') + d_{T}(u', v) \quad \text{(2.6)} \\
d_{T}(x, u) &= d_{T}(x, u') + d_{T}(u', u).
\end{align*}
\]

From (2.4)-(2.6), we obtain

\[
d_{T}(u', v') > d_{T}(u', v).
\] (2.7)

Also inequality (2.4) together with equations (2.6) and (2.7) gives

\[
d_{T}(u', v) \geq d_{T}(u', u).
\] (2.8)

We consider following three cases:

**Case 1.** When $P$ and $(x, v')$-path have a vertex in common. If $u''$ lies on $(x, v)$-path then by using (2.7), we get

\[
\begin{align*}
d_{T}(u, v') &= d_{T}(u, u') + d_{T}(u', v') \\
&> d_{T}(u, u') + d_{T}(u', v) \\
&= d_{T}(u, v) = \mathrm{diam}(T).
\end{align*}
\]

This contradicts the fact that $P$ is a diametrical path.

**Case 2.** If $u''$ lies on $(x, u)$-path then using (2.7) and (2.8), we obtain

\[
\begin{align*}
d_{T}(v, v') &= d_{T}(v, u') + d_{T}(u', v') \\
&> d_{T}(v, u') + d_{T}(u', v) \\
&= d_{T}(u, v) = \mathrm{diam}(T).
\end{align*}
\]
This is again a contradiction.

**Case 3.** When $P$ and $(x, v')$-path have no vertex in common. We denote $(u, v')$-path by $P'$. Let $w' \in V(P')$ such that $d_T(x, w') = \min \{d_T(x, w) \mid w \in V(P') \}$. Then

$$d_T(x, v') = d_T(x, w') + d_T(w', v') \tag{2.9}$$

$$d_T(x, v) = d_T(x, w') + d_T(w', v). \tag{2.10}$$

Inequality (2.4) along with equations (2.9) and (2.10) gives

$$d_T(w', v') > d_T(w', v). \tag{2.11}$$

Using (2.11), we obtain

$$d_T(u, v') = d_T(u, w') + d_T(w', v')$$

$$> d_T(u, w') + d_T(w', v)$$

$$= d_T(u, u') + d_T(u', w') + d_T(w', v') + d_T(u', v)$$

$$= d_T(u, v) + 2d_T(u', w') \geq \text{diam}(T),$$

which is a contradiction. The proof is complete.

In the next result, we construct a new tree from the given tree with larger total-eccentricity index.

**Lemma 2.2.** Let $T \cong P_n$ be an $n$-vertex tree, $n \geq 4$, and $u, v$ be the end-vertices of a diametrical path in $T$. Take a pendant vertex $x$ of $T$ distinct from $u$ and $v$ and let $y$ be the unique neighbour of $x$. Construct a tree $T' \cong \{T - \{xy\}\} \cup \{xu\}$. Then $\tau(T) < \tau(T').$
Proof. We note that \((x, v)\)-path is a diametrical path in \(T\) and
\[
e_T(x) = e_T(u) + 1 = \text{diam}(T) + 1 > e_T(x).
\] (2.12)

By the construction of \(T\), we have
\[
d_T^*(w, v) = d_T(w, v) \quad \forall \ w \in V(T) \setminus \{x\} \tag{2.13}
d_T^*(w, x) = d_T(w, u) + 1 \quad \forall \ w \in V(T) \setminus \{x\}. \tag{2.14}
\]

By Proposition 2.1, we have
\[
e_T(w) = \max \{d_T(w, u), d_T(w, v)\} \quad \forall \ w \in V(T) \tag{2.15}
e_T^*(w) = \max \{d_T^*(w, x), d_T^*(w, v)\} \quad \forall \ w \in V(T). \tag{2.16}
\]

Thus for each \(w \in V(T) \setminus \{x\}\), equations (2.13)-(2.16) imply
\[
e_T^*(w) = \max \{d_T^*(w, x), d_T^*(w, v)\} = \max \{d_T^*(w, u) + 1, d_T^*(w, v)\}
\geq \max \{d_T^*(w, u), d_T^*(w, v)\} = e_T(w). \tag{2.17}
\]

Thus, from inequalities (2.12)-(2.17), we obtain
\[
\tau(T^*) = \sum_{w \in V(T) \setminus \{x\}} e_T^*(w) + e_T^*(x)
> \sum_{w \in V(T) \setminus \{x\}} e_T(w) + e_T(x)
= \tau(T).
\]

This completes the proof. \(\square\)

Now we find the trees with minimal and maximal total-eccentricity index among the class of \(n\)-vertex trees. We devise an algorithm to reduce a given tree into a path. Let \(T\) be an \(n\)-vertex tree, \(n \geq 4\) and let \(u, v \in V(T)\) be the end-vertices of a diametrical path in \(T\). Define
\[
A_{u,v} = \{xy \in E(T) \mid d_T(x) = 1, x \in V(T) \setminus \{u, v\}\}. \tag{2.18}
\]

**Algorithm 1**

| input:   | An \(n\)-vertex tree \(T\), \(n \geq 4\). |
| output:  | The tree \(P_n\). |
| Step 0:  | Take a diametrical \((u, v)\)-path in \(T\) and define \(A_{u,v}\) by (2.18). |
| Step 1:  | If \(A_{u,v} = \emptyset\) then Stop. |
| Step 2:  | For an \(xy \in A_{u,v}\) define \(T := \{T - \{xy\}\} \cup \{ux\}\). Set \(u := x\) and update \(A_{u,v}\) by (2.18); go to Step 1. |

Next, we discuss the termination and correctness of Algorithm 1. When the algorithm goes from Step A to Step B, we will use the notation [Step A \(\rightarrow\) Step B].

**Theorem 2.1** (Termination). The Algorithm 1 terminates after a finite number of iterations.
Proof. Initially $A_{u,v}$ is defined at Step 0 and modified at Step 2 in each iteration. Modification of $A_{u,v}$ at Step 2 implies that if a pendant edge is removed from $A_{u,v}$, it will not appear again in $A_{u,v}$ in the subsequent iterations of Algorithm 1. Thus [Step 2 $\rightarrow$ Step 1] is executed at most $n - 1$ times. Hence Algorithm 1 terminates after a finite number of iterations. \hfill \Box

Theorem 2.2 (Correctness). If Algorithm 1 terminates then it outputs $P_n$.

Proof. We can obviously see that after the execution of Step 2 in any iteration of Algorithm 1, the modified graph $T$ at Step 2 is again an $n$-vertex tree. Also, by definition of $A_{u,v}$, we see that $T$ has exactly two pendant vertices when $A_{u,v} = \emptyset$. Thus, when Algorithm 1 terminates at Step 1, the tree $T$ has exactly two pendant vertices, that is, $T = P_n$. \hfill \Box

Using Lemma 2.2 and Algorithm 1, we prove the following theorem.

Theorem 2.3. Let $n \geq 4$. Then among the $n$-vertex trees, the path $P_n$ has the maximal total-eccentricity index. Thus for any $n$-vertex tree $T$, we have $\tau(T) \leq \tau(P_n)$.

Proof. Let $T \not\cong P_n$ be an $n$-vertex tree. By Lemma 2.2, the total-eccentricity index of the modified tree $T$ strictly increases at Step 2 in each iteration of Algorithm 1. The Algorithm 1 terminates when $T \cong P_n$. This shows that $P_n$ has the maximal total-eccentricity index. \hfill \Box

Corollary 2.4. Let $T$ be a tree on $n$ vertices, then

$$\tau(T) \leq \frac{3n^2}{4} - \frac{n}{2}, \quad \text{(2.19)}$$

where equality holds when $T$ is a path on $n$ vertices and $n \equiv 0 \text{(mod2)}$.

Proof. The result follows by using Theorem 2.3 and equation (1.6).\hfill \Box

By Lemma 2.2, we see that when the Algorithm 1 goes from Step 2 to Step 1, the total-eccentricity index of the modified tree strictly increases. Thus, if the Algorithm 1 terminates after $k$ iterations, it generates a sequence of trees $T_1, T_2, \ldots, T_k$, of same order $n$ satisfying (2.1).

Example 1. Consider a tree $T$ of order 9 shown in Figure 3. The Algorithm 1 will generate a sequence of trees $T_1, T_2, T_3 \cong P_9$ such that $\tau(T) < \tau(T_1) < \tau(T_2) < \tau(T_3) = \tau(P_9)$. We remark that this sequence is not unique. The modification of the tree at Step 2 depends upon the choice of pendant edge $xy$.

Figure 3: Sequence of trees generated by Algorithm 1 at Step 2 in each iteration.
Next we propose an algorithm to reduce a given tree into a star. Let $T$ be an $n$-vertex tree and $c \in V(T)$ with $e_T(c) = \text{rad}(T)$. We define $A_r$ by

$$A_r = \{ xy \in E(T) \mid d_T(x, c) = \text{rad}(T) \}. \quad (2.20)$$

**Algorithm 2**

**Input:** An $n$-vertex tree $T$, $n \geq 4$.

**Output:** The tree $S_n$.

**Step 0:** Find $\text{rad}(T)$ by (1.1), a vertex $c \in V(T)$ with $e_T(c) = \text{rad}(T)$ and define $A_r$ by (2.20).

**Step 1:** If $\text{rad}(T) = 1$, then Stop.

**Step 2:** For an edge $xy \in A_r$, define $T' := T - \{yx\} \cup \{cx\}$ and $A_r' := A_r \setminus \{xy\}$.

**Step 3:** If $A_r' \neq \emptyset$ then go to Step 2; else define $\text{rad}(T)$ by (1.1) and $A_r'$ by (2.20); go to Step 1.

Next, we discuss the correctness and termination of the Algorithm 2.

**Theorem 2.5** (Termination). The Algorithm 2 terminates after a finite number of iterations.

**Proof.** Note that initially $\text{rad}(T)$ and $A_r$ are defined at Step 0. The set $A_r$ reduces at Step 2. If [Step 3 $\rightarrow$ Step 2] is executed then $A_r$ reduces. Thus [Step 3 $\rightarrow$ Step 2] can be executed for a finite number of times. If $A_r = \emptyset$ at Step 3 then $r$ decreases at Step 3. Thus [Step 3 $\rightarrow$ Step 1] can be executed for a finite number of times. Therefore the algorithm will terminate after a finite number of iterations. $\square$

**Theorem 2.6** (Correctness). If Algorithm 2 terminates then it outputs $S_n$.

**Proof.** When Algorithm 2 terminates at Step 1 then $\text{rad}(T) = 1$ and $c$ remains the central vertex of $T$, that is, $d_T(c, x) = 1$ for all $x \in V(T) \setminus \{c\}$. This shows that $T \cong S_n$. $\square$

The following theorem gives trees with minimal total-eccentricity index.

**Theorem 2.7.** Among all $n$-vertex trees with $n \geq 4$, the star $S_n$ has minimal total-eccentricity index.

**Proof.** Let $T \not\cong S_n$ be an $n$-vertex tree, $n \geq 4$ and let $c$ be a central vertex of $T$. Define $A_r$ by (2.20). We construct a new set of edges not in $E(T)$ by

$$\tilde{A}_r = \{ cx \mid x \in V(T) \text{ with } d_T(x, c) = \text{rad}(T) \}$$

and define a tree $T'$ by

$$T' \cong \{ T - A_r \} \cup \tilde{A}_r.$$

Then we note that $\text{rad}(T') = \text{rad}(T) - 1$. Thus by the construction of $T'$, we observe that

$$e_{T'}(u) \leq e_T(u) \quad \forall u \in V(T). \quad (2.21)$$

Moreover, $c$ is a central vertex of $T'$, that is,

$$e_{T'}(c) = \text{rad}(T) - 1 < e_T(c). \quad (2.22)$$
From (2.21) and (2.22), we obtain
\[ \tau(T') < \tau(T). \]
In fact, if \( T \) is a tree at Step 1 with \( \text{rad}(T) > 1 \) in any iteration of Algorithm 2, then \( T' \) is a tree at Step 3 when \( A_r = \emptyset \). Thus when \( \text{Step 3} \rightarrow \text{Step 1} \) is executed, the total-eccentricity index strictly decreases. Since Algorithm 2 outputs \( S_n \), we have \( \tau(S_n) < \tau(T) \). Thus the assertion holds.

**Corollary 2.8.** For an \( n \)-vertex tree \( T \), we have
\[ \tau(T) \geq 2n - 1. \] (2.23)

**Proof.** By Theorem 2.7 and equation (1.5), the proof is obvious. \( \square \)

From the proof of Theorem 2.7, we note that when \( \text{Step 3} \rightarrow \text{Step 1} \) is executed, the total-eccentricity index of the modified tree strictly decreases. Thus, if the Algorithm 2 terminates after \( l \) iterations, it generates a sequence of trees \( T'_1, T'_2, \ldots, T'_l \), of same order \( n \) satisfying (2.2).

**Example 2.** Consider a tree \( T \) of order 14 shown in Figure 4. The Algorithm 2 will generate a sequence of trees \( T'_1, T'_2, T'_3 \equiv S_{14} \) such that \( \tau(T) > \tau(T'_1) > \tau(T'_2) > \tau(T'_3) = \tau(S_{14}) \). We remark that this sequence is not unique. The modification of the tree at Step 2 depends upon the choice of pendant edge \( xy \). The step-wise procedure is explained in Figure 4.

![Figure 4: Sequence of trees generated by Algorithm 2 when [Step 2 \rightarrow Step 1] is executed.](image)

3 Extremal unicyclic and bicyclic graphs with respect to total-eccentricity index

In this section, we find graphs with minimal and maximal total-eccentricity index among the \( n \)-vertex unicyclic and bicyclic graphs. In the next theorem, we find the graph with minimal total-eccentricity index among all unicyclic graphs.

**Theorem 3.1.** Among all \( n \)-vertex unicyclic graphs, \( n \geq 4 \), the graph \( U_1 \) shown in Figure 5 has the minimal total-eccentricity index.
Proof. Let $U \ngeq U_1$ be an $n$-vertex unicyclic graph, $n \geq 4$. Then $e_U(u) \geq 2$ for each $u \in V(U)$. Note that $e_{U_1}(u) \leq 2$ for each $u \in V(U_1)$. Thus

$$\tau(U) \geq \tau(U_1).$$

The proof is complete.

Corollary 3.2. For any unicyclic graph $U$, $\tau(U) \geq 2n - 1$.

Proof. After simple computation we see that $\tau(U_1) = 2n - 1$. Thus the proof is obvious by using Theorem 3.1.

In the next theorem, we find an $n$-vertex unicyclic graph with maximal total-eccentricity index.

Theorem 3.3. Among all $n$-vertex unicyclic graphs, $n \geq 4$, the graph $U_2$ shown in Figure 5 has maximal total-eccentricity index.

Figure 5: Extremal unicyclic graphs $U_1$ and $U_2$ with respect to total-eccentricity index.

Proof. Let $T \ngeq P_n$ be an $n$-vertex tree and $T_1 \cong U_2 - \{v_1v_2\}$. We show that $\tau(T) \leq \tau(T_1)$. There exists a pendant vertex $u_1 \in V(T)$ such that $e_T(u) = e_{T-u_1}(u)$ for all $u \in V(T) \setminus \{u_1\}$. Then from Theorem 2.3, we obtain

$$\tau(T - u_1) \leq \tau(T_1 - v_1). \quad (3.1)$$

Note that $e_{T_1-v_1}(u) = e_{T_1}(u)$ for each $u \in V(T_1) \setminus \{v_1\}$ and $e_{T_1}(v_1) = n - 2$. Thus

$$\tau(T_1) = \tau(T_1 - v_1) + n - 2. \quad (3.2)$$

Also, $e_{T-u_1}(u) = e_{T}(u)$ for each $u \in V(T) \setminus \{u_1\}$ and $e_T(u_1) \leq n - 2$. Thus

$$\tau(T) \leq \tau(T - u_1) + n - 2. \quad (3.3)$$

From (3.1)-(3.3), we obtain

$$\tau(T) \leq \tau(T_1).$$

Also observe that $\tau(T_1) = \tau(U_2)$. Thus $\tau(T) \leq \tau(U_2)$. Now, if we join any two non-adjacent vertices in $T$, it gives us a unicyclic graph $U$ and $\tau(U) \leq \tau(T)$. Thus, $\tau(U) \leq \tau(U_2)$. This completes the proof. \qed
Corollary 3.4. For any unicyclic graph $U$, we have $\tau(U) \leq \frac{n(n-1)}{2} - 1$.

Proof. After simple computation, we see that $\tau(U) = \frac{n(n-1)}{2} - 1$. Thus the proof is obvious by using Theorem 3.3.

Now we find the extremal bicyclic graphs with respect to total-eccentricity index. The following remark can be obtained by simple computation.

Remark 3.1. Let $B_1, B'_1, B_2$ and $B'_2$ be $n$-vertex bicyclic graphs shown in Figure 6. Then the total-eccentricity index of these graphs is given by

1. $\tau(B_1) = \tau(B'_1) = 2n - 1$.

2. $\tau(B_2) = \begin{cases} \frac{3}{4}n^2 - \frac{3}{2}n - 2 & \text{when } n \text{ is even} \\ \frac{3}{4}n^2 - \frac{3}{2}n - \frac{9}{4} & \text{when } n \text{ is odd.} \end{cases}$

3. $\tau(B'_2) = \begin{cases} \frac{3}{4}n^2 - n - 2 & \text{when } n \text{ is even} \\ \frac{3}{4}n^2 - n - \frac{7}{4} & \text{when } n \text{ is odd.} \end{cases}$

Remark 3.2. Let $G$ be a connected graph and $C_k$ be a cycle of length $k$ in $G$. Then each diametrical path in $G$ contains at most $\lfloor \frac{k}{2} \rfloor + 1$ vertices of $C_k$ and at most $\lfloor \frac{k}{2} \rfloor$ edges of $C_k$.

![Figure 6: Bicyclic graphs $B_1, B'_1, B_2$ and $B'_2$.](image)

Theorem 3.5. Among all $n$-vertex bicyclic graphs, $n \geq 5$, the graph $B_1$ shown in Figure 6 has minimal total-eccentricity index.

Proof. Consider a bicyclic graph $B \not\cong B_1$. Then $e_B(v) \geq 2$ for all $v \in V(B)$. Since $e_{B_1}(v) \leq 2$ for all $v \in V(B_1)$. Thus, $\tau(B_1) \leq \tau(B)$.

Corollary 3.6. For any bicyclic graph $B$, we have $\tau(B) \geq 2n - 1$.

Proof. By Remark 3.1 and Theorem 3.5, the proof is obvious.

Let $B_1$ denotes the class of those $n$-vertex bicyclic graphs which have exactly two cycles, $n \geq 5$. Then the maximal graph with respect to total-eccentricity index in $B_1$ is obtained in the next result.
Lemma 3.1. Among all \(n\)-vertex bicyclic graphs in \(\mathcal{B}_1\), \(n \geq 5\), the graph \(B_2\) shown in Figure 6 has the maximal total-eccentricity index.

Proof. First note that \(B_2 - v \cong U_2\) and \(\tau(B_2) = \tau(U_2) + n - 3\), where \(U_2\) is the \(n - 1\) vertex unicyclic graph shown in Figure 5. Let \(B \in \mathcal{B}_1\) be any \(n\)-vertex bicyclic graph. Then there exist two disjoint edges \(e_1, e_2 \in E(B)\) such that \(B - \{e_1, e_2\}\) is a tree and \(B - \{e_1, e_2\}\) has at least four pendant vertices. Let \(T \cong B - \{e_1, e_2\}\). Then

\[e_T(v) \leq n - 3, \quad \forall \ v \in V(T). \tag{3.4}\]

Obviously \(\tau(B) \leq \tau(T)\). Since \(T \not\cong P_n\), using Lemma 2.1 there exists a pendant vertex \(u_1 \in V(T)\) such that

\[e_T(u) = e_{T-u_1}(u), \quad \forall \ u \in V(T) \setminus \{u_1\}. \tag{3.5}\]

Note that \(T - u_1 \not\cong P_{n-1}\). Then as shown in the proof of Theorem 3.3 that

\[\tau(T - u_1) \leq \tau(U_2). \tag{3.6}\]

From (3.4) and (3.5), we obtain

\[\tau(T) \leq \tau(T - u_1) + n - 3. \tag{3.7}\]

From (3.6) and (3.7), we have

\[\tau(B) \leq \tau(T - u_1) + n - 3 \leq \tau(U_2) + n - 3 = \tau(B_2).\]

The proof is complete. \(\square\)

Let \(\mathcal{B}_2\) denotes the class of all \(n\)-vertex bicyclic graphs which have exactly three cycles, \(n \geq 5\). Then we have the following result.

Lemma 3.2. Among all \(n\)-vertex bicyclic graphs in \(\mathcal{B}_2\), \(n \geq 5\), the graph \(B'_2\) shown in Figure 6 has the maximal total-eccentricity index.

Proof. Let \(B'_2 \in \mathcal{B}_2\) be the graph shown in Figure 6. Note that \(B'_2 - v \cong P_{n-1}\) and

\[\tau(B'_2) = \tau(P_{n-1}) + n - 3. \tag{3.8}\]

We show that, \(B'_2\) has maximal total-eccentricity index in \(\mathcal{B}_2\). Let \(B \in \mathcal{B}_2\) with cycles \(C_{k_1}, C_{k_2}\) and \(C_{k_3}\). Without loss of generality, assume that \(k_1 \leq k_2 \leq k_3\). Then \(3 \leq k_1, k_2 \leq n - 1\) and \(4 \leq k_3 \leq n\). Since \(B\) is not a path, it holds that \(\text{diam}(B) \leq n - 2\).

![Figure 7: A bicyclic graph \(B \in \mathcal{B}_2\). Here at most \(y\) or \(z\) are of degree 2.](image)

Case 1. When \(\text{diam}(B) = n - 2\). Let \(P\) be a diametrical path in \(B\). By Remark 3.2, \(P\) contains at most \(\lfloor \frac{k_2}{2} \rfloor + 1\) vertices of \(C_{k_3}\). With similar arguments, we have \(k_1 = k_2 = 3\). Since
length of $P$ is $n-2$, there is exactly one vertex, say $x$, of $C_{k_3}$ which does not belong to $V(P)$. Then $x$ is a common vertex in $C_{k_1}$, $C_{k_2}$ and $C_{k_3}$ and $e_B(x) \leq n - 3$. The graph in this case is shown in Figure 7. We see that $B - x \cong P_{n-1}$ and

$$\tau(B) = \tau(P_{n-1}) + e_B(x)$$

$$\leq \tau(P_{n-1}) + (n-1)$$

$$= \tau(B'_2).$$

**Case 2.** When $\text{diam}(B) \leq n - 3$. Then there exist two edges $e_1, e_2 \in E(B)$ such that $T \cong B - \{e_1, e_2\}$ is a tree and

$$e_T(v) \leq n - 3 \quad \forall \ v \in V(T).$$

Following Lemma 3.1, we can show that $\tau(B) \leq \tau(B'_2)$. This completes the proof.  

From Lemma 3.1 and Lemma 3.2, we have the following result.

**Theorem 3.7.** Among all $n$-vertex bicyclic graphs, $n \geq 5$, the graph $B'_2$ shown in Figure 6 has the maximal total-eccentricity index.

**Proof.** Since $\tau(B_2) < \tau(B'_2)$, the assertion follows from Lemmas 3.1 and 3.2.

**Corollary 3.8.** For any bicyclic graph $B$, we have $\tau(B) \leq \frac{3}{4}n^2 - n - 2$.

**Proof.** By using Remark 3.1 and Lemmas 3.1 and 3.2, the proof is obvious.

### 4 Extremal conjugated trees with respect to total-eccentricity index

Consider a conjugated $n$-vertex tree $T$ with perfect a matching $M$, where $n \geq 2$. It can be observed that $|M| = \frac{n}{2}$. We define some families of trees which will be used in the later discussion. A subdivided star $S_{n,2}$, of order $2n - 1$ is obtained by subdividing every edge in $S_n$ once. A double star $DS_{k,n-k}$, where $k \geq 2$ and $n-k \geq 2$, of order $n$ is obtained by joining the centers of the stars $S_k$ and $S_{n-k}$ by an edge. The graphs $S_{n,2}$ and $DS_{k,n-k}$ are shown in Figure 8.

The following results will be required to find extremal conjugated trees with respect to total-eccentricity index. We construct a tree $S_*$ by deleting a pendant vertex from $S_{n,2}$ as shown in Figure 8. We will see that $S_*$ is the unique conjugated tree of order $2(n-1)$ with $\frac{2(n-1)}{2}$ pendant vertices.

**Lemma 4.1.** Let $T$ be an $n$-vertex tree with $n \geq 4$. When $\text{diam}(T) = 3$ then $T \cong DS_{k,n-k}$, where $2 \leq k \leq n - 2$.

**Proof.** When $\text{diam}(T) = 3$, we consider a diametrical path $v_1v_2v_3v_4$. Since $\text{diam}(T) = 3$, the remaining $n - 4$ vertices are adjacent to $v_2$ or $v_3$. Thus $T \cong DS_{k,n-k}$ for $2 \leq k \leq n - 2$.

**Remark 4.1.** The total-eccentricity index of $S_{n,2}$, $S_*$ and $DS_{k,n-k}$ is given by

$$\tau(S_{n,2}) = \frac{7n}{2} - \frac{3}{2}, \quad \tau(S_*) = \frac{7n}{2} - 2 \quad \text{and} \quad \tau(DS_{k,n-k}) = 3n - 2.$$
Remark 4.2. An \(n\)-vertex conjugated tree, \(n \geq 4\), can have at most \(\frac{n}{2}\) pendant vertices. If \(T\) is an \(n\)-vertex conjugated tree with exactly \(\frac{n}{2}\) pendant vertices then \(T \cong S_\ast\), where \(S_\ast\) is shown in Figure 8.

Let \(T\) be an \(n\)-vertex conjugated tree, \(n \geq 4\), with a perfect matching \(M\) and let \(c\) be a vertex in \(V(T)\) with \(e_T(c) = \text{rad}(T)\). Let \(w \in V(T)\) such that \(d_T(c, w) = 1\) and \(vw \in M\). We denote the set of all such paths of length 2 in \(T\) by \(B_r\) and define it as follows.

\[
B_r = \{uv \mid uvw \text{ is a path in } T \text{ with } d_T(c, w) = 1\}.
\]

Now we proceed to find the conjugated trees with minimal total-eccentricity index. We first device an algorithm to construct the tree \(S_\ast\) from a given \(n\)-vertex tree \(T\), \(n \geq 4\).

**Algorithm 3**

\begin{itemize}
  \item **input:** An \(n\)-vertex conjugated tree \(T\), \(n \geq 4\).
  \item **output:** The tree \(S_\ast\).
  \item **Step 0:** Find \(\text{rad}(T)\) by (1.1), a vertex \(c \in V(T)\) with \(e_T(c) = \text{rad}(T)\) and define \(B_r\) by (4.1).
  \item **Step 1:** If \(\text{rad}(T) = 2\), then Stop.
  \item **Step 2:** For an edge \(uv \in B_r\), define \(T := \{T - \{uv\}\} \cup \{cv\}\) and \(B_r := B_r \setminus \{uv\}\).
  \item **Step 3:** If \(B_r \neq \emptyset\) then go to Step 2; else define \(\text{rad}(T)\) by (1.1) and \(B_r\) by (4.1); go to Step 1.
\end{itemize}

Now we discuss the correctness and termination of Algorithm 3.

**Theorem 4.1** (Termination). The Algorithm 3 terminates after a finite number of iterations.

**Proof.** The proof follows from Theorem 2.5. \(\square\)

**Theorem 4.2** (Correctness). If the Algorithm 3 terminates then it outputs \(S_\ast\).

**Proof.** Let \(T\) be an \(n\)-vertex conjugated tree, \(n \geq 4\), with a perfect matching \(M\). Let \(c \in V(T)\) such that \(e_T(c) = \text{rad}(T)\). Define \(B_r\) by (4.1) and let \(uv \in B_r\). Then there exists \(w \in V(T)\) such that \(d_T(w) = 1\) and \(vw \in M\). Since \(T\) is conjugated, we have \(d_T(v) = 2\) and \(uv \notin M\). Therefore \(\{T - \{uv\}\} \cup \{cv\}\) is also a conjugated tree with a perfect matching \(M\). This shows that after the execution of Step 2 in any iteration of Algorithm 3, the modified graph at Step 2 is again an \(n\)-vertex conjugated tree. Thus, when Algorithm 3 terminates at Step 1, it
outputs an $n$-vertex conjugated tree. We finally show that when the algorithm terminates at Step 1, then $T \cong S_*$.

By the modifications of the tree at Step 2, the vertex $c$ remains the central vertex of the modified tree when $[\text{Step 3 } \rightarrow \text{Step 1}]$ is executed. If Algorithm 3 terminates at Step 1 then $\text{rad}(T) = 2$ and $e_T(c) = 2$. This shows that $d_T(c, x) \leq 2$ for each $x \in V(T)$ at Step 1. Since $T$ is also a conjugated tree at Step 1, there is exactly one pendant vertex adjacent to $c$. This shows that $T \cong S_*$. \qed

**Theorem 4.3.** Among all $n$-vertex conjugated trees, $n \geq 4$, the graph $S_*$ shown in Figure 8 has the minimal total-eccentricity index.

**Proof.** Let $T \not\cong S_*$ be an $n$-vertex conjugated tree, $n \geq 4$, and let $c$ be a central vertex of $T$. Define $B_r$ by (4.1). We construct a new set of edges not in $E(T)$ by

$$\tilde{B}_r = \{cv \mid uv \in B_r, v, w \in V(T)\}$$

and define a new conjugated tree $T'$ by

$$T' \cong \{T - B_r\} \cup \tilde{B}_r.$$ 

Then we note that $\text{rad}(T')$ is $r - 1$ or $r - 2$. By the construction of $T'$, we observe that

$$e_{T'}(x) \leq e_T(x) \quad \forall x \in V(T). \quad (4.2)$$

Moreover, since $c$ is a central vertex of $T'$, we have

$$e_{T'}(c) \leq \text{rad}(T) - 1 < e_T(c). \quad (4.3)$$

From (4.2) and (4.3), we obtain

$$\tau(T') < \tau(T).$$

In fact, if $T$ is conjugated tree at Step 1 with $\text{rad}(T) > 2$ in any iteration of Algorithm 3, then $T'$ is a conjugated tree at Step 3 when $B_r = \emptyset$. Thus when $[\text{Step 3 } \rightarrow \text{Step 1}]$ is executed, the total-eccentricity index strictly decreases. Since Algorithm 3 outputs $S_*$, we have $\tau(S_*) < \tau(T)$. \qed

**Corollary 4.4.** Let $T$ be an $n$-vertex conjugated tree, then

$$\tau(T) \leq \frac{7n}{2} - 2, \quad (4.4)$$

where equality holds when $T \cong S_*$. \quad \Box

**Proof.** The result follows by using Remark 4.1 and Theorem 4.3. \quad \Box

Among the class of all $n$-vertex conjugated trees, the maximal conjugated tree with respect to the total-eccentricity index in presented in the next theorem.

**Theorem 4.5.** Among all $n$-vertex conjugated trees, the path $P_n$ has the maximal total-eccentricity index.

**Proof.** The proof is obvious from Theorem 2.3. \quad \Box
5 Conclusion and open problems

In this paper, we studied the maximal and minimal graphs with respect to total-eccentricity index among trees, unicyclic and bicyclic graphs. Moreover, we studied the extremal conjugated trees with respect to total-eccentricity index. It will be interesting to study the extremal conjugated unicyclic and bicyclic graphs with respect to total-eccentricity index.

Acknowledgements

The first and second author are thankful to the Higher Education Commission of Pakistan for supporting this research under the grant 20-3067/NRPU/R&D/HEC/12/831.

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