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On the Extremal Mostar Indices of Trees with a Given Segment Sequence

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Abstract
Given a graph G and an edge $e = xy$ in G, let $n_x(e)$ and $n_y(e)$ be the number of vertices that have the distance to x less than that to y, and the number of vertices that have the distance to y less than that to x, respectively. The contribution of e is defined as $|n_x(e) - n_y(e)|$. The Mostar index of G is the sum of all edge contributions in G. A segment in a given tree T is a path, each of whose inner vertices has degree exactly 2, and none of whose two ends has the degree 2. The segment sequence of T is the length sequence of all segments in T. In this paper, we focus on the tree set with a fixed segment sequence, and the tree set with a fixed size together with a fixed segment number. We completely determine the graphs with the greatest Mostar index among the two sets, respectively. The graphs with the least Mostar index among the second set are also identified.

Keywords Segment sequence · Mostar index

Mathematics Subject Classification 92E10 · 05C30 · 05C90

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1 Introduction

Let G be an undirected simple graph. Let V_G and E_G be its vertex set and edge set, respectively. Then $n(G) = |V_G|$ and $\varepsilon(G) = |E_G|$ are its *order* and *size*, respectively. Let u, v be in V_G and $e = xy$ be in E_G. The distance between u and v is denoted by $d(u, v)$. Let $n_x(e) = \{w \in V_G | d(w, x) < d(w, y)\}$ and $n_y(e) = \{w \in V_G | d(w, y) < d(w, x)\}$. Then $\phi(e) = |n_x(e) - n_y(e)|$ is the *contribution* of e. The sum $Mo(G) = \sum_{e \in E_G} \phi(e)$ is called the *Mostar index* of G.

The Mostar index was proposed by Došlić et al. [12], which was defined to measure how far a graph is from distance-balanced, where a *distance-balanced* graph [6,11,18,20,21] is one of Mostar index zero. In [12], the extremal unicyclic graphs and trees respect to the Mostar index were obtained, respectively. After that, with respect to the extremal value of the index, the bicyclic graphs [24], cacti [14], trees with given parameters [9,15], hexagonal chains [17,25,26], tree-like benzenoid compounds [7,10], chemical trees [8] and so on were studied. The edge version of the index was also studied [1,5,19,23] recently. The most recent article [2] stated more modifications and generalizations of the Mostar index.

Let T be a tree, v be in V_T and $d(v)$ be the degree of v. Then v is a *d-vertex* if $d(v) = d$ and is a *d^+-vertex* if $d(v) \geq d$. Each 1-vertex in T is called a *leaf*; each 3^+-vertex is called a *branch vertex*. A *segment* in T is a path, where the inner vertices are all 2-vertices, and none of the ends is a 2-vertex. A segment is *pendent* if it has a pendent edge and is *non-pendent* otherwise. The length sequence of all segments in T in order from largest to smallest is called its *segment sequence*.

The tree set $\mathcal{T}^L$ with a fixed segment sequence L, and the tree set $\mathcal{T}(\varepsilon, k)$ with a fixed size ε and together with a fixed segment number k, have attracted more and more researchers' attentions, with respect to many extremal problems [3,4,22,27,28]. For a graph set $\mathcal{X}$, let $\mathcal{X}^{\max}$ and $\mathcal{X}^{\min}$ be its subsets with the greatest and the least Mostar indices, respectively. Let $Mo(\mathcal{X}^{\max})$ and $Mo(\mathcal{X}^{\min})$ be the Mostar indices of graphs in the corresponding sets. This paper completely determines $\mathcal{T}^{L\max}$, $\mathcal{T}^{\max}(\varepsilon, k)$ and $\mathcal{T}^{\min}(\varepsilon, k)$, and their Mostar indices.

First, we find $\mathcal{T}^{L\max}$ and their Mostar index. Let $L = (l_1, l_2, \ldots, l_k)$ where $k \geq 3$, each l_i $(i = 1, 2, \ldots, k)$ is a positive integer, and $l_i \geq l_j$ whenever $i < j$. Then, the sum $\varepsilon(L) = \sum_{i=1}^{k} l_i$ is called the *size* of L. The unique tree T_S^L, in $\mathcal{T}^L$, which has exactly one branch vertex is called a *starlike tree*, as shown in Fig. 1a.

Theorem 1.1 *Let T be in $\mathcal{T}^L$, where $L = (l_1, l_2, \ldots, l_k)$, $k \geq 3$ and $l_i \geq l_j$ whenever $i < j$. Let $\varepsilon = \varepsilon(L)$. Then*

$$Mo(T) \leq \begin{cases} \varepsilon(\varepsilon+1) - 2\sum_{i=1}^{k}\sum_{j=1}^{l_i} j, & \text{if } l_1 \leq (\varepsilon+1)/2; \\ \sum_{j=1}^{l_1} |\varepsilon+1-2j| + (\varepsilon+1)(\varepsilon-1) - 2\sum_{i=2}^{k}\sum_{j=1}^{l_i} j, & \text{if } l_1 \geq (\varepsilon+1)/2+1, \end{cases}$$

where the equality holds if and only if $T \cong T_S^L$.

Second, we obtain $\mathcal{T}^{\max}(\varepsilon, k)$ and their Mostar index, based on Theorem 1.1. Let $3 \leq k \leq \varepsilon$. Suppose $\varepsilon = \alpha k + \beta$, where $0 \leq \beta \leq k-1$. Let $L_S(\varepsilon, k) = (\alpha, \ldots, \alpha, \alpha +$

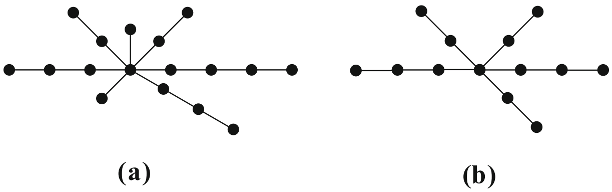

Fig. 1 **a** T_S^L where $L = (4, 3, 3, 2, 2, 1, 1)$; **b** $T_S(12, 5)$

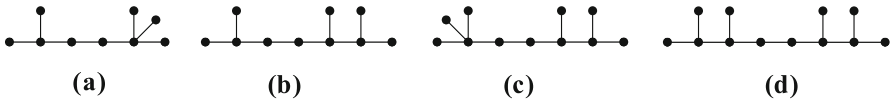

Fig. 2 **a** $T_C(8, 6)$; **b** $T_C(9, 7)$; **c** $T_C(10, 8)$; **d** $T_C(11, 9)$

$1, \ldots, \alpha + 1)$ be a segment sequence of size ε with k integers. Let $T_S(\varepsilon, k) = T_S^{L_S(\varepsilon,k)}$ for short. Figure 1b shows the graph $T_S(12, 5)$.

Theorem 1.2 *Let $T \in \mathcal{T}(\varepsilon, k)$ $(3 \le k \le \varepsilon)$, where $\varepsilon = \alpha k + \beta$, with α, β being nonnegative integers, and $0 \le \beta \le k - 1$. Then*

$$Mo(T) \le (\varepsilon + 1)^2 - (\beta + \varepsilon + 1)(\alpha + 1)$$

where the equality holds if and only if $T \cong T_S(\varepsilon, k)$.

Third, we obtain $\mathcal{T}^{\min}(\varepsilon, k)$ and their Mostar index. A tree is called a *caterpillar* if its 2^+-vertices induce a path. Let $L_C(\varepsilon, k) = (\varepsilon - k + 1, 1, 1, \ldots, 1)$ be a sequence of size ε with k integers. A tree in $\mathcal{T}^{L_C(\varepsilon,k)}$ is called a *balanced caterpillar* (denoted by $T_C(\varepsilon, k)$) if the followings hold: (1) $T_C(\varepsilon, k)$ is a caterpillar; (2) there is exactly one 4^+-vertex when $k = 2t$ for some integer t, and there is no 4^+-vertex otherwise; (3) the numbers ε_1 and ε_2 of edges in the resulted two non-empty components after deleting the longest segment satisfy that $|\varepsilon_1 - \varepsilon_2| \le 2$. Figure 2a–d shows $T_C(8, 6)$, $T_C(9, 7)$, $T_C(10, 8)$ and $T_C(11, 9)$, respectively.

Theorem 1.3 *Let T be a tree in $\mathcal{T}(\varepsilon, k)$, where $3 \le k \le \varepsilon$. Then*

$$Mo(T) \ge \begin{cases} \lfloor \frac{\varepsilon^2}{2} \rfloor + 2, & \text{if} \quad k = 3; \\ 12, & \text{if} \quad k = 4 \text{ and } \varepsilon = 4; \\ \lfloor \frac{\varepsilon^2}{2} \rfloor + 6, & \text{if} \quad k = 4 \text{ and } \varepsilon \ge 5; \\ \lceil \frac{(\varepsilon+1)^2}{2} \rceil - (\varepsilon + 1) + \frac{(k-1)^2}{4}, & \text{if} \quad k = 4t + 1 \ (t \ge 1); \\ \lceil \frac{(\varepsilon+1)^2}{2} \rceil - \varepsilon + \frac{(k-1)^2}{4}, & \text{if} \quad k = 4t + 3 \ (t \ge 1); \\ \lceil \frac{(\varepsilon+1)^2}{2} \rceil - \varepsilon + \frac{(k-1)^2+5}{4}, & \text{if} \quad k = 2t \ (t \ge 3) \end{cases}$$

where the equality holds if and only if $T \cong T_C(\varepsilon, k)$.

In Sect. 2, we introduce the moving operations and their properties. By using these properties, Theorems 1.1, 1.2 are proved in Sect. 3, and Theorem 1.3 is shown in Sect. 4. The last section gives some conclusion remarks.

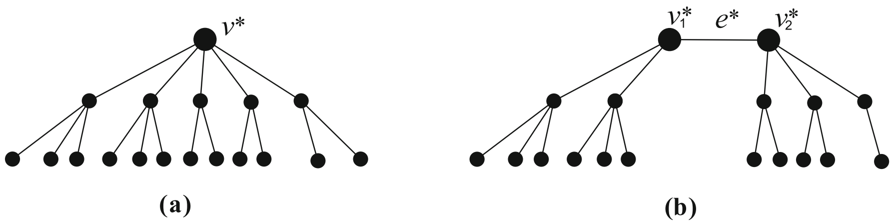

Fig. 3 **a** A tree central at v^*; **b** a tree edge central at e^*

2 Preliminaries and Moving Operations

Let T be a tree of size ε and order $n = \varepsilon + 1$. T is *central* at v^* if there is a vertex v^*, such that $(T - v^*)$ consists of components of order less than $n/2$. Then v^* is called the *center*. T is *edge central* at e^*, if there is an edge $e^* = v_1^* v_2^*$, such that $(T - e^*)$ consists of two components of order exactly $n/2$. Then e^* is called the *edge center*. Figure 3 shows examples of the (edge) central tree. One has that every tree is either central or edge central, as stated early in [13].

Let $u, w \in V_T$, $e = uu_1$, $f = ww_1 \in E_T$, and $F \subseteq E_T$. $N(v)$ and $E(v)$ are the neighbor set and incident edge set of v, respectively. Let $P_{u,w}$ be the path with ends u, w. Suppose $d(w, u) < d(w, u_1)$ and $d(u, w) < d(u, w_1)$; then, we define $P_{x,y} = P_{w,u}$ to be the path between x and y for $(x, y) = (e, f), (w, e), (u, f)$, and let $d(x, y) = |E_{P_{x,y}}|$. For short, let $P(x)$ be the path from x to the (edge) center if x is a vertex or an edge, and let $d(x) = |E_{P(x)}|$.

Each element in $V_{P(v)}$ and $E_{P(v)}$ is called an *ancestor* and an *ancestor edge* of v, respectively. If v is in $P(u)$, then each element in $V_{P_{v,u}}$ and $E_{P_{v,u}}$ is called a *successor* and a *successor edge* of v, respectively. Let $S(v)$ and $ES(v)$ be the successor set and successor edge set of v, respectively. Let $S(e) = S(u_1)$ where we assume $d(u) < d(u_1)$. Let $S(F) = \cup_{e' \in F} S(e')$. Let $\sigma(v) = |S(z)|$ for $z = v$, e and F, respectively.

Suppose T is central at v^*. Let $v_i \in N(v^*)$. The graph T_{v_i} induced by $S(v_i)$ is called a v_i-*successor subtree*, and the graph $T_{v_i v^*}$ induced by $(S(v_i) \cup \{v^*\})$ is called a v_i-*extended successor subtree*.

Suppose T is edge central at $e^* = v_1^* v_2^*$. For $i = 1, 2$, the v_i^*-*extended successor subtree* $T_{v_i^*}$ is the one induced by $S(v_i^*)$.

Definition 1 Suppose $F = \{e_i | e_i = uu_i, i = 1, 2, \ldots, t\} \subseteq (E(u) \cap ES(u))$ and $v \in (V_T \setminus S(F))$. The *moving operation on* (F, v) is the following transformation: first delete F, and second add the edges $\{vu_i | i = 1, 2, \ldots, t\}$. Let $T(F^-, v^+)$ be the newly obtained graph.

Definition 2 Suppose $e_1 = w_1 w_2, e_2 = w_3 w_4$ are two edges other than the edge center, such that $d(w_i) < d(w_{i+1})$ for $i = 1, 3$. The *moving operation on* (e_1, e_2) is the following transformation: first delete e_1, e_2, and second add the edges $w_3 w_2$ and $w_1 w_4$ (let $e_1 = w_2 w_1$ and $e_2 = w_1 w_4$, too). Let $T(e_1, e_2)$ be the newly obtained graph.

Figure 4 shows examples for the graph transformations in Definitions 1 and 2.

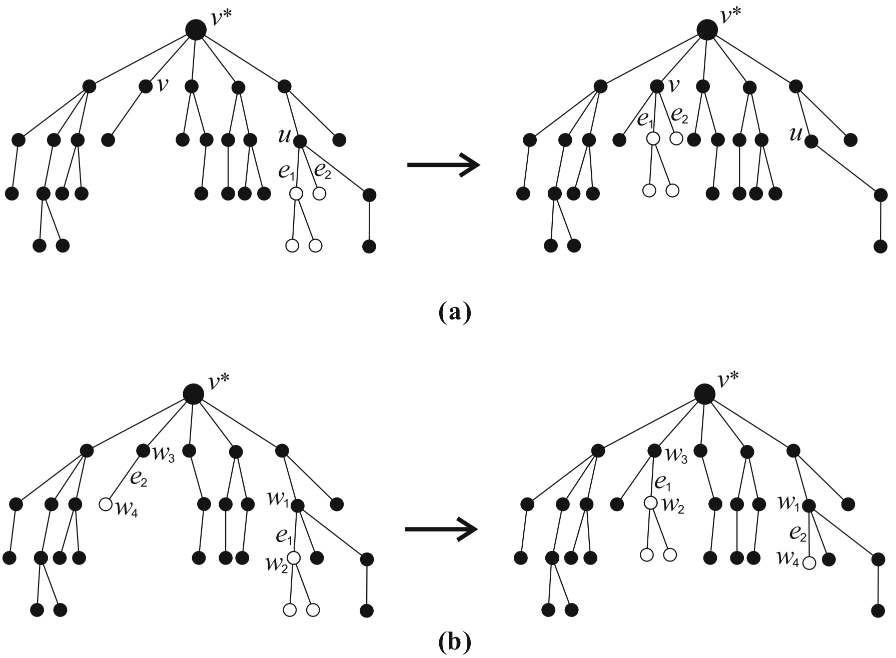

Fig. 4 **a** Moving operation on (F, v); **b** moving operation on (e_1, e_2)

Lemma 2.1 ([9]) *Let T be a tree with a being the center v^* or edge center $e^* = v_1^* v_2^*$. Choose $u, v \in V_T$, $F \subseteq [E(u) \cap ES(u)]$ such that $v \notin S(F)$. Let $T_1 = T(F^-, v^+)$.*

(1) *If u, v are in the same extended branch and u is not the center when T is central, then $Mo(T_1) = Mo(T) + 2\sigma(F)(d(u, a) - d(v, a))$.*
(2) *Suppose T is v^*-central and u, v are in distinct branches T_{v_1} and T_{v_2}, respectively.*

- *If $\sigma(v_2) \leq \lceil n/2 \rceil - \sigma(F) - 1$, then $Mo(T_1) = Mo(T) + 2\sigma(F)(d(u, v^*) - d(v, v^*))$.*
- *If n is even and $\sigma(v_2) = n/2 - \sigma(F)$ and $d(u, v^*) = d(v, v^*)$, then T_1 is $v^* v_2$-edge central and $Mo(T_1) = Mo(T)$.*
- *If n is odd and $\sigma(v_2) = (n + 1)/2 - \sigma(F)$, then $Mo(T_1) = Mo(T) + 2\sigma(F)(d(u, v^*) - d(v, v^*) + 1)$.*
- *If $\sigma(v_2) \geq \lceil n/2 \rceil - \sigma(F)$ and $d(u, v^*) > d(v, v^*)$, then $Mo(T_1) > Mo(T)$.*

(3) *Suppose T is $v_1^* v_2^*$-edge central, $u \in V_{T_{v_1^*}}$, $v \in V_{T_{v_2^*}}$*

- *If $d(u, v_1^*) \geq d(v, v_2^*)$, then $Mo(T_1) > Mo(T)$.*
- *If $d(u, v_1^*) = d(v, v_2^*) - 1$ and T_1 is v_2^*-central, then $Mo(T_1) = Mo(T)$.*

Lemma 2.2 (1) *Suppose T is a tree of order n which is central at v^*. Let v_1 and v_2 be two vertices adjacent to v^*. Suppose u and v are in $T_{v^* v_1}$ and T_{v_2}, respectively. Let F be a subset of $[(E(u) \cap ES(u)) \setminus \{v^* v_2\}]$.*

- *If $|T_{v_2}| > \lceil n/2 \rceil - \sigma(F)$ and $d(u) \geq d(v)$, then $Mo(T(F^-, v^+)) > Mo(T)$.*

- *If* $|T_{v_2}| = n/2 - \sigma(F)$ *and* $d(u) \le d(v) - 1$, *then* $T(F^-, v^+)$ *is edge central at* v^*v_2 *and* $Mo(T(F^-, v^+)) < Mo(T)$.

(2) *Suppose* T *is central at* v^*, *which admits at least three neighbors* v_1, v_2, v_3. *Let* $e_i = v^*$ *for* $i = 1, 2, 3$. *Let* $e_4 = w_1w_2$ *be an edge in* T_{v_1} *with* $d(w_1) < d(w_2)$.

- *Suppose* $|T_{v_2}| \ge |T_{v_1}|$ *and* $F \subseteq (E(v^*) \setminus \{e_1, e_2\})$. *Then* $Mo(T(F^-, w_1^+)) < Mo(T)$.
- *Suppose* $|T_{v_1}| \le |T_{v_2}|$ *and* $|T_{v_1}| \le |T_{v_3}|$. *Then* $Mo(T(e_2, e_4)) < Mo(T)$ *and* $Mo(T(e_3, e_4)) < Mo(T)$.

(3) *Suppose* u *and* v *belong to two different extended successor subtrees of* T, *or* u *is the center. Let* F *be a subset of* $[E(u) \cap ES(u)]$ *such that* F *contains no edge of the extended successor subtree that contains* v.

- *If* $d(v) \ge d(u) + \sigma(F)$, *then* $Mo(T(F^-, v^+)) \le Mo(T)$.
- *If* $d(v) \ge d(u) + \sigma(F) + 1$, *then* $Mo(T(F^-, v^+)) < Mo(T)$.

Proof Let $\phi(e)$ be the contribution of e in T.

(1) Let $\phi_1(e)$ be the contribution of e in $T(F^-, v^+)$. Then $\phi_1(e) = \phi(e)$ for each $e \in (E_T \setminus E_{P_{u,v}})$. If $|T_{v_2}| > \lceil n/2 \rceil - \sigma(F)$ and $d(u) \ge d(v)$, then the (edge) center of $T(F^-, v^+)$ is in $P_{v_2,v}$. One has $\phi_1(e) = \phi(e) + 2\sigma(F)$ for $e \in E_{P_{v^*,u}}$; $\phi_1(e) = |\phi(e) - 2\sigma(F)| \ge \phi(e) - 2\sigma(F)$ for $e \in E_{P_{v_2,v}}$. What is more, $\phi_1(v^*v_2) = |\phi(v^*v_2) - 2\sigma(F)| = |n - 2\sigma(v_2) - 2\sigma(F)| > n - 2\sigma(v_2) - 2\sigma(F) = \phi(v^*v_2) - 2\sigma(F)$ since $|T_{v_2}| > \lceil n/2 \rceil - \sigma(F)$. Thus, $Mo(T(F^-, v^+)) > Mo(T)$ since $d(u) \ge d(v) > d(v_2, v)$. If $|T_{v_2}| = n/2 - \sigma(F)$ and $d(u) \le d(v) - 1$, then $T(F^-, v^+)$ is edge central at v^*v_2. So $0 = \phi_1(v^*v_2) < \phi(v^*v_2)$ and $\phi_1(e) = \phi(e) + 2\sigma(F)$ for $e \in E_{P_{v^*,u}}$. Note that $\phi_1(e) = \phi(e) - 2\sigma(F)$ for $e \in E_{P_{v_2,v}}$. Thus, $Mo(T(F^-, v^+)) < Mo(T)$ since $d(u) \le d(v) - 1 = d(v_2, v)$.

(2) One has that the (edge) center of $T(F^-, w_1^+)$, $T(e_2, e_4)$ and $T(e_3, e_4)$ is in P_{w_1,v^*}. Let $\phi_1(e)$ be the contribution of e in $T(F^-, w_1^+)$. Let $\phi_2(e)$ be the contribution of e in $T(e_2, e_4)$. Then $\phi_i(e) = \phi(e)$ $(i = 1, 2)$ for $e \in (E_T \setminus E_{P_{w_1,v^*}})$. For the first item, if $|T_{v_1}| \le |T_{v_2}|$, then $\sigma_T(e_2) \ge \sigma_T(e_1) > \sigma_T(e_4) > 0$. Then for each $e \in E_{P_{w_1,v^*}}$, one has $\phi_1(e) = \phi(e) - 2\sigma_T(F)$ or $\phi_1(e) \le n - 2\sigma_T(e_2) - 2 \le n - 2\sigma_T(e_1) - 2 \le \phi(e) - 2$. So $Mo(T(F^-, w_1^+)) < Mo(T)$. Thus, the first item holds. For the second item, it is sufficient to show the conclusion for $T(e_2, e_4)$. For each $e \in E_{P_{w_1,v^*}}$, one has $\sigma_{T(e_2,e_4)}(e) = \sigma_T(e) + (\sigma_T(e_2) - \sigma_T(e_4)) > \sigma_T(e)$ or $\sigma_{T(e_2,e_4)}(e) \ge \sigma_T(e_3) + \sigma_T(e_4) > \sigma_T(e)$. That is $\phi_2(e) = n - 2\sigma_{T(e_2,e_4)}(e) < n - 2\sigma_T(e) = \phi(e)$. So $Mo(T(e_2, e_4)) < Mo(T)$. Thus, the second item also holds.

(3) Let $T_1 = T(F^-, v^+)$ and $\phi_1(e)$ be the contribution of e in T_1.

Case 1 If $d(v) \ge d(u) + \sigma(F)$.

Let P be the path between v and the (edge) center of T. Note that the (edge) center a_1 of T_1 is in P. One has $\phi_1(e) = \phi(e)$ for $e \in (E_T \setminus E_{P_{u,v}})$; $\phi_1(e) = \phi(e) + 2\sigma(F)$ for e in $P_{u,a}$. Similarly, $\phi_1(e) = \phi(e) - 2\sigma(F)$ for e in $P_{a_1,v}$.

Suppose T is central at v^*, $u \in V_{T_{v^*v_1}}$ and $v \in V_{T_{v_2}}$ where $v_1, v_2 \in N(v^*)$. If T_1 is central at w^*, let w^*w_1 be the edge in P_{v^*,w^*}. Let $\sigma_t = |S_T(v_2) \setminus (S_T(w^*) \cup V_{P_{v_2,w_1}})|$.

Then $\sigma_t + |P_{v_2,w_1}| < \sigma(F)$, since $\sigma_{T_1}(w_1) \leq (n-1)/2$ (because T_1 is central at w^*) and $(|T| - \sigma_T(v_2)) \geq (n+1)/2$ (because T is central at v^*). Note that

$$\begin{aligned}\phi_1(w^*w_1) &= n - 2\sigma_{T_1}(w_1)\\ &= n - 2[n - \sigma_T(v_2) - \sigma_T(F) + (\sigma_t + |P_{v_2,w_1}|)]\\ &= 2[\sigma_T(v_2) + \sigma_T(F) - (\sigma_t + |P_{v_2,w_1}|)] - n\\ &= 2[\sigma_T(F) - (\sigma_t + |P_{v_2,w_1}|)] - (n - 2\sigma_T(v_2))\\ &= 2[\sigma_T(F) - (\sigma_t + |P_{v_2,w_1}|)] - \phi(v^*v_2).\end{aligned}$$

Then, for $e \in E_{P_{v^*,w^*}}$, one has

$$\begin{aligned}\phi_1(e) &\leq \phi(w^*w_1) + 2(\sigma_t + d(e, w^*))\\ &= 2[\sigma_T(F) - (\sigma_t + |P_{v_2,w_1}|)] - \phi(v^*v_2) + 2(\sigma_t + d(e, w^*))\\ &= 2(\sigma_T(F) - |P_{v_2,w_1}|) - \phi(v^*v_2) + 2d(e, w^*),\end{aligned}$$

whereas for $\bar{e} \in E_{P_{v^*,w^*}}$, one has

$$\phi(\bar{e}) \geq \phi(v^*v_2) + 2d(\bar{e}, v^*).$$

So for $e, \bar{e} \in E_{P_{v^*,w^*}}$ satisfying $d(v^*, e) = d(w^*, \bar{e})$, one has

$$\begin{aligned}\phi_1(e) - \phi(\bar{e}) &\leq 2(\sigma_T(F) - |P_{v_2,w_1}|) - 2\phi(v^*v_2)\\ &\leq 2(\sigma_T(F) - |P_{v_2,w_1}| - 1)\\ &= 2(\sigma_T(F) - d(v^*, w^*)).\end{aligned}$$

This gives

$$\begin{aligned}Mo(T_1) &\leq Mo(T) + 2d(u, v^*)\sigma(F)\\ &\quad +2d(v^*, w^*)(\sigma(F) - d(v^*, w^*)) - 2d(w^*, v)\sigma(F)\\ &= Mo(T) + 2d(u, v^*)\sigma(F) + 2d(v^*, w^*)(\sigma(F) - d(v^*, w^*))\\ &\quad -2(d(v^*, v) - d(v^*, w^*))\sigma(F)\\ &\leq Mo(T) + 2d(u, v^*)\sigma(F) + 2d(v^*, w^*)(\sigma(F) - d(v^*, w^*))\\ &\quad -2(d(v^*, u) + 2\sigma(F) - d(v^*, w^*))\sigma(F)\\ &= Mo(T) - 2(\sigma(F))^2 + 2d(v^*, w^*)(2\sigma(F) - d(v^*, w^*))\\ &= Mo(T) - 2(\sigma(F) - d(v^*, w^*))^2.\end{aligned}$$

So $Mo(T_1) \leq Mo(T)$.

If T_1 is edge central at $w_1^*w_2^*$ where $d(w_1^*, v^*) < d(w_2^*, v^*)$, let $\sigma_t = |S_T(v_2) \setminus (S_T(w_2^*) \cup V_{P_{v_2,w_1^*}})|$. Then $\sigma_t + |P_{v_2,w_1^*}| < \sigma(F)$, since $\sigma_{T_1}(w_1^*) = n/2$ (because T_1 is edge central at $w_1^*w_2^*$) and $(|T| - \sigma(v_2)) \geq (n+2)/2$. That is $d(v^*, w_2^*) \leq \sigma(F) - \sigma_t$. Note that $\phi_1(e) \leq \phi(\bar{e}) + 2\sigma_t$ for $e, \bar{e} \in E_{P_{v^*,w_2^*}}$ satisfying $d(v^*, e) = d(w^*, \bar{e})$. So

$$\begin{aligned}Mo(T_1) &\leq Mo(T_1) + 2d(u, v^*)\sigma(F) + 2d(v^*, w_2^*)\sigma_t - 2d(w_2^*, v)\sigma(F)\\ &\leq Mo(T_1) + 2d(u, v^*)\sigma(F) + 2(\sigma(F) - \sigma_t)\sigma_t\\ &\quad -2(d(v^*, v) - d(v^*, w_2^*))\sigma(F)\end{aligned}$$

$$\begin{aligned}&\leq Mo(T_1) + 2d(u, v^*)\sigma(F) + 2(\sigma(F) - \sigma_t)\sigma_t\\&\quad -2(d(u, v^*) + \sigma(F) - (\sigma(F) - \sigma_t))\sigma(F)\\&= Mo(T_1) - 2\sigma_t^2.\end{aligned}$$

So one also has $Mo(T_1) \leq Mo(T)$.

Suppose T is edge central at $v_1^* v_2^*$, and u, v are in $T_{v_1^*}$ and $T_{v_2^*}$, respectively. If T_1 is central at w^*, let $w^* w_1$ be the edge in P_{v^*, w^*}. Put $\sigma_t := |S_T(v_2^*) \setminus (S_T(w^*) \cup V_{P_{v_2^*, w_1}})|$. Then $\sigma_t + |P_{v_2^*, w_1}| < \sigma(F)$, since $(|T| - \sigma_T(v_2)) \geq n/2$ (because T is edge central at $v_1^* v_2^*$) and $\sigma_{T_1}(w_1) \leq (n-2)/2$ (because T_1 is central at w^*). Note that

$$\begin{aligned}\phi_1(w^* w_1) &= n - 2\sigma_{T_1}(w_1)\\&= n - 2[\tfrac{n}{2} - \sigma_T(F) + (\sigma_t + |P_{v_2^*, w_1}|)]\\&= 2[\sigma_T(F) - (\sigma_t + |P_{v_2^*, w_1}|)]\\&= 2[\sigma_T(F) - (\sigma_t + d(v_1^*, w^*) - 1)].\end{aligned}$$

If $e \in E_{P_{v_1^*, w^*}}$, then

$$\begin{aligned}\phi_1(e) &\leq \phi(w^* w_1) + 2(\sigma_t + d(e, w^*))\\&= 2[\sigma_T(F) - (\sigma_t + d(v_1^*, w^*) - 1)] + 2(\sigma_t + d(e, w^*))\\&= 2[\sigma_T(F) - (d(v_1^*, w^*) - 1)] + 2d(e, w^*).\end{aligned}$$

If $\bar{e} \in E_{P_{v_1^*, w^*}}$, then

$$\phi(\bar{e}) \geq 2d(\bar{e}, v_1^*).$$

If $e, \bar{e} \in E_{P_{v_1^*, w^*}}$ satisfy $d(v^*, e) = d(w^*, \bar{e})$, then

$$\phi_1(e) - \phi(\bar{e}) \leq 2[\sigma_T(F) - (d(v_1^*, w^*) - 1)].$$

This gives us

$$\begin{aligned}Mo(T_1) &\leq Mo(T) + 2d(u, v_1^*)\sigma(F) + 2d(v_1^*, w^*)[\sigma_T(F) - (d(v_1^*, w^*) - 1)]\\&\quad -2d(w^*, v)\sigma(F) = Mo(T) + 2d(u, v_1^*)\sigma(F) + 2d(v_1^*, w^*)(\sigma_T(F)\\&\quad -d(v_1^*, w^*))\\&\quad +2d(v_1^*, w^*) - 2(d(v_2^*, v) - d(v_2^*, w^*))\sigma(F)\\&\leq Mo(T) + 2d(u, v_1^*)\sigma(F) + 2d(v_1^*, w^*)(\sigma_T(F)\\&\quad -d(v_1^*, w^*)) + 2d(v_1^*, w^*)\\&\quad -2(d(v_1^*, u) + \sigma(F) - d(v_1^*, w^*) + 1)\sigma(F)\\&= Mo(T) - 2(\sigma(F))^2 + 2d(v_1^*, w^*)(2\sigma(F) - d(v_1^*, w^*))\\&\quad +2d(v_1^*, w^*) - 2\sigma(F)\\&= Mo(T) - 2(\sigma(F) - d(v_1^*, w^*))(\sigma(F) - d(v_1^*, w^*) + 1).\end{aligned}$$

That is $Mo(T_1) \leq Mo(T)$.

If T_1 is edge central at $w_1^* w_2^*$ where $d(v_1^*, w_1^*) < d(v_1^*, w_2^*)$, let $\sigma_t = |S_T(v_2^*) \setminus (S_T(w_2^*) \cup V_{P_{v_2^*, w_1^*}})|$. Then $\sigma_t + |P_{v_2^*, w_1^*}| = \sigma(F)$, since $\sigma_{T_1}(w_1^*) = n/2 = \sigma_T(v_1^*)$. That is $d(v_2^*, w_1^*) = \sigma(F) - \sigma_t - 1$. If $e, \bar{e} \in E_{P_{v_2^*, w_1^*}}$ satisfy $d(v_2^*, e) = d(w_1^*, \bar{e})$, then $\phi_1(e) \leq \phi(\bar{e}) + 2\sigma_t$. So

$$\begin{aligned}
Mo(T_1) &\leq Mo(T_1) + 2d(u, v_1^*)\sigma(F) + 2d(v_2^*, w_1^*)\sigma_t - 2d(w_2^*, v)\sigma(F) \\
&= Mo(T_1) + 2d(u, v_1^*)\sigma(F) + 2(\sigma(F) - \sigma_t - 1)\sigma_t \\
&\quad -2(d(v_2^*, v) - d(v_2^*, w_2^*))\sigma(F) \\
&\leq Mo(T_1) + 2d(u, v^*)\sigma(F) + 2(\sigma(F) - \sigma_t - 1)\sigma_t \\
&\quad -2[d(u, v_1^*) + \sigma(F) - (\sigma(F) - \sigma_t)]\sigma(F) \\
&= Mo(T_1) - 2(\sigma_t + 1)\sigma_t
\end{aligned}$$

That is $Mo(T_1) \leq Mo(T)$.

This completes the proof of Case 1.

Case 2 $d(v) \geq d(u) + \sigma(F) + 1$. By the proof in Case 1, one always has $Mo(T_1) \leq Mo(T) - 2\sigma(F)$. That is $Mo(T_1) < Mo(T)$.

This completes our proof. □

3 Greatest Mostar Index in $\mathcal{T}^L$ and $\mathcal{T}(\varepsilon, k)$

In this section, we prove Theorems 1.1 and 1.2, which determine $\mathcal{T}^{L\max}$, $\mathcal{T}^{\max}(\varepsilon, k)$ and their Mostar indices.

Proof of Theorem 1.1 Let $T \in \mathcal{T}^{L\max}$ where L has size ε and let $n = \varepsilon + 1$. Suppose T is not a starlike tree. Then each branch vertex is in some non-pendent segment.

Case 1 T is central at v^*.

If v^* is a branch vertex (this happens only when $l_1 < n/2$), let P_{v^*, w_1} be the non-pendent segment with ends v^* and w_1. Let $F = (E(w_1) \setminus E_{P_{v^*, w_1}})$. Then $T(F^-, (v^*)^+)$ is also in $\mathcal{T}^L$. Then $Mo(T(F^-, (v^*)^+)) > Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\max}$.

If v^* is a 2-vertex in some non-pendent segment P_{w_1, w_2}. Then n is odd since T is central, and the branch containing w_i has $(n-1)/2$ vertices for $i = 1, 2$. Without loss of generality, suppose $d(v^*, w_1) \leq d(v^*, w_2)$. If both w_1 and w_2 are branch vertices, let $F = (E(w_2) \setminus E_{P_{v^*, w_2}})$ and $P_{w_1, w}$ be a segment incident to w_1 where $w \neq w_2$. Then $T(F^-, w^+)$ is in $\mathcal{T}^L$ and $Mo(T(F^-, w^+)) > Mo(T)$ by Lemma 2.1 (ii), contradicted to $T \in \mathcal{T}^{L\max}$. So P_{w_1, w_2} is pendent (which implies $l_1 > n/2$ and P is the unique segment of length l_1). Suppose w_1 is a branch vertex without loss of generality. By assumption, there exists a non-pendent segment P_{w_1, w_3}. Let $F = (E(w_3) \setminus E_{P_{w_1, w_3}})$. Then $T(F^-, w_1^+) \in \mathcal{T}^L$ and $Mo(T(F^-, w_1^+)) > Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\max}$. Thus, T is a starlike tree in this case.

Case 2 T is central at e^* (then n is even) where e^* is in some segment P_{w_1, w_2}.

If both w_1 and w_2 are branch vertices, then $l_1 < n/2$. Suppose $d(w_1, e^*) \leq d(w_2, e^*)$ without loss of generality. Let $F = (E(w_2) \setminus E_{P_{v^*, w_2}})$. Then $T(F^-, w_1^+) \in \mathcal{T}^L$ and $Mo(T(F^-, w_1^+)) > Mo(T)$ by Lemma 2.1 (iii), contradicted to $T \in \mathcal{T}^{L\max}$.

So P is a pendent segment (which implies $l_1 \geq n/2$ and P_{w_1,w_2} is the unique segment of length l_1). Suppose w_1 is a branch vertex without loss of generality. By assumption, there exists an non-pendent segment P_{w_1,w_3}. Let $F = (E(w_3) \setminus E_{P_{w_1,w_3}})$. Then $T(F^-, w_1^+) \in \mathcal{T}^L$ and $Mo(T(F^-, w_1^+)) > Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\max}$. Thus, T is also a starlike tree of L in this case.

So one always has that T is a starlike tree of L.

On the other hand, one has $Mo(T) = \sum_{i=1}^{k}\sum_{j=1}^{l_i}|n-2j|$. So if $l_1 \leq n/2$, then

$$Mo(T) = n(n-1) - 2\sum_{i=1}^{k}\sum_{j=1}^{l_i} j.$$

If $l_1 \geq n/2+1$, then

$$Mo(T) = \sum_{j=1}^{l_1}|n-2j| + n(n-2) - 2\sum_{i=2}^{k}\sum_{j=1}^{l_i} j.$$

Since $n = \varepsilon + 1$, one has

$$Mo(T) = \begin{cases} \varepsilon(\varepsilon+1) - 2\sum_{i=1}^{k}\sum_{j=1}^{l_i} j, & \text{if } l_1 \leq (\varepsilon+1)/2; \\ \sum_{j=1}^{l_1}|\varepsilon+1-2j| + (\varepsilon+1)(\varepsilon-1) - 2\sum_{i=2}^{k}\sum_{j=1}^{l_i} j, & \text{if } l_1 \geq (\varepsilon+1)/2+1. \end{cases}$$

This completes our proof. □

Proof of Theorem 1.2 Suppose $T \in \mathcal{T}^{\max}(\varepsilon, k)$ $(3 \leq k \leq \varepsilon)$ and $n = \varepsilon + 1$, where $\varepsilon = \alpha k + \beta$, with α, β being nonnegative integers, and $0 \leq \beta \leq k-1$. Let $L = (l_1, l_2, \ldots, l_k)$ be the segment sequence of T, where $l_i \geq l_j$ whenever $i < j$. By Theorem 1.1, one has $T \cong T_S^L$.

Let v be the unique branch vertex and let P_{v,w_1}, P_{v,w_k}, respectively, be the segments of lengths l_1 and l_k in T_S^L. Assume $e_1 \in E(w_1)$ and let $T_1 = T(e_1^-, w_k^+)$ which is also in $\mathcal{T}(\varepsilon, k)$. If T is edge central at some edge e^* in P_{v,w_1}, then $d(e^*, e_1) = (n-4)/2 \geq d(w_k, e^*)$ since $k \geq 3$. Then $Mo(T_1) > Mo(T)$ by Lemma 2.1 (iii), contradicted to $T \in \mathcal{T}^{\max}(\varepsilon, k)$.

If T is central at some vertex v^* in $(V_{P_{v,w_1}} \setminus \{v\})$, then $d(v^*, e_1) = (n-5)/2 \geq d(v^*, w_k)$ since $k \geq 3$ and each branch has exactly $(n-1)/2$ vertices. Then $Mo(T_1) > Mo(T)$ by Lemma 2.1 (ii), contracted to $T \in \mathcal{T}^{\max}(\varepsilon, k)$. So T is central at v.

If $l_k \leq l_1 - 2$, then $Mo(T_1) > Mo(T)$ by Lemma 2.1 (ii), contradicted to $T \in \mathcal{T}^{\max}(\varepsilon, k)$. Thus, $T \cong T_S(\varepsilon, k)$.

On the other hand, by a direct calculation one has

$$\begin{aligned} Mo(T_S(\varepsilon, k)) &= (k-\beta)\sum_{i=1}^{\alpha}(n-2i) + \beta\sum_{i=1}^{\alpha+1}(n-2i) \\ &= n^2 - (n+\beta)(\alpha+1) \end{aligned}$$

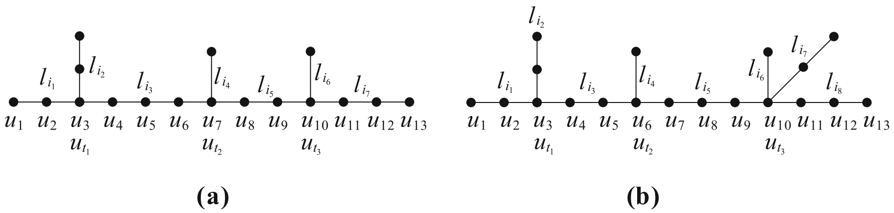

Fig. 5 **a** The balanced caterpillar-like tree $T^L_{(2,2,4,1,3,1,3)}$ where $L = (4, 3, 3, 2, 2, 1, 1)$; **b** the balanced caterpillar-like tree $T^L_{(2,2,3,1,4,1,2,3)}$ where $L = (4, 3, 3, 2, 2, 2, 1, 1)$

$$= (\varepsilon + 1)^2 - (\varepsilon + \beta + 1)(\alpha + 1).$$

This completes our proof. □

4 Trees with Least Mostar Indices in $\mathcal{T}(\varepsilon, k)$

In this section, $\mathcal{T}^{\min}(\varepsilon, k)$ and their Mostar index are completely determined. First, some properties of trees in $\mathcal{T}^{L\min}$ are given.

Let $L = (l_1, l_2, \ldots, l_k)$ $(k \geq 5)$ be a segment sequence. A tree is *balanced caterpillar-like* if replacing each segment with an edge will result a balanced caterpillar. Figure 5 shows examples for balanced caterpillar-like trees.

For convenience, a path or a starlike tree with 3 or 4 segments is also called a balanced caterpillar-like tree. Let $\mathcal{T}^L_C \subseteq \mathcal{T}^L$ be the caterpillar-like tree set. Let $T^L_{(l_{i_1}, l_{i_2}, \ldots, l_{i_k})} \in \mathcal{T}^L_C$ with spine path $P = u_1u_2 \ldots u_s$ where u_{t_j} $(j \in [1, \lfloor k/2 \rfloor - 1]$ and $1 = t_1 < t_2 < \cdots < t_{\lfloor k/2 \rfloor} = s)$ is a 3-vertex, u_s is a 3-vertex if k is odd or a 4-vertex if k is even, such that the two pendent segments attached at u_{t_1} have the lengths l_{i_1} and l_{i_2}, respectively, the segment connecting $u_{t_{j-1}}$ $(j \in [2, \lfloor k/2 \rfloor])$ and u_{t_j} has the length $l_{i_{2j-1}}$, the pendent segment attached at u_{t_j} $(j \in [2, \lfloor k/2 \rfloor - 1])$ has the length $l_{i_{2j}}$, and the pendent segments attached at u_s have the length $l_{i_{k-r}}$ $(r = 0, 1$ if k is odd or $r = 0, 1, 2$ if k is even). See Fig. 5a, b.

Lemma 4.1 *Let $T \in \mathcal{T}^{L\min}$ with $L = (l_1, l_2, \ldots, l_k)$, $k \geq 3$ and $l_i \geq l_j$ whenever $i < j$.*

(1) • *If T is central at v^*, let $T_{v_1v^*}$ be an arbitrary extended successor subtree. Then, $T_{v_1v^*}$ is isomorphic to a balanced caterpillar-like tree with v^* being a leaf. What is more, if there are at least five segments in $T_{v_1v^*}$, then v^* is in some pendent segment incident to some spine end of $T_{v_1v^*}$ of degree 3;*
• *If T is edge central at $v_1^*v_2^*$, let $T_1' = T[V_{T_{v_1^*}} \cup \{v_2^*\}]$ and $T_2' = T[V_{T_{v_2^*}} \cup \{v_1^*\}]$. Then T_i' $(i = 1, 2)$ is isomorphic to a balanced caterpillar-like tree with $v_1^*v_2^*$ being a pendent edge. What is more, if there are at least five segments in T_i', then $v_1^*v_2^*$ is in some pendent segment incident to some spine end of T_i' of degree 3.*

(2) *Let $P_{w_{1,1},w_{1,2}}$ and $P_{w_{2,1},w_{2,2}}$ be two segments of T in a common extended successor subtree where $d(w_{i,1}) < d(w_{i,2})$ and $l_{x_i} = |E_{P_{w_{i,1},w_{i,2}}}|$ $(i = 1, 2)$.*

- *If $w_{1,2} = w_{2,1}$, then $l_{x_1} \geq l_{x_2}$.*
- *If $P_{w_{1,1},w_{1,2}}$ and $P_{w_{2,1},w_{2,2}}$ are both pendent segments with $d(w_{1,1}) < d(w_{2,1})$, then $l_{x_1} \leq l_{x_2}$.*
- *If T is edge central, or is central at a 2-vertex, then the segment containing the (edge) center has the length l_1.*
- *If $k \geq 5$ and T is central at a branch vertex v^*, then $d(v^*) \leq 4$ with equality only if $k = 6$ and all segments in T have the same length. What is more, if $d(v^*) = 3$, then v^* admits exactly one pendent segment length of l_k and two non-pendent segments.*

(3) *At most one extended successor subtree of T has a vertex of degree 4.*

Proof (1) When T is edge central, it is sufficient to show the conclusion holds for T_1'. Let $\hat{T} = T_{v_1 v^*}$ or T_1', and let $a = v^*$ or $v_1^* v_2^*$. The conclusion holds easily if $\hat{T}$ contains at most four segments. So we consider that $\hat{T}$ contains at least five segments in what follows.

Let v be a branch vertex in $\hat{T}$ (then $v \neq v^*$ or v_2^*). If v is incident to at least two non-pendent segments (P_{v,w_1} and P_{v,w_2}) in T where $w_1, w_2 \in S(v)$, then without loss of generality, assume that $d(w_1) \leq d(w_2)$. Let $F = (E(w_1) - E_{P_{v,w_1}})$ and w be a leaf in $S(w_2)$. Then $T(F^-, w^+) \in \mathcal{T}^L$ and $Mo(T(F^-, w^+)) < Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\min}$.

Next we consider that v is incident to exactly one non-pendent segment P_{v,w_1} in T such that $w_1 \in S(v)$. If $d(v) \geq 4$, let $e \in (E(v) - E_{P_{v,w_1}} - E_{P_{v^*,v}})$. Then $T(e^-, w_1^+) \in \mathcal{T}^L$, and $Mo(T(e^-, w_1^+)) < Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\min}$. So $d(v) = 3$.

Now we consider that there does not exist branch vertex in $(S(v) \setminus \{v\})$. Let P_{v,w_1} be a pendent segment such that $w_1 \in S(v)$. If $d(v) \geq 5$, let $F = \{e_1, e_2\}$ where $e_1, e_2 \in (E(v) - E_{P(v)} - E_{P_{v,w_1}})$. Then $T(F^-, w_1^+) \in \mathcal{T}^L$, and $Mo(T(F^-, w_1^+)) < Mo(T)$ by Lemma 2.1 (i), a contradiction. So $d(v) \leq 4$.

Thus, (1) holds.

(2) Suppose $w_{1,2} = w_{2,1}$. Then $P_{w_{1,1},w_{1,2}}$ is a non-pendent segment. If $l_{x_1} < l_{x_2}$, then choose $w \in V_{P_{w_{2,1},w_{2,2}}}$ such that $d(w_{1,1}, w) = l_{x_2}$. Put $F := (E(w_{1,2}) - E_{P_{w_{1,1},w_{2,2}}})$. Then $T(F^-, w^+) \in \mathcal{T}^L$, and $Mo(T(F^-, w^+)) < Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\min}$. So $l_{x_1} \geq l_{x_2}$ and the first item holds.

Suppose both $P_{w_{1,1},w_{1,2}}$ and $P_{w_{2,1},w_{2,2}}$ are pendent segments with $d(w_{1,1}) < d(w_{2,1})$. If $l_{x_1} > l_{x_2}$, then choose $e \in E_{P_{w_{1,1},w_{1,2}}}$ such that $d(w_{1,1}, e) = l_{x_2}$. Then $T(e^-, w_{2,2}^+) \in \mathcal{T}^L$, and $Mo(T(e^-, w_{2,2}^+)) < Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\min}$. So $l_{x_1} \leq l_{x_2}$ and the second item holds.

Suppose T is edge central or central at a 2-vertex. Let P_{w_1,w_2} be the segment containing the (edge) center which has length l_{x_1}. If $l_1 \geq n/2$, then it is easy to see $|E_{P_{w_1,w_2}}| = l_1$. Suppose $l_1 < n/2$. Then P_{w_1,w_2} is a non-pendent segment. Let $P_{w_i,w_{i+2}}$ $(i = 1, 2)$ be the segment other than P_{w_1,w_2}, which has the greatest length among all segments incident to w_i. Let $l_{z_i} = |E_{P_{w_i,w_{i+2}}}|$ $(i = 1, 2)$. If $l_{x_1} < l_{z_1}$, then choose a vertex w in P_{w_1,w_3} such that $d(w, w_2) = l_{z_1}$ and let $F = (E(w_1) - E_{P_{w_1,w_3}} - E_{P_{w_1,w_2}})$. Then $T(e^-, w^+) \in \mathcal{T}^L$, and $Mo(T(e^-, w^+)) < Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{L\min}$. So $l_{x_1} \geq l_{z_1}$. Similarly, one has $l_{x_1} \geq l_{z_2}$. So $l_{x_1} = l_1$ and the third item holds.

For the fourth item, suppose $k \geq 5$ and T is central at a branch vertex v^*.

If $d(v^*) \geq 5$, then choose $v_1, v_2, v_3, v_4, v_5 \in N(v^*)$ such that $|T_{v_1}| \leq |T_{v_2}| \leq |T_{v_3}| \leq |T_{v_4}| \leq |T_{v_5}|$. Thus, $|T_{v_1}| + |T_{v_3}| < n/2$. Let P_{v^*,w_i} $(i = 1, 2, 3, 4, 5)$ be the segment in $T_{v^*v_i}$ incident to v^*. Let $T_1 = T(v^*v_1^-, w_3^+)$ and $T_2 = T_1(v^*v_2^-, w_3^+)$. Then T_1 is also central at v^*, $T_2 \in \mathcal{T}^L$ and $Mo(T_1) < Mo(T)$ by Lemma 2.1 (ii). If w_3 is a branch vertex, then $T_1 \in \mathcal{T}^L$, contradicted to $T \in \mathcal{T}^{L\min}$. If w_3 is a leaf, then $d(v^*, w_3) = |T_{v_3}| \geq d(v^*, w_2)$, which implies $Mo(T_2) \leq Mo(T_1) < Mo(T)$ by Lemma 2.2 (iii), also contradicted to $T \in \mathcal{T}^{L\min}$. So $d(v^*) \leq 4$.

Case 1 $d(v^*) = 4$. Then, let $N(v^*) = \{v_1, v_2, v_3, v_4\}$ and P_{v^*,w_i} $(i = 1, 2, 3, 4)$ be the segment of length l_{x_i} in $T_{v^*v_i}$ incident to v^*. Suppose $\sigma(v_1) \leq \sigma(v_2) \leq \sigma(v_3) \leq \sigma(v_4)$. Then $\sigma(v_1)+\sigma(v_2) \leq \sigma(v_3)+\sigma(v_4)$ and $\sigma(v_1)+\sigma(v_3) \leq \sigma(v_2)+\sigma(v_4)$. If w_3 is a branch vertex, then $T(v^*v_1^-, w_3^+) \in \mathcal{T}^L$ is also central at v^*, and $Mo(T(v^*v_1^-, w_3^+)) < Mo(T)$ by Lemma 2.1 (ii), contradicted to $T \in \mathcal{T}^{L\min}$. So w_3 is a leaf. By a similar discussion, one concludes that w_i $(i = 1, 2)$ is also a leaf. So w_4 is a branch vertex since $k \geq 5$.

If $l_{x_4} < l_{x_3}$, suppose w is a vertex in P_{v^*,w_3} such that $d(w_4, w) = l_{x_3}$. Let $F = \{v^*v_1, v^*v_2\}$. Then $T(F^-, w^+) \in \mathcal{T}^L$ and $Mo(T(F^-, w^+)) < Mo(T)$ by Lemma 2.2 (ii), contradicted to $T \in \mathcal{T}^{L\min}$. So $l_{x_4} \geq l_{x_3}$.

Let $P_{w_4,w_{4,1}}$ and $P_{w_4,w_{4,2}}$ be two segments of length $l_{4,1}$ and $l_{4,2}$, respectively, which is incident to w_4, where $w_{4,i} \neq v^*$ $(i = 1, 2)$. Without loss of generality, suppose $P_{w_4,w_{4,1}}$ is pendent and $l_{4,1} \leq l_{4,2}$, by the first and the second item of Lemma 4.1 (2). If $l_{4,1} < l_{x_3}$, let e be the edge in P_{v^*,w_3} such that $d(v^*, e) = l_{4,1}$. Then $T(e^-, w_{4,1}^+) \in \mathcal{T}^L$ and $Mo(T(e^-, w_{4,1}^+)) < Mo(T)$ by Lemma 2.2 (iii), contradicted to $T \in \mathcal{T}^{L\min}$. Then $l_{4,1} \geq l_{x_3}$, and $l_{4,1} + l_{4,2} + l_{x_4} \geq l_{x_1} + l_{x_2} + l_{x_3}$, which implies $k = 6$ and all the segments in T have the same length, since T is central at v^*.

Case 2 $d(v^*) = 3$. Then let $N(v^*) = \{v_1, v_2, v_3\}$ and P_{v^*,w_i} $(i = 1, 2, 3)$ be the segment of length l_{x_i} in $T_{v^*v_i}$ incident to v^*. Suppose $\sigma(v_1) \leq \sigma(v_2) \leq \sigma(v_3)$. If w_1 is a branch vertex, let $e \in (E(w_1) \setminus E_{P_{v^*,w_1}})$. Then $T(v^*v_2, e) \in \mathcal{T}^L$ and $Mo(T(v^*v_2, e)) < Mo(T)$ by Lemma 2.2 (ii), contradicted to $T \in \mathcal{T}^{L\min}$. So w_1 is a leaf.

If w_2 is also a leaf, then w_3 is a branch vertex since $k \geq 5$. If $l_{x_3} < l_{x_2}$, choose a vertex w in P_{v^*,w_2} such that $d(w_3, w) = l_{x_2}$. Then $T(v^*v_1^-, w^+) \in \mathcal{T}^L$ and $Mo(T(v^*v_1^-, w^+)) < Mo(T)$ by Lemma 2.2 (ii), contradicted to $T \in \mathcal{T}^{L\min}$. So $l_{x_3} \geq l_{x_2}$.

Let $P_{w_3,w_{3,1}}$ and $P_{w_3,w_{3,2}}$ be two segments of length $l_{3,1}$ and $l_{3,2}$, respectively, which is incident to w_3, where $w_{3,i} \neq v^*$ $(i = 1, 2)$. Without loss of generality, suppose $P_{w_3,w_{3,1}}$ is pendent and $l_{3,1} \leq l_{3,2}$, by the first and the second item of Lemma 4.1 (2). If $l_{3,1} < l_{x_2}$, let e be the edge in P_{v^*,w_2} such that $d(v^*, e) = l_{3,1}$. Then $T(e^-, w_{3,1}^+) \in \mathcal{T}^L$ and $Mo(T(e^-, w_{3,1}^+)) < Mo(T)$ by Lemma 2.2 (iii), contradicted to $T \in \mathcal{T}^{L\min}$. So $l_{3,1} \geq l_{x_2}$. Then $l_{3,1} + l_{3,2} + l_{x_3} > l_{x_1} + l_{x_2}$, contracted to the fact that T is central at v^*. So w_2 is a branch vertex.

If $l_{x_2} < l_{x_1}$, choose w be the vertex in P_{v^*,w_1} with $d(w_2, w) = l_{x_1}$. Then $T(v^*v_3^-, w^+) \in \mathcal{T}^L$ and $Mo(T(v^*v_3^-, w^+)) < Mo(T)$ by Lemma 2.2 (ii), contradicted to $T \in \mathcal{T}^{L\min}$. Then, $l_{x_2} \geq l_{x_1}$. Let $P_{w_2,w_{2,1}}$ and $P_{w_2,w_{2,2}}$ be two segments of length $l_{2,1}$ and $l_{2,2}$, respectively, which is incident to w_2, where $w_{2,i} \neq v^*$ $(i = 1, 2)$. Without loss of generality, suppose $P_{w_2,w_{2,1}}$ is pendent and $l_{2,1} \leq l_{2,2}$, by the first and the second item of Lemma 4.1 (2). If $l_{2,1} < l_{x_1}$, let e be the edge in P_{v^*,w_1} such that $d(v^*, e) = l_{2,1}$. Then $T(e^-, w^+_{2,1}) \in \mathcal{T}^L$ and $Mo(T(e^-, w^+_{2,1})) < Mo(T)$ by Lemma 2.2 (iii), contradicted to $T \in \mathcal{T}^{L\min}$. So $l_{2,1} \geq l_{x_1}$. So $l_{x_1} = l_k$.

Thus, we have (2) holds.

(3) By (1) and (2), if $k \leq 6$ the conclusion holds directly. Suppose $k \geq 7$. Let $\tilde{T}_1$ and $\tilde{T}_2$ be arbitrary two extended successor subtrees of T, and a be the (edge) center of T. By (1), there is at most one 4-vertex in $\tilde{T}_i$ $(i = 1, 2)$ which would be the end of the spine in $\tilde{T}_i$ which is at a longer distance from a. If there are two 4-vertices w_1 and w_2 in $\tilde{T}_1$ and $\tilde{T}_2$, respectively, then the (edge) center is in some non-pendent segment by (2).

For $i = 1, 2$; $j = 1, 2, 3$, let $P_{w_i,w_{i,j}}$ be the pendent segment incident to w_i whose length is $l_{i,j}$. Without loss of generality, suppose $l_{i,j_1} \leq l_{i,j_2}$ $(i = 1, 2)$ whenever $j_1 < j_2$, and $d(w_{1,1}, a) \leq d(w_{2,3}, a)$. Let $e_{i,j}$ $(i = 1, 2;\ j = 1, 2, 3)$ be the edge in $P_{w_i,w_{i,j}}$ which is incident to w_i. Let $T_1 = T(e^-_{2,2}, w^+_{2,3})$ and $T_2 = T_1(e^-_{1,1}, w^+_{2,3})$. Then $T_2 \in \mathcal{T}^L$ and a is also the (edge) center of T_1. Note that $Mo(T_2) \leq Mo(T_1)$ by Lemma 2.2 (iii), and $Mo(T_1) < Mo(T)$ by Lemma 2.1 (i) or Lemma 2.2 (ii), contradicted to $T \in \mathcal{T}^{L\min}$. So there is at most one extended successor subtree of T having a vertex of degree 4. Thus, (3) also holds. □

Corollary 4.2 *Let T be a tree in $\mathcal{T}^{L\min}$ with $L = (l_1, l_2, \ldots, l_k)$ and $k \geq 5$. Then T is caterpillar-like tree, where there is a non-pendent segment of length l_1 in the spine which contains the center or edge center. What is more, let $P = u_1u_2\ldots u_s$ be the spine of T, and u_{t_j} $(j \in [1, \lfloor (k-1)/2 \rfloor])$ be a branch vertex). Then*

(1) *Suppose T is central at a branch vertex u_{t_λ} $(\lambda \in [1, k])$. Then $d(u_{t_\lambda}) = 4$ if and only if $k = 6$ and all segments in T have the same length. If $d(u_{t_\lambda}) = 3$, then $k \geq 7$, T admits exactly two non-pendent segments, $l_{i_{2\lambda}} \leq l_{i_{2\lambda-2}} \leq l_{i_{2\lambda-4}} \leq \cdots \leq l_{i_2} \leq l_{i_1} \leq l_{i_3} \leq \cdots \leq l_{i_{2\lambda-1}}$, and $l_{i_{2\lambda}} \leq l_{i_{2\lambda+2}} \leq l_{i_{2\lambda+4}} \leq \cdots \leq l_{i_{k-1}} \leq l_{i_k} \leq l_{i_{k-2}} \leq \cdots \leq l_{i_{2\lambda+3}} \leq l_{i_{2\lambda+1}}$ if k is odd or $l_{i_{2\lambda}} \leq l_{i_{2\lambda+2}} \leq l_{i_{2\lambda+4}} \leq \cdots \leq l_{i_{k-2}} \leq l_{i_{k-1}} \leq l_{i_k} \leq l_{i_{k-3}} \leq \cdots \leq l_{i_{2\lambda+3}} \leq l_{i_{2\lambda+1}}$ if k is even.*

(2) *Suppose T is central at a 2-vertex u_λ, or T is edge central at $u_\lambda u_{\lambda+1}$. Let $y = \max\{j | t_j \leq \lambda\}$. Then $l_{i_{2y}} \leq l_{i_{2y-2}} \leq \cdots \leq l_{i_2} \leq l_{i_1} \leq l_{i_3} \leq \cdots \leq l_{i_{2y-1}} \leq l_{i_{2y+1}}$, and $l_{i_{2y+2}} \leq l_{i_{2y+4}} \leq \cdots \leq l_{i_{k-1}} \leq l_{i_k} \leq l_{i_{k-2}} \leq \cdots \leq l_{i_{2y+3}} \leq l_{i_{2y+1}}$ if k is odd or $l_{i_{2y+2}} \leq l_{i_{2y+4}} \leq \cdots \leq l_{i_{k-2}} \leq l_{i_{k-1}} \leq l_{i_k} \leq l_{i_{k-3}} \leq \cdots \leq l_{i_{2y+3}} \leq l_{i_{2y+1}}$ if k is even.*

Proof If $k = 3$ or 4, then T is a caterpillar-like tree by definition. If $k \geq 5$ and T is edge central or central with the center being a 2-vertex, then T is a caterpillar-like tree by Lemma 4.1 (1) and (3); if $k \geq 5$ and T is central with the center being a branch vertex, then T is a caterpillar-like tree by Lemma 4.1 (1), (2) and (3).

For the rest conclusions in Corollary 4.2, if T is edge central or central at a 2-vertex, then they hold directly by the first, second and third items of Lemma 4.1 (2). If T is central at a branch vertex, then they hold directly by the first, second and fourth items of Lemma 4.1 (2). □

Proof of Theorem 1.3 Let $T \in \mathcal{T}^{\min}(\varepsilon, k)$ $(3 \le k \le \varepsilon)$ and $n = \varepsilon + 1$. Let $L = (l_1, l_2, \ldots, l_k)$ be the segment sequence of T, where $l_i \ge l_j$ whenever $i < j$. Let a be the (edge) center of T.

If $(\varepsilon, k) = (3, 3), (4, 3), (4, 4)$ or $(5, 4)$, then $\mathcal{T}(\varepsilon, k)$ has a unique tree. Suppose $k = 3$ and $\varepsilon \ge 5$, or $k = 4$ and $\varepsilon \ge 6$. Then $l_1 \ge 2$. Let P_{v,w_i} $(i = 1, 2, 3, 4)$ be a segment of length l_i, $w_i w_i'$ be the pendent edge incident to w_i and $e_i \in (E_{P_{v,w_i}} \cap E(v))$. Then P_{v,w_1} contains the (edge) center. Let $F = (E(v) \setminus \{e_1, e_2\})$. If $l_2 \ge 2$, then $T(F^-, w_2'^+) \in \mathcal{T}(\varepsilon, k)$ and $Mo(T(F^-, w_2'^+)) < Mo(T)$ by Lemma 2.1 (i) or Lemma 2.2 (ii), contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$. So $l_2 = 1$ and $T \cong T_C(\varepsilon, k)$.

Suppose $k \ge 5$. Then T is a balanced caterpillar-like tree satisfying Corollary 4.2.

If $n = k + 1$, then T is the unique tree $T_C(\varepsilon, k)$ in $\mathcal{T}_C^L$ where $L = (1, 1, \ldots, 1)$ of length k.

If $n = k + 2$, then $(k - 1)$ segments have a length one, and the rest segment $w_1 w_2 w_3$ of length 2 contains the (edge) center of T by Corollary 4.2. Without loss of generality, suppose $\zeta(w_1) \le \zeta(w_3)$, where $\zeta(w_i)$ $(i = 1, 3)$ is the vertex number of the component in $(T - \{w_1 w_2, w_2 w_3\})$ that contains w_i. Then T is central at w_2 if and only if $\zeta(w_1) = \zeta(w_3)$ and $k = 4t + 1$ $(t \ge 1)$; T is edge central at $w_2 w_3$ if and only if $\zeta(w_1) = \zeta(w_3) - 1$ and k is an even integer at least 6; T is central at w_3 if and only if $\zeta(w_1) = \zeta(w_3) - 2$ and $k = 4t + 3$ $(t \ge 1)$. That is $T \cong T_C(\varepsilon, k)$.

If $n \ge k + 3$, then first we have the following claims.

Claim 1 *Suppose $n \ge k + 3$ with $k \ge 5$. Let T_b be an extended successor subtree of T. If T_b contains at least one branch vertex other than the center, then each segment of T in T_b other than the one which contains the (edge) center has the length one.*

Proof Let w_1 be one branch vertex other than the center, such that $d(w_1)$ is minimal. Let P_{w_1,w_2} be the longest segment incident to w_1 in T_b such that $V_{P_{w_1,w_2}} \subseteq S(w_1)$ and $w_2 w_2' \in E_{P_{w_1,w_2}}$. Then P_{w_1,w_2} is the longest segment in T_b other than the one containing the (edge) center, by Corollary 4.2. Let P_{w_1,w_3} be the other segment such that $V_{P_{w_1,w_3}} \subseteq \sigma(w_1)$ and $w_1 w_3' \in E_{P_{w_1,w_3}}$. If $|E_{P_{w_1,w_2}}| \ge 2$, then $T(w_1 w_3'^-, w_2'^+) \in \mathcal{T}(\varepsilon, k)$ and $Mo(T(w_1 w_3'^-, w_2'^+)) < Mo(T)$ by Lemma 2.1 (i), contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$. This implies $|E_{P_{w_1,w_2}}| = 1$ and so all segments in T_b other than the one containing the (edge) center are of length one. □

Claim 2 *Suppose T is central at v^*, $k \ge 5$ and $n \ge k + 3$. Then $d(v^*) = 2$.*

Proof By the proof of Corollary 4.2, if v^* is incident to exactly one non-pendent segment, then $k = 6$, $d(v^*) = 4$ and each segment has a common length l where $l \ge 2$ since $n \ge k + 3$. However, let P and P' be two pendent segments incident to v^*, and let e be a pendent edge in P and w be a leaf in P'. Then $T(e^-, w^+) \in \mathcal{T}(\varepsilon, k)$ and $Mo(T(e^-, w^+)) < Mo(T)$ by Lemma 2.1 (ii), contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$. So v^* is incident to two non-pendent segments (supposed to be P_{v^*,w_1} and P_{v^*,w_2} of length l_1 and l_2, respectively, by Corollary 4.2). Then $k \ge 7$.

Let $P_{v^*,w_3} = v^* w_3$ be the pendent segment of length one, by Claim 1 and Corollary 4.2. Let $w_1 w \in E_{P_{v^*,w_1}}$. Then $T(v^* w_3^-, w^+) \in \mathcal{T}(\varepsilon, k)$. Let T_{v_i} $(i = 1, 2)$ be the branch containing w_i. Note that one has either $l_1 \ge 3$ holds, or $l_1, l_2 \ge 2$

holds. If $l_1 \geq 3$, then $Mo(T(v^*w_3^-, w^+)) < Mo(T)$ by Lemma 2.2 (iii), contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$. If $l_1 \geq 2$ and $l_2 \geq 2$, without loss of generality, suppose $\sigma(v_1) \leq \sigma(v_2)$. Then again, $Mo(T(v^*w_3^-, w^+)) < Mo(T)$ by Lemma 2.2 (iii), also contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$. □

By Claim 2 and Corollary 4.2, T is either edge central at some edge in a non-pendent segment of length l_1, or central at some 2-vertex in a non-pendent segment of length l_1. So by Claim 1, each segment other than the non-pendent segment containing the center or edge center has a length one. That is, $L = (l_1, 1, 1, \ldots, 1)$.

Let $P = w_1w_2\ldots w_{n-k+1}$ be the non-pendent segment containing the (edge) center. Let $\zeta(w_i)$ $(i = 1, n-k+1)$ be the number of vertices in the connected component in $(T - E_P)$ containing w_i. Without loss of generality, suppose $\zeta(w_1) \leq \zeta(w_{n-k+1})$. Note that there is at least one branch vertex in each of $S(v_1)$ and $S(w_{n-k+1})$. If $k = 5$, 6 or 7, then $T \cong T_C(\varepsilon, k)$. If $k \geq 8$, then $d(w_{n-k+1}) = 3$. Let e_1 be the pendent edge incident to w_{n-k+1} and $w_1w_2 \in E_{P_{w_1,a}}$. Then $T_1 = T(e_1^-, w_2^+) \in \mathcal{T}(\varepsilon, k)$.

If $k = 4t + 1$ $(t \geq 2)$, then $\zeta(w_1) = \zeta(w_{n-k+1})$. Otherwise, one has $\zeta(w_1) \geq \zeta(w_{n-k+1}) - 4z$ for some $z \geq 1$ which implies $d(w_1) \leq d(w_{n-k+1}) + 4$ (that is $d(w_2) \leq d(w_{n-k+1}) + 3$). When $n \leq k + 4$, it is a contradiction to Claim 2; When $n \geq k + 5$, $Mo(T_1) < Mo(T)$ by Lemma 2.2 (iii), contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$.

If $k = 4t + 3$ $(t \geq 2)$, then $\zeta(w_1) = \zeta(w_{n-k+1}) - 2$. Otherwise, one has $\zeta(w_1) \geq \zeta(w_{n-k+1}) - 4z - 2$ for some $z \geq 1$ which implies $d(w_1) \leq d(w_{n-k+1}) + 6$ (that is $d(w_2) \leq d(w_{n-k+1}) + 5$). When $n \leq k + 5$, it is a contradiction to Claim 2; when $n \geq k + 6$, $Mo(T_1) < Mo(T)$ by Lemma 2.2 (iii), contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$.

If $k = 2t$ $(t \geq 4)$, then $\zeta(w_1) = \zeta(w_{n-k+1}) - 1$. Otherwise, one has $\zeta(w_1) \geq \zeta(w_{n-k+1}) - 2z - 1$ for some $z \geq 1$ which implies $d(w_1) \leq d(w_{n-k+1}) + 3$ (that is $d(w_2) \leq d(w_{n-k+1}) + 2$). When $n \leq k + 3$, it is a contradiction to Claim 2; when $n \geq k + 4$, $Mo(T_1) < Mo(T)$ by Lemma 2.2 (iii), contradicted to $T \in \mathcal{T}^{\min}(\varepsilon, k)$.

Thus, $T \cong T_C(\varepsilon, k)$ also holds when $k \geq 5$ and $n \geq k + 3$.

On the other hand,

(1) If $k = 3$, then

$$Mo(T) = 2(n-2) + \sum_{i=1}^{n-3} |n - 2(2i-1)| = \left\lfloor \frac{(n-1)^2}{2} \right\rfloor + 2.$$

(2) If $k = 4$ and $n = 5$, one has $Mo(T) = 12$; If $k = 4$ and $n \geq 6$, then

$$Mo(T) = 3(n-2) + \sum_{i=1}^{n-4} |n - 2(2i-1)| = \left\lfloor \frac{(n-1)^2}{2} \right\rfloor + 6.$$

(3) If $k = 4t + 1$ $(t \geq 1)$ and $(n - k)$ is odd, then

$$Mo(T) = 2t \cdot (n-2) + 2\sum_{i=1}^{t} [n - 2(2i-1)] + 2 \sum_{i=1}^{\frac{n-k-1}{2}} (2i)$$

$$= \frac{n^2}{2} - n + \frac{(k-1)^2}{4}.$$

If $k = 4t + 1$ ($t \geq 1$) and $(n - k)$ is even, then

$$\begin{aligned} Mo(T) &= 2t \cdot (n-2) + 2\sum_{i=1}^{t}[n - 2(2i-1)] + 2\sum_{i=1}^{\frac{n-k}{2}}(2i-1) \\ &= \frac{n^2+1}{2} - n + \frac{(k-1)^2}{4}. \end{aligned}$$

(4) If $k = 4t + 3$ ($t \geq 1$) and $(n - k)$ is odd, one has

$$\begin{aligned} Mo(T) &= (2t+1) \cdot (n-2) + 2\sum_{i=1}^{t+1}[n - 2(2i-1)] + \sum_{i=1}^{\frac{n-k-3}{2}}(2i) + \sum_{i=1}^{\frac{n-k-1}{2}}(2i) \\ &= \frac{n^2}{2} - n + \frac{(k-1)^2}{4} + 1. \end{aligned}$$

If $k = 4t + 3$ ($t \geq 1$) and $(n - k)$ is even, one has

$$\begin{aligned} Mo(T) &= (2t+1) \cdot (n-2) + 2\sum_{i=1}^{t+1}[n - 2(2i-1)] + \sum_{i=1}^{\frac{n-k-2}{2}}(2i-1) + \sum_{i=1}^{\frac{n-k}{2}}(2i-1) \\ &= \frac{n^2+1}{2} - n + \frac{(k-1)^2}{4} + 1. \end{aligned}$$

(5) If $k = 4t + 2$ ($t \geq 1$) and $(n - k)$ is odd, then

$$\begin{aligned} Mo(T) &= (2t+2) \cdot (n-2) + \sum_{i=1}^{t}[n - 2(2i-1)] + \sum_{i=2}^{t}[n - 2(2i)] \\ &\quad + \sum_{i=1}^{\frac{n-k+1}{2}}(2i-1) + \sum_{i=1}^{\frac{n-k-1}{2}}(2i-1) \\ &= \frac{n^2+1}{2} - n + \frac{(k-1)^2+7}{4}. \end{aligned}$$

If $k = 4t + 2$ ($t \geq 1$) and $(n - k)$ is even, then

$$\begin{aligned} Mo(T) &= (2t+2) \cdot (n-2) + \sum_{i=1}^{t}[n - 2(2i-1)] + \sum_{i=2}^{t}[n - 2(2i)] \\ &\quad + \sum_{i=1}^{\frac{n-k+2}{2}}(2i) + \sum_{i=1}^{\frac{n-k-2}{2}}(2i) \end{aligned}$$

$$= \frac{n^2}{2} - n + \frac{(k-1)^2+7}{4}.$$

(6) If $k = 4t + 4$ $(t \geq 1)$ and $(n-k)$ is odd, then

$$\begin{aligned} Mo(T) &= (2t+3)\cdot(n-2) + \sum_{i=1}^{t+1}[n-2(2i-1)] + \sum_{i=2}^{t}[n-2(2i)] \\ &+ \sum_{i=1}^{\frac{n-k+1}{2}}(2i-1) + \sum_{i=1}^{\frac{n-k-1}{2}}(2i-1) \\ &= \frac{n^2+1}{2} - n + \frac{(k-1)^2+7}{4}. \end{aligned}$$

If $k = 4t + 4$ $(t \geq 1)$ and $(n-k)$ is even, then

$$\begin{aligned} Mo(T) &= (2t+3)\cdot(n-2) + \sum_{i=1}^{t+1}[n-2(2i-1)] + \sum_{i=2}^{t}[n-2(2i)] \\ &+ \sum_{i=1}^{\frac{n-k}{2}}(2i) + \sum_{i=1}^{\frac{n-k-2}{2}}(2i) \\ &= \frac{n^2}{2} - n + \frac{(k-1)^2+7}{4}. \end{aligned}$$

So for $3 \leq k \leq \varepsilon$, one has

$$Mo(T) = \begin{cases} \lfloor \frac{(n-1)^2}{2} \rfloor + 2, & \text{if} \quad k = 3; \\ 12, & \text{if} \quad k = 4 \text{ and } n = 5; \\ \lfloor \frac{(n-1)^2}{2} \rfloor + 6, & \text{if} \quad k = 4 \text{ and } n \geq 6; \\ \lceil \frac{n^2}{2} \rceil - n + \frac{(k-1)^2}{4}, & \text{if} \quad k = 4t+1 (t \geq 1); \\ \lceil \frac{n^2}{2} \rceil - n + \frac{(k-1)^2}{4} + 1, & \text{if} \quad k = 4t+3 (t \geq 1); \\ \lceil \frac{n^2}{2} \rceil - n + \frac{(k-1)^2+7}{4}, & \text{if} \quad k = 2t (t \geq 3). \end{cases}$$

That is,

$$Mo(T) = \begin{cases} \lfloor \frac{\varepsilon^2}{2} \rfloor + 2, & \text{if} \quad k = 3; \\ 12, & \text{if} \quad k = 4 \text{ and } \varepsilon = 4; \\ \lfloor \frac{\varepsilon^2}{2} \rfloor + 6, & \text{if} \quad k = 4 \text{ and } \varepsilon \geq 5; \\ \lceil \frac{(\varepsilon+1)^2}{2} \rceil - (\varepsilon + 1) + \frac{(k-1)^2}{4}, & \text{if} \quad k = 4t + 1 \ (t \geq 1); \\ \lceil \frac{(\varepsilon+1)^2}{2} \rceil - \varepsilon + \frac{(k-1)^2}{4}, & \text{if} \quad k = 4t + 3 \ (t \geq 1); \\ \lceil \frac{(\varepsilon+1)^2}{2} \rceil - \varepsilon + \frac{(k-1)^2+5}{4}, & \text{if} \quad k = 2t \ (t \geq 3). \end{cases}$$

This completes the proof. □

5 Concluding Remarks and Further Research Problems

In this paper, we determine the trees having the greatest Mostar index among the tree set with a given segment sequence and among the tree set with a given size and together with a given segment number, respectively. We also identify the trees having the least Mostar index among the later set.

Quite recently, as a generalization of the Mostar index, the *edge-Mostar index* [5] was introduced:

$$Mo_e(G) = \sum_{e=uv \in E_G} |m_u(e|G) - m_v(e|G)|,$$

where $m_u(e|G) = \{e'|d(e', u) < d(e', v)\}$ and $m_v(e|G) = \{e'|d(e', v) < d(e', u)\}$, respectively. The edge Mostar index of some polycyclic aromatic structures [5] and some other chemical graphs [1,19,23] have been studied. It is a natural problem to look for extremal graphs among all kinds of graph sets respect to the edge Mostar index, as those have been studied respect to the Mostar index. It seems that as the number of cycles in graphs increases, the extremal graphs are quite different respect to the two distinct indices.

One can also consider the extremal problems respect to the Mostar index, among trees or general graphs given parameters related to all kinds of vertex sequences [16]. For example, consider the graphs with given Grundy domination number which is the maximum length of a dominating sequence [16].

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