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*Research Article*

# An inequality for the Mostar index of line graphs of trees

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**Abstract:** Consider a simple connected graph $G$ with the vertex set $V(G)$ and edge set $E(G)$. The Mostar index $M_\circ(G)$ of $G$ is defined as $M_\circ(G) = \sum_{e=xy\in E(G)} |n_x - n_y|$, where $n_x$ and $n_y$ represent the number of vertices that lie closer to $x$ than to $y$ and the number of vertices that lie closer to $y$ than to $x$, respectively. In this paper, we prove that if $G$ is a tree, then $M_\circ(L_G) < M_\circ(G)$, where $L_G$ is the line graph. In order to provide an example supporting this result, we develop three algorithms (and implement them using Python) to calculate the Mostar index of trees of order at most 8 and their line graphs.

**Keywords:** Mostar Index, line graph, trees, graph transformation, algorithmic graph analysis.

**AMS Subject classification:** 05C12, 05C35, 05C81

## 1. Introduction

Consider a simple connected graph $G$ with a vertex set $V(G)$ and an edge set $E(G)$. The *degree* of a vertex $x$, denoted as $d_x$, is the number of edges incident to $x$. The *distance* $d(a, b)$ between two vertices $a$ and $b$ in the graph $G$ is defined as the minimum number of edges that must be traversed to travel from vertex $a$ to vertex $b$. Various numerical quantities, commonly referred to as structural invariants, molecular

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descriptors, topological descriptors, and topological indices, have been developed and studied to elucidate and summarize the information embedded in graph connectivity patterns [26, 28]. An essential aspect of mathematical chemistry is the use of molecular descriptors, particularly for investigating quantitative structure-property relationships (QSPR). One of the earliest molecular descriptors introduced by Wiener is the Wiener index [31]. This concept is particularly significant in mathematical chemistry, especially in chemical graph theory. The Wiener index is defined as:

$$W(G) = \sum_{u<v} d(u,v).$$

When applied to trees, the Wiener index can be stated as:

$$W(G) = \sum_{e=ab\in E(G)} n_a n_b,$$

where $n_a$ and $n_b$ represent, respectively, the number of vertices that lie closer to $a$ than to $b$ and the number of vertices that lie closer to $b$ than to $a$. This formulation also defines the Szeged index, which was introduced and defined by Gutman [16]:

$$S(G) = \sum_{e=ab\in E(G)} n_a n_b.$$

The two indices do not coincide for general graphs. However, when applied to trees, both the Wiener index and the Szeged index yield identical results. For graphs containing cycles, the inequality $W(G) \leq S(G)$ holds, with equality if every block of the graph is complete. The Szeged index belongs to the category of bond-additive indices. Numerous bond-additive indices exist, among which the first and second Zagreb indices are precisely specified in [19]:

$$M_1(G) = \sum_{e=ab\in E(G)} (d_a + d_b) \quad \text{and} \quad M_2(G) = \sum_{e=ab\in E(G)} d_a d_b.$$

Another metric, the irregularity of $G$, is defined based on the edges' contributions as follows:

$$Irr(G) = \sum_{e=ab\in E(G)} |d_a - d_b|.$$

Došlić et al. [14] introduced a novel bond-additive structural invariant known as the Mostar index $M_\circ(G)$, which is defined as:

$$M_\circ(G) = \sum_{e=ab\in E(G)} |n_a - n_b|. \tag{1.1}$$

In the case of a vertex-transitive graph, $M_\circ(G) = 0$ [14]. The Mostar index is an enhanced method for determining the extent to which specific bonds (edges) are located on the periphery of a graph. A global measure of a graph's peripherality is obtained by summing the contributions of each edge in the graph. An edge is identified as being on the periphery when a significant number of vertices are closer to one of its endpoints than to the other. For further information, we now discuss several recent publications on the Mostar index.

Hayat and Zhou [23] employed graph transformations to manipulate the Mostar index, either decreasing or increasing it. They identified groups of trees of order $n$ that satisfy specific criteria, such as maximum degree, diameter, or number of pendant vertices. These families included both the trees with the lowest and highest Mostar indices. This was achieved by applying graph transformations that make the Mostar index either decrease or increase. Dehgardi and Azari [11] determined an exact lower bound for the Mostar indices of trees, taking order and maximal degree into account. Furthermore, the researchers identified the precise trees that meet these reduced constraints. Huang, Li, and Zhang [24] effectively distinguished the extremal hexagonal chains and established precise upper and lower limits on the Mostar indices for hexagonal chains with $n$ hexagons. Hayat and Zhou [22] investigated cacti with the highest Mostar index. They successfully identified all such cacti and provided a precise upper limit for the Mostar index in these cases, focusing on cacti of order $n$ with $k$ cycles. In their investigation, Deng and Li [12] observed that tree-type hexagonal systems with the smallest and second smallest Mostar indices exhibited correspondingly low values. They also demonstrated how several common properties can characterize tree-type hexagonal structures with the highest Mostar index. Additionally, they identified the tree-type hexagonal system with exactly one full hexagon and determined which graph had the highest Mostar index among those systems. These findings generalize some previously obtained information on extremal hexagonal chains. Xiao et al. [32] characterized the related extremal graphs through certain transformations on hexagonal chains and identified the three lowest values of the Mostar index across all hexagonal chains containing $h$ hexagons. Deng and Li [13] succeeded in identifying chemical trees of order $n$ with the highest Mostar index. For recent research on the Mostar index, readers are encouraged to consult the following articles: [1, 2, 4, 5, 15, 25, 29, 30].

The graph denoted by the notation $L_G$ for a given graph $G$ is a line graph whose vertices are the edges of $G$. Adjacent vertices in $L_G$ are those whose incident edges in $G$ share a common vertex [20, 27]. The subsequent Lemma is advantageous in determining the degree of the vertices of $L_G$.

**Lemma 1.** *[21] Let $G$ be a graph with $a, b \in V(G)$ and $f \in E(G)$. Then*

$$d_f = d_a + d_b - 2.$$

Research on the properties of $M_\circ(G)$ and $M_\circ(L_G)$ is motivated by theoretical chemistry. The Mostar index $M_\circ(G)$ has gained attention in both complex network analysis and classical chemical graph theory due to its utility in determining the surface area of octane isomers and exploring the topological characteristics of fullerene morphologies [3]. Bertz [6] was the first to propose that line graphs can be used to depict relevant features of molecular structures (also see [7, 8]). Line graphs have also been employed in other chemical research [18].

A *tree* $T$ is a connected, acyclic graph. In 1996, Gutman studied the relationship between the Wiener index of a tree $T$ and the Wiener index of its line graph $L_T$ [17], as initially stated by Buckley [10]. Buckley's formula, which is used in various academic disciplines, is:

$$W(T) = W(L_T) + \binom{n}{2}$$

valid for trees, and it immediately implies $W(T) > W(L_T)$. In [17], the following extension of Buckley's formula to all connected graphs $G$ was deduced:

$$W(G) \leq W(L_G) + \frac{1}{2}m(m+1) - n(n-1)$$

from which we see that the expression $W(G) > W(L_G)$ holds, provided the graph $G$ has a sufficient number of edges.

This work aims to determine that if $G$ is a tree, then $M_\circ(L_G) < M_\circ(G)$. We establish relations between $M_\circ(G)$ and $M_\circ(L_G)$ for certain classes of tree graphs. Furthermore, we verify the theorem for all trees with fewer than 9 vertices. For undefined notations and terminologies, please refer to the book by Bollobás [9].

## 2. Main Results

This section aims to present the proof of our main results. A tree that exhibits the characteristic of having only one vertex with a degree exceeding 2 is commonly referred to as a *star-like tree*. Suppose $T$ is a star-like tree. We indicate its maximum degree by $r$ ($r \geq 3$), and the length (number of edges) of its branches is indicated by $b_1, b_2, \ldots, b_m$. By convention, $b_1 \geq b_2 \geq \cdots \geq b_m$. Since $b_1 + b_2 + \cdots + b_m = n-1$, the structure of star-like tree $T$ is fully determined by the partition $T = (b_1, b_2, \ldots, b_m)$ of $n-1$. In view of this, a star-like tree will be denoted by $T(b_1, b_2, \ldots, b_m)$. If $b_1 = b_2 = \cdots = b_m = 1$, then the respective tree is a *simple star*. Some examples of star-like trees are given in Figure 1 and the third is a simple star.

**Theorem 1.** *Let $T(b_1, b_2, \ldots, b_m)$ (or simply $T_n$) be a star-like tree on $n$ vertices and the length of its branches is $l$. Then*

$$M_\circ(L_{T_n}) < M_\circ(T_n).$$

*Proof.* Suppose $T_n$ is a star-like tree with exactly one vertex, a degree greater than 2, $m$ branches, and $l$ length for each branch. We denote these branches by $b_1, b_2, \ldots, b_m$ and one vertex with a degree greater than 2 by $v_0$. The cardinality of the sets of

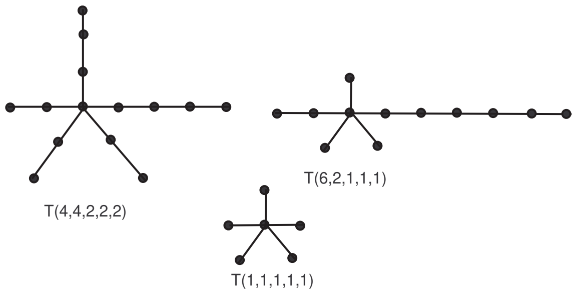


**Figure 1.** **Star-like tree examples.**

vertices and edges is $|V(T_n)| = n = lm+1$ and $|E(T_n)| = n-1 = lm$, respectively. The vertices of these $m$ branches can be listed in order $b_1 = \{v_0, v_{11}, v_{12}, \ldots, v_{1l}\}$, $b_2 = \{v_0, v_{21}, v_{22}, \ldots, v_{2l}\}$, $\ldots$, $b_m = \{v_0, v_{m1}, v_{m2}, \ldots, v_{ml}\}$ such that the edges are $b_1 = \{v_0v_{11}, v_{1(i-1)}v_{1i}\}$, $b_2 = \{v_0v_{21}, v_{2(i-1)}v_{2i}\}$,$\ldots$, $b_m = \{v_0v_{m1}, v_{m(i-1)}v_{mi}\}$, where $2 \le i \le l$. Let $u, v \in T_n$, then

$$M_\circ(T_n) = \sum_{e=uv\in E(b_1)} |n_u - n_v| + \sum_{e=uv\in E(b_2)} |n_u - n_v| + \sum_{e=uv\in E(b_3)} |n_u - n_v| + \cdots + \sum_{e=uv\in E(b_m)} |n_u - n_v|. \tag{2.1}$$

Consider

$$\begin{aligned}
\sum_{e=uv\in E(b_1)} |n_u - n_v| &= \sum_{e=v_0v_{11}\in E(b_1)} |n_{v_0} - n_{v_{11}}| + \sum_{e=v_{11}v_{12}\in E(b_1)} |n_{v_{11}} - n_{v_{12}}| + \cdots \\
&\quad + \sum_{e=v_{1l-1}v_{1l}\in E(b_1)} |n_{v_{1l-1}} - n_{v_{1l_n}}| \\
&= |(m-1)l - (l-1)| + |((m-1)l+1) - (l-2)| \\
&\quad + |((m-1)l+2) - (l-3)| \\
&\quad + \cdots + |((m-1)l + (l-1)) - (l-l)| \\
&= \sum_{i=0}^{l-1} |((m-1)l+i) - (l-(i+1))| \\
&= \sum_{i=0}^{l-1} |lm + 2i - 2l + 1|.
\end{aligned}$$

Similarly,

$$\sum_{e=uv\in E(b_2)} |n_u - n_v| = \sum_{i=0}^{l-1} |lm + 2i - 2l + 1|. \tag{2.2}$$

$$\sum_{e=uv\in E(b_3)} |n_u - n_v| = \sum_{i=0}^{l-1} |lm + 2i - 2l + 1|. \tag{2.3}$$

$$\vdots$$

$$\sum_{e=uv\in E(b_m)} |n_u - n_v| = \sum_{i=0}^{l-1} |lm + 2i - 2l + 1|. \tag{2.4}$$

Now by adding the above Equations in Equation (2.1), we get

$$\begin{aligned} M_\circ(T_n) &= \sum_{i=0}^{l-1} |lm+2i-2l+1| + \sum_{i=0}^{l-1} |lm+2i-2l+1| + \cdots + \sum_{i=0}^{l-1} |lm+2i-2l+1| \\ &= m \times \sum_{i=0}^{l-1} |lm+2i-2l+1| \\ &= m(l^2(m-1)). \end{aligned} \tag{2.5}$$

Since in $T_n$, we have vertices of degrees $m$, 2, 1, and edges of types $(m, 2)$, $(1, 2)$, $(2, 2)$. Hence, in terms of Lemma 1, in $L_{T_n}$, we have vertices of degrees $m$, 2 and 1. Since $|E(T_n)| = |V(L_{T_n})|$. The line graph $L(T_n)$ of $T_n$ is formed by a complete graph $K_m$ with $m$ vertices, to which $m$ pendent paths of length $l-1$ are attached. The vertices of these $m$ paths can be listed in order $P_1 = \{v_{11}, v_{12}, \ldots, v_{1(l-1)}\}$, $P_2 = \{v_{21}, v_{22}, \ldots, v_{2(l-1)}\}$, $\ldots$, $P_m = \{v_{m1}, v_{m2}, \ldots, v_{m(l-1)}\}$ and the edges are $P_1 = \{v_{1(i-1)}v_{1(i)}\}$, $P_2 = \{v_{2(i-1)}v_{2i}\}$,$\ldots$, $b_m = \{v_{m(i-1)}v_{mi}\}$, where $1 \le i \le l-1$. The complete graph $K_m$ consists of a collection of vertices indicated as $\{v_{11}, v_{21}, \ldots, v_{m1}\}$. In a complete graph, every vertex is next to every other vertex, and the total number of edges may be calculated using the formula $\frac{m(m-1)}{2}$. If $u, v \in L_{T_n}$, then

$$\begin{aligned} M_\circ(L_{T_n}) &= \sum_{e=uv\in E(K_m)} |n_u - n_v| + \sum_{e=uv\in E(P_1)} |n_u - n_v| \\ &\quad + \sum_{e=uv\in E(P_2)} |n_u - n_v| + \cdots + \sum_{e=uv\in E(P_m)} |n_u - n_v|. \end{aligned} \tag{2.6}$$

If $u, v \in K_m$, then

$$\sum_{e=uv\in E(K_m)} |n_u - n_v| = 0, \tag{2.7}$$

because the graph is a vertex-transitive. Now let $u, v \in P_1$, then

$$\begin{aligned}
\sum_{e=uv\in E(P_1)} |n_u - n_v| &= \sum_{e=v_{11}v_{12}\in E(P_1)} |n_{v_{11}} - n_{v_{12}}| + \sum_{e=v_{12}v_{13}\in E(P_1)} |n_{v_{12}} - n_{v_{13}}| + \cdots \\
&\quad + \sum_{e=v_{1l-2}v_{1l-1}\in E(b_1)} |n_{v_{1l-2}} - n_{v_{1l-1}}| \\
&= |(m-1)l - (l-2)| + |((m-1)l+1) - (l-3)| \\
&\quad + |((m-1)l+2) - (l-4)| + \cdots \\
&\quad + |((m-1)l + (l-2)) - (l-l)| \\
&= \sum_{i=0}^{l-2} |((m-1)l+i) - (l-(i+2))| \\
&= \sum_{i=0}^{l-2} |ml - 2l + 2i + 2|.
\end{aligned}$$

Similarly, we infer

$$\sum_{e=uv\in E(P_2)} |n_u - n_v| = \sum_{i=0}^{l-2} |ml - 2l + 2i + 2|. \tag{2.8}$$

$$\sum_{e=uv\in E(P_3)} |n_u - n_v| = \sum_{i=0}^{l-2} |ml - 2l + 2i + 2|. \tag{2.9}$$

$$\vdots$$

$$\sum_{e=uv\in E(P_m)} |n_u - n_v| = \sum_{i=0}^{l-2} |ml - 2l + 2i + 2|. \tag{2.10}$$

Now by putting the above equations in Equation (2.6), we get

$$\begin{aligned}
M_\circ(L_{T_n}) &= 0 + \sum_{i=0}^{l-2} |ml - 2l + 2i + 2| + \sum_{i=0}^{l-2} |ml - 2l + 2i + 2| + \cdots + \sum_{i=0}^{l-2} |ml - 2l + 2i + 2| \\
&= m(\sum_{i=0}^{l-2} |ml - 2l + 2i + 2|) \\
&= m(l(m-1)(l-1)).
\end{aligned} \tag{2.11}$$

In light of (2.5) and (2.11), we deduce

$$M_\circ(L_{T_n}) < M_\circ(T_n).$$

□

**Remark 1.** Let $T(b_1, b_2, \ldots, b_m)$ (or simply $T_n$) be a star-like tree on $n = lm+1$ vertices and $b_1 = b_2 = \cdots = b_m = l$. Then

$$M_\circ(T_n) = M_\circ(L_{T_n}) + ml(m-1).$$

A tree that possesses precisely two non-pendant vertices is referred to as a *double star*. The notation $S_{k_{1,n},k_{1,n}}$ is used to represent a double-star tree with a degree sequence of $(n+1, n+1, 1, \ldots, 1)$. For example, the double star tree $S_{k_{1,5},k_{1,5}}$ and its line graph are depicted in Figure 2. The double star tree $S_{k_{1,n},k_{1,n}}$ has a total of $2n+2$ vertices and $2n+1$ edges. In the following, we denote the double star tree simply by $T_n$.

**Theorem 2.** *Let $T_n$ be a double star tree on $2n+2$ vertices and $2n+1$ edges. Then*

$$M_\circ(L_{T_n}) < M_\circ(T_n).$$

*Proof.* Let $T_n$ be a tree with $2n+2$ vertices and $2n+1$ edges. The set of vertices and edges is $V(T_n) = \{v_1, u_1, \underbrace{v_{11}, v_{12}, \ldots, v_{1n}}_{n}, \underbrace{u_{11}, u_{12}, \ldots, u_{1n}}_{n}\}$ and $E(T_n) = v_1u_1 \cup v_1v_{1i} \cup u_1u_{1i}$ $(1 \leq i \leq n)$, respectively. If $u, v \in T_n$, then

$$\begin{aligned} M_\circ(T_n) &= \sum_{e=u_1v_1\in E(T_n)} |n_{u_1} - n_{v_1}| + \sum_{e=v_1v_{1i}\in E(T_n)} |n_{v1} - n_{v1i}| + \sum_{e=u_1u_{1i}\in E(T_n)} |n_{u1} - n_{u1i}| \\ &= |n-n| + (|2n-0| + |2n-0| + \cdots + |2n-0|) + (|2n-0| + |2n-0| + \cdots + |2n-0|) \\ &= n|2n| + n|2n| = 4n^2. \end{aligned} \tag{2.12}$$

Since in $T_n$, we have vertices of degree $n+1$, $1$, and edges of types $(n+1, n+1)$, $(1, n+1)$. By virtue of Lemma 1, in $L(T_n)$ we have $2n+1$ vertices in which $|d_n| = 2n$ and $|d_{2n}| = 1$. Since $|\ V(L_{T_n})\ |=|\ E(T_n)\ |$, the line graph $L_{T_n}$ is equal to the two complete graphs with one common vertex between them (see Figure 2). We denote the common vertex with $x$ and the vertices of two complete graphs except the common vertex are denoted by $v_1, v_2, \ldots, v_n$ and $u_1, u_2, \ldots, u_n$, respectively. Let $u, v \in V(L_{T_n})$, then

$$\begin{aligned} M_\circ(L_{T_n}) &= \sum_{e=u_iu_i\in E(T_n)} |n_{u_i} - n_{u_i}| + \sum_{e=v_1v_i\in E(T_n)} |n_{vi} - n_{vi}| + \sum_{e=u_ix\in E(T_n)} |n_{ui} - n_x| \\ &\quad + \sum_{e=v_ix\in E(T_n)} |n_{vi} - n_x| \qquad (2.13) \\ &= 0 + 0 + (|(n-1)-(n-1)+n| + |(n-1)-(n-1)+n| + \cdots \\ &\quad + |(n-1)-(n-1)+n|) + (|(n-1)-(n-1)+n| \\ &\quad + |(n-1)-(n-1)+n| + \cdots + |(n-1)-(n-1)+n|) \\ &= n|n| + n|n| = 2n^2. \end{aligned} \tag{2.14}$$

By means of (2.12) and (2.13), we get $M_\circ(L_{T_n}) < M_\circ(T_n)$. □

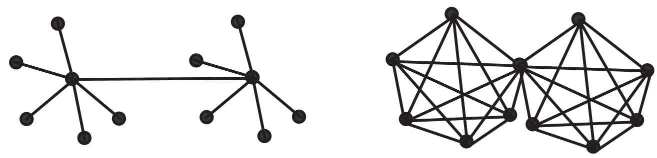

**Figure 2.** **A double star tree $S_{k_{1,5},k_{1,5}}$ and its line graph.**

**Remark 2.** Let $T_n$ be a double star tree on $2n+2$ vertices. Then

$$M_\circ(T_n) = 2M_\circ(L_{T_n}).$$

In the field of graph theory, a tree referred to as a *caterpillar tree* is characterized by the property that all of its vertices are situated at a maximum distance of 1 from a central path. For the sake of simplicity in the exposition, we adopt the notation $C_{b_2,b_3,\ldots,b_t}$ for a caterpillar tree with a central path of $t$ vertices and such that the ith-vertex of the path has a degree equal to $d(b_i)+2$, for $i \in \{2,3,\ldots,t-1\}$, while the first and last vertices of the path have degrees equal to 1 each. See Figure 3 for an illustration of a caterpillar tree.

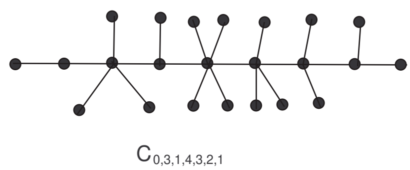


**Figure 3.** **Example of caterpillar tree.**

**Theorem 3.** *Let $C_b := C_{b_2,b_3,\ldots,b_{t-1}}$ (or simply $T_n$) be a caterpillar tree and $b_2 = b_3 = \cdots = b_{t-1} = l$. Then*

$$M_\circ(L_{T_n}) < M_\circ(T_n).$$

*Proof.* Given $T_n$ is a caterpillar tree and $b_2 = b_3 = \cdots = b_{t-1} = l$ or $b_i = l$, where $2 \le l \le t-1$. The set of vertices of the central path of a caterpillar tree is denoted by $P_t = u_1, u_2, \ldots, u_t$. The cardinality of vertices in caterpillar tree $T_n$ is $t+(t-2)l$. If $u, v \in T_n$, then

$$M_\circ(T_n) = \sum_{e=uv\in E(P_t)} |n_u - n_v| + \sum_{u\in V(P_t), v\in V(b_i)} |n_u - n_v|. \tag{2.15}$$

Suppose $t$ is even and consider

$$
\begin{aligned}
&\sum_{e=uv\in E(P_t)} |n_u - n_v| \\
= \;& |0-(t-2)l+(t-2)| + |(t-(t-1))l+(t-(t-1))-(t-3)l+(t-3)| \\
& +|(t-(t-2))l+(t-(t-2))-(t-4)l+(t-4)| + \cdots + |(t-2)l+(t-2)-0| \\
= \;& \sum_{i=o}^{\frac{t}{2}-2}(((t-(t-i))l+(t-(t-i)))-(t-(i+2))l+(t-(i+2))) \\
& + \sum_{i=o}^{\frac{t}{2}-2}((t-(i+2))l+(t-(i+2))-((t-(t-i))l+(t-(t-i)))) \\
= \;& 2\sum_{i=o}^{\frac{t}{2}-2}((t-(i+2))l+(t-(i+2))-((t-(t-i))l+(t-(t-i)))) \\
= \;& \frac{1}{2}lt^2 - lt + \frac{1}{2}t^2 - t. \qquad (2.16)
\end{aligned}
$$

Similarly, if $t$ is odd, then

$$
\begin{aligned}
\sum_{e=uv\in E(P_t)} |n_u - n_v| &= 2\sum_{i=o}^{\frac{t-3}{2}}((t-(i+2))l+(t-(i+2))-((t-(t-i))l+(t-(t-i)))) \\
&= \frac{1}{2}lt^2 - lt + \frac{1}{2}l + \frac{1}{2}t^2 - t + \frac{1}{2}. \qquad (2.17)
\end{aligned}
$$

Now consider

$$
\begin{aligned}
\sum_{u\in V(P_t), v\in V(b_i)} |n_u - n_v| &= |(((t-3)l+(t-1)+(l-1))l)(t-2)| \\
&= l^2t^2 - 4l^2t + lt^2 + 4l^2 - 4lt + 4l. \qquad (2.18)
\end{aligned}
$$

For odd $t$, putting Equations (2.17) and (2.18) in (2.15), we get

$$M_\circ(T_n) = (t^2-4t+4)l^2 + (\frac{3}{2}t^2 - 5t + \frac{9}{2})l + (\frac{1}{2}t^2 - t + \frac{1}{2}).$$

For even $t$, putting Equations (2.16) and (2.18) in (2.15), we yield

$$M_\circ(T_n) = (t^2-4t+4)l^2 + (\frac{3}{2}t^2 - 5t + 4)l + (\frac{1}{2}t - 1)t.$$

The line graph $L_{T_n}$ is a maximal sequence of complete graphs $K_{l+2}$, i.e., $K_1, K_2, \ldots, K_{t-2}$ in which each $K_i$ has a vertex next to a vertex of $K_{i+1}$ $(1 \le i \le t-3)$

(see Figure 4 ). If $u, v \in V(K_i)$ $(1 \leq i \leq t-2)$ and $u, v \notin V(K_i) \cap V(K_{i+1})$ $(1 \leq i \leq t-3)$, then

$$\sum_{e=uv\in E(K_i),uv\notin V(K_i\cap k_{i+1})} |n_u - n_v| = 0 \tag{2.19}$$

because it is a vertex-transitive. Now let $u \in V(K_i) \cap V(K_{i+1})$ $(1 \leq i \leq t-3)$, $v \in V(K_i)$ $(1 \leq i \leq t-2)$ and $t$ is odd then

$$\begin{aligned}
& \sum_{e=u\in V(K_i)\cap V(K_{i+1})v\in K_i} |n_u - n_v| \\
= \ & (l|(l+1)(t-3)| + l|(l+1)| + |(l+1) - (l+1)(t-4)|) + (l|(l+1)(t-4)| \\
& + l|2(l+1)| + |2(l+1) - (l+1)(t-5)|) + \cdots \\
= \ & 2(l+1)|(l+1)(t-3)| + 2l\sum_{i=4}^{\frac{t+1}{2}} |(l+1)(t-i)| + \sum_{i=1}^{\frac{(t-3)}{2}} l|i(l+1)| \\
& + 2\sum_{i=1}^{\frac{t-5}{2}} |(l+1)(t-(i+3)) - i(l+1)| \\
= \ & (t^2 - 5t + 6)l^2 + (\frac{3}{2}t^2 - 7t + \frac{15}{2})l + (\frac{1}{2}t^2 - 2t + \frac{3}{2}).
\end{aligned} \tag{2.20}$$

Now adding Equations (2.19) and (2.20), we get

$$M_\circ(L_{T_n}) = (t^2 - 5t + 6)l^2 + (\frac{3}{2}t^2 - 7t + \frac{15}{2})l + (\frac{1}{2}t^2 - 2t + \frac{3}{2}).$$

Similarly, let $u, v \in L(T_n)$ and $t$ is even, then

$$\begin{aligned}
M_\circ(L_{T_n}) \ = \ & 2(l+1)|(l+1)(t-3)| + 2l\sum_{i=4}^{\frac{t}{2}+1} |(l+1)(t-i)| \\
& + \sum_{i=1}^{\frac{t}{2}-2} l|i(l+1)| + 2\sum_{i=1}^{\frac{t}{2}-2} |(l+1)(t-(i+3)) - i(l+1)| \\
= \ & (t^2 - 5t + 6)l^2 + (\frac{3}{2}t^2 - 7t + 8)l + (\frac{1}{2}t^2 - 2t + 2). \qquad \square
\end{aligned}$$

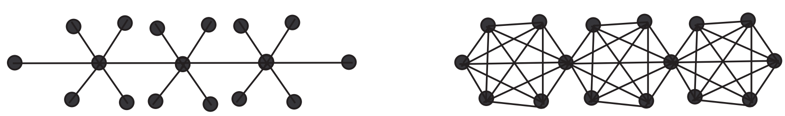

**Figure 4.** **A caterpillar tree and its line graph.**

**Remark 3.** Let $C_b := C_{b_2,b_3,\ldots,b_{n-1}}$ (or simply $T_n$) be a caterpillar tree and $b_2 = b_3 = \cdots = b_{n-1} = l$. Then

$$M_\circ(T_n) = M_\circ(L_{T_n}) + l^2(t-2) + (2t-3)l + (t-1); \text{ if } t \text{ is odd.}$$

$$M_\circ(T_n) = M_\circ(L_{T_n}) + l^2(t-2) + (2t-4)l + (\frac{1}{2}t^3 - \frac{1}{2}t^2 + t - 2); \text{ if } t \text{ is even.}$$

Let $P_n$, $K_n$ denote the path and complete graph with order $n$, respectively. It is clear that $L_{P_n} = P_n - 1$.

**Theorem 4.** *Suppose $T$ is a tree with $n$ vertices and $n > 2$. Then $M_\circ(L_T) < M_\circ(T)$.*

*Proof.* Let $T$ be a tree with $n$ vertices. The line graph $L_T$ of $T$ is defined such that each vertex of $L_T$ represents an edge of $T$, and two vertices of $L_T$ are adjacent if and only if their corresponding edges in $T$ share a common vertex.
Since $E(T) = V(L_T)$, each vertex $v$ of $T$ with degree $d_v$ gives rise to a complete graph $K_{d_v}$ in $L_T$. Specifically, every edge of $L_T$ is counted exactly once because two edges of $T$ intersect at most once.
The line graphs of trees are block graphs where each block corresponds to the star subgraph induced by the edges incident to each vertex of $T$. Each block in $L_T$ is a complete subgraph $K_{d_v}$ for some vertex $v$ in $T$ (see Figure 5).
Consider the structure of $L_T$. Each block $K_{d_v}$ in $L_T$ has a Mostar index of zero because $M_\circ(K_n) = 0$ for any complete graph $K_n$. The only contributions to the Mostar index of $L_T$ come from the cut vertices that connect different blocks.
In contrast, the Mostar index of the tree $T$ depends on the differences in path lengths between pairs of vertices across all edges. Since $T$ is acyclic and more sparse compared to its line graph, there are more significant variations in path lengths, resulting in a higher Mostar index.
Therefore, for any tree $T$ with $n > 2$, the Mostar index of its line graph $L_T$ is less than the Mostar index of $T$, formally, $M_\circ(L_T) < M_\circ(T)$.
This conclusion is supported by the fact that the structure of $L_T$ minimizes the differences in path lengths due to its block graph nature, reducing the overall Mostar index compared to the original tree $T$. □

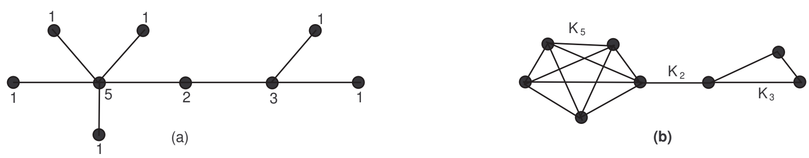


Figure 5. Illustration of a tree and its corresponding line graph. (a) A tree structure. (b) The line graph derived from the tree.

## 3. Computational Verification of the Theorem

To further substantiate the theoretical proof, we calculated the Mostar index for all trees with fewer than 9 vertices and their corresponding line graphs using a computer program. The results are presented below (see Figure 6 and Table 1), demonstrating that for each tree, the Mostar index of its line graph is consistently less than the Mostar index of the tree itself.

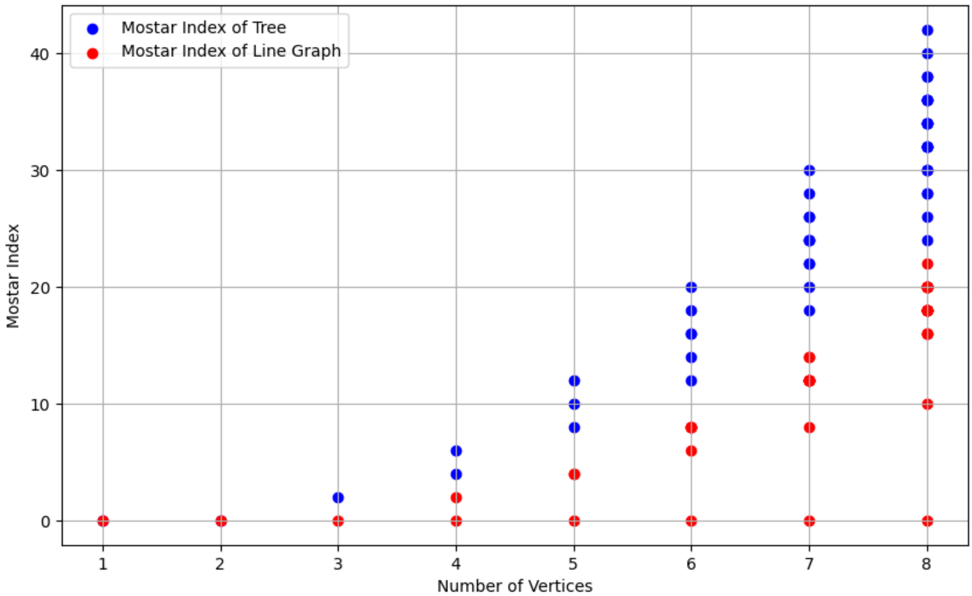


**Figure 6.** **Mostar index of trees and their line graphs.**

Table 1: Mostar index of trees and their line graphs with fewer than 9 vertices.

| Vertices | $M_\circ(T)$ | $M_\circ(L_T)$ | Vertices | $M_\circ(T)$ | $M_\circ(L_T)$ |
|---|---|---|---|---|---|
| 1 | 0 | 0 | 7 | 30 | 0 |
| 2 | 0 | 0 | 7 | 28 | 8 |
| 3 | 2 | 0 | 7 | 26 | 12 |
| 4 | 6 | 0 | 7 | 26 | 12 |
| 4 | 4 | 2 | 7 | 24 | 12 |
| 5 | 12 | 0 | 7 | 24 | 14 |
| 5 | 10 | 4 | 7 | 24 | 12 |
| 5 | 8 | 4 | 7 | 22 | 14 |
| 6 | 20 | 0 | 7 | 22 | 12 |
| 6 | 18 | 6 | 7 | 20 | 12 |
| 6 | 16 | 8 | 7 | 18 | 12 |
| 6 | 16 | 8 | 8 | 42 | 0 |
| 6 | 14 | 8 | 8 | 40 | 10 |
| 6 | 12 | 8 | 8 | 38 | 16 |
| 8 | 38 | 16 | 8 | 36 | 16 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 36 | 18 | 8 | 36 | 20 |
| 8 | 34 | 20 | 8 | 32 | 18 |
| 8 | 30 | 18 | 8 | 34 | 20 |
| 8 | 34 | 20 | 8 | 32 | 22 |
| 8 | 32 | 20 | 8 | 30 | 20 |
| 8 | 30 | 20 | 8 | 28 | 20 |
| 8 | 28 | 20 | 8 | 28 | 18 |
| 8 | 26 | 18 | 8 | 24 | 18 |

The computational process involved three main algorithms. The Algorithm 1 calculates the Mostar Index of a given graph by iterating through each edge and summing the absolute differences in the number of vertices that are closer to one endpoint of the edge than the other. The Algorithm 2 generates all unique trees with a specified number of vertices by constructing graphs from all possible combinations of edges and retaining those that form trees and are not isomorphic to any previously generated tree. The Algorithm 3 uses the previous two algorithms to collect and compute the Mostar Index for all unique trees with up to 10 vertices and their corresponding line graphs, storing the results in a DataFrame for analysis.

**Algorithm 1** Calculate Mostar Index of a Graph

**Input:** Graph $G$<br>
**Output:** Mostar Index of $G$<br>
Initialize `mostar` to 0<br>
**for** each edge $(u, v)$ in $G$ **do**<br>
    Compute $n_u = \sum_{w \in G}[\text{shortest\_path\_length}(G, u, w) < \text{shortest\_path\_length}(G, v, w)]$<br>
    Compute $n_v = \sum_{w \in G}[\text{shortest\_path\_length}(G, v, w) < \text{shortest\_path\_length}(G, u, w)]$<br>
    Update `mostar` by adding $|n_u - n_v|$<br>
**end for**<br>
**return** `mostar`

**Algorithm 2** Generate All Unique Trees with $n$ Vertices

**Input:** Number of vertices $n$<br>
**Output:** List of unique trees with $n$ vertices<br>
**if** $n == 1$ **then**<br>
    **return** list containing a single graph with one self-loop edge<br>
**else**<br>
    Initialize an empty list `trees`<br>
    **for** each set of $n - 1$ edges from the combination of $\binom{n}{2}$ edges **do**<br>
        Create a graph `graph` from these edges<br>
        **if** `graph` is a tree and is not isomorphic to any tree in `trees` **then**<br>
            Add `graph` to `trees`<br>
        **end if**<br>
    **end for**<br>
    **return** `trees`<br>
**end if**

**Algorithm 3** Collect and Compute Mostar Index for Trees and Their Line Graphs

```
Input: Range of number of vertices 1 to 8
Output: DataFrame containing Mostar indices for trees and their line graphs
Initialize an empty list results
for n in range 1 to 8 do
    Generate all unique trees with n vertices
    for each tree in generated trees do
        Compute mostar_tree = Calculate Mostar Index of tree
        Compute line graph of tree
        Compute mostar_line_graph = Calculate Mostar Index of line graph
        Append (n, mostar_tree, mostar_line_graph) to results
    end for
end for
Convert results to DataFrame with columns ["Vertices", "Mostar_Tree", "Mostar_Line_Graph"]
return DataFrame
```

## 4. Conclusion

This work presents an analysis of Mostar index of the line graph of trees. Specifically, the mostar index of trees and their line graphs for special types of trees are computed, and it proved that $M_\circ(L_T) < M_\circ(T)$. It seems to be true for all other classes of graphs except the cycle graph and complete graph. The line graph of $C_n$ is another cycle graph $C_n$, so $L_{C_n}$ and $C_n$ are isomorphic to each other. The line graph $L_{K_n}$ is another regular graph on $\frac{n(n-1)}{2}$ vertices, where the degree of each vertex is $2n-4$. So the Mostar index for these two particular classes of graphs and their line graphs are equal. To further substantiate our theoretical findings, we execute computational verification by Python, where the proposed algorithms are implemented to calculate the Mostar index for all trees with fewer than 9 vertices and their corresponding line graphs. The computational results consistently supported our theoretical proof.
Based on our study, we propose the following conjecture for further investigation.

**Conjecture 5.** Let $G$ be a simple connected graph on $n$ vertices. Then

$$M_\circ(L_G) \leq M_\circ(G).$$

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