Minimizing Degree-based Topological Indices for Trees with Given Number of Pendent Vertices

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Abstract

We derive sharp lower bounds for the first and the second Zagreb indices ($M_1$ and $M_2$ respectively) for trees with the given number of pendent vertices and find optimal trees. $M_1$ is minimized by a tree with all internal vertices having degree 4, while $M_2$ is minimized by a tree where each “stem” vertex is incident to 3 or 4 pendent vertices and one internal vertex, while the rest internal vertices are incident to 3 other internal vertices. The technique is shown to generalize to the weighted first Zagreb index, the zeroth order general Randić index, as long as to many other degree-based indices.

Introduction

Topological graph indices are widely used in mathematical chemistry to predict properties of chemical compounds. They have been intensively studied in recent years. Dozens of various indices were suggested [1] to describe topology of complex molecules, among the earliest and the most famous being the first and the second Zagreb indices – $M_1$ and $M_2$ respectively [9].

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The popular research problem is to find lower and upper bounds of an index over a certain set of graphs and to characterize extremal graphs in this set.

The typical set to study is that of all graphs (trees, bipartite or unicyclic graphs, “cacti”, etc) of the fixed order (i.e. with the fixed number of vertices). Extremal graphs on these sets often appear to be degenerate. For example, the chain minimizes Zagreb indices, while the star maximizes them over the set of trees of order $N$ (see [4, 10]). Even when the set of admissible graphs is cut (by limiting degrees, chromatic or matching numbers, etc), extremal graphs are typically found on the “boundary” of the set. For instance, the “broom” (i.e., the star $K_{1,\Delta}$ with the path of length $N - \Delta - 1$ attached to any pendant vertex) minimizes $M_2$ over the set of trees with the fixed maximum degree $\Delta$ (see [16]), the path of length $N - k$ attached to the cycle of length $k$ minimizes both $M_1$ and $M_2$ over the set of all unicyclic graphs of order $N$ and girth $k$ (see [5]), etc.

We optimize indices over the set of trees with the fixed number of pendant vertices. If hydrogen atoms are not suppressed from Sachs diagrams [15], this set can be interpreted as that of all acyclic molecules with the fixed number of hydrogen atoms. In hydrogen-suppressed diagrams of paraffins pendant vertices stand for methyl groups $\text{CH}_3$.

This set of graphs is of interest as it provides a “vertex-number vs degree” trade-off for degree-based indices, resulting in optimality of nontrivial internal solutions. Note that such “internal” solutions do not arise even when one studies the set of graphs parameterized by the number of pendant vertices $n$ and the total number of vertices $N$. For example, the star $K_{1,n}$ with $n$ (roughly equal) paths attached to its rays maximizes $M_2$ over the set of trees with fixed $n$ and $N$ [13]. The root of the star in this graph has the maximum possible degree $n$ while all other internal vertices have the minimum possible degree 2. Unicyclic graphs with minimum possible vertex degrees (no more than 3) minimize both $M_1$ and $M_2$ over the set of “cacti” with fixed $n$ and $N$ [12]. For more results on extremal trees with fixed $N$ and $n$ for the Randić index (which is closely related to $M_2$) one can refer to [14].

Below we show that in the tree minimizing $M_1$ over the set of all trees with $n$ pendant vertices almost all internal vertices have degree 4, which is strictly greater than the minimum possible degree 3 but less than the maximum possible degree $n$. We also show that in a tree, which minimizes $M_2$, internal vertices have degrees 3, 4 and 5. Even more surprising structures are shown to minimize the generalized Randić index or the multiplicative Zagreb indices $\Pi_1$ and $\Pi_2$. 

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1 The First Zagreb Index

Let $G$ be a simple connected undirected graph with the vertex set $V(G)$ and the edge set $E(G)$. Denote by $d_G(v)$ the degree of a vertex $v \in V(G)$ in the graph $G$, i.e., the number of vertices being incident to $v$ in $G$. The first Zagreb index is defined in [9] as

$$M_1(G) := \sum_{v \in V(G)} d_G(v)^2,$$  \hspace{1cm} (1)

while the second Zagreb index – as

$$M_2(G) := \sum_{uv \in E(G)} d_G(u)d_G(v).$$  \hspace{1cm} (2)

The vertex $v \in V(G)$ with $d_G(v) = 1$ is called a pendent vertex. Denote the set of pendent vertices of the graph $G$ with $W(G)$. A connected graph $T$ with $N$ vertices and $N - 1$ edges is called a tree.

**Theorem 1** For any tree $T$ with $n \geq 2$ pendent vertices $M_1(T) \geq 9n - 16$ if $n$ is even. The equality holds if $T$ is a 4-tree (with $d_T(m) = 4$ for all $m \in V(G) \setminus W(G)$). If $n$ is odd, then $M_1(T) \geq 9n - 15$, and the equality holds if $T$ is a tree with all internal vertices having degree 4 except the one of degree 3.

**Proof** For $n = 2$ the optimal tree is the complete graph $K_2$, and the theorem obviously holds. If $n > 2$, there must be at least one internal vertex in a tree.

Note that the tree $T$ cannot minimize $M_1(T)$ over the set of all trees with $n$ vertices if it contains an internal vertex of degree 2. Actually, the index is reduced by eliminating such a vertex and shortcutting its incident vertices. So, below we restrict attention to the trees with internal vertex degrees at least 3.

For an arbitrary tree with $n > 2$ pendent vertices and $q > 0$ internal vertices of degrees $d_1, ..., d_q$ the following identity holds:

$$n - 2 = \sum_{i=1}^{q} (d_i - 2).$$  \hspace{1cm} (3)

Thus, minimization of $M_1$ for fixed $n$ and $q$ reduces to minimization of $n1^2 + \sum_{i=1}^{q} d_i^2$ over all $d_i = 3, 4, ..., i = 1, ..., q$ satisfying (3). Ignoring integer
constraints from the first order conditions we obtain an obvious solution of this convex program: \( d_i = 2 + (n - 2)/q \) for all \( i = 1, \ldots, q \). Then, to find optimal \( q \) we minimize \( n + q(2 + (n - 2)/q)^2 \) over all \( q = 1, \ldots, n - 2 \) (the range follows from (3)). Relaxing the integer constraint from the first order condition find optimal \( q = (n - 2)/2 \) and \( d_i = 4 \). Thus, as we relaxed some integer constraints during minimization, \( M_1(T_{\text{even}}) = 9n - 16 \). It follows from (3) that the tree \( T_{\text{even}} \) with \( q = (n - 2)/2 \) internal vertices of degree 4 exists for even \( n \). An obvious calculation gives \( M_1(T_{\text{even}}) = 9n - 16 \).

For odd \( n \) it follows from (3) that no 4-tree exists and, thus, the lower-bound estimate \( 9n - 16 \) cannot be achieved. At the same time, there exists a tree \( T_{\text{odd}} \) with all internal vertices having degree 4 except the one of degree 3 with \( M_1(T_{\text{odd}}) = 9n - 15 \). As the index \( M_1 \) is integer-valued, \( T_{\text{odd}} \) is optimal for odd \( n \).

The above theorem says that, at least in the considered stylized setting, carbon of valency 4 is the best connector for any given number of hydrogen atoms (if hydrogen atoms are not suppressed from the molecular graph) or methyl groups \( \text{CH}_3 \) (in hydrogen-suppressed diagrams) in terms of minimization of the first Zagreb index. In both cases \( M_1 \) is minimized by alkanes \( \text{C}_m\text{H}_{2m+2} \).

Let us account for heterogeneity of atoms by adding to every term \( d_G(v)^2 \) in \( M_1(G) \) a weight depending on the vertex degree (the valency of an atom in a molecule). The following theorem gives the lower bound for the generalized index \( C(G) := \sum_{v \in V(G)} c(d_G(v)) \), where \( c(\cdot) \) is an arbitrary non-negative function of the vertex degree. As we minimize \( C(G) \), it is natural to call it the cost of the graph \( G \), and to call \( c(d_G(m)) \) the cost of the vertex \( m \) in the graph \( G \).

**Theorem 2** For \( n \geq 2 \)

\[
C(T) \geq C(n) := nc(1) + (n - 2) \frac{c(\Delta(n))}{\Delta(n) - 2} \tag{4}
\]

for an arbitrary tree \( T \) with \( n \) pendant vertices, where

\[
\Delta(2) = 3, \Delta(n) \in \text{Argmin}_{d=3,\ldots,n} \frac{c(d)}{d - 2} \text{ for } n > 2. \tag{5}
\]

When \( q(n) := \frac{n-2}{\Delta(n)-2} \) is integer, the equality in (4) is achieved at an arbitrary tree, where all internal vertices have degree \( \Delta(n) \). □
Proof Fix an arbitrary pendent vertex $w \in W(T)$ in a tree $T$. Then $C(T) = c(1) + \sum_{v \in V(T) \setminus \{w\}} c(d_T(v))$. Let us call the tree $T$ with the selected pendent vertex $w$ the attached tree with the root $w$ and define the cost of this attached tree as $C_a(T, w) := C(T) - c(1)$. So, the root is still a pendent vertex of an attached tree, but the cost of the root is not included in the cost of the attached tree. We will also refer to the vertex incident to the root as to the “sub-root”.

The set of trees with $n$ pendent vertices coincides with that of attached trees with $n$ pendent vertices, and their costs differ only by a constant. So, the problem of cost minimization for a tree with $n$ pendent vertices is equivalent to cost minimization for an attached tree with $n$ pendent vertices. Below we prove by induction that for any attached tree $T$ with $n \geq 2$ pendent vertices

$$C_a(T, \cdot) \geq C_a(n) := (n - 1)c(1) + (n - 2)\frac{c(\Delta(n))}{\Delta(n) - 2}. \tag{6}$$

For $n = 2$ (6) is satisfied as equality, as the optimal attached tree is a complete graph $K_2$ with $C_a(K_2, \cdot) = c(1)$ (remember the cost of the root is not counted). Suppose (6) is valid for all $n' < n$. Let us prove that it is also valid for any attached tree $T$ with $n$ pendent vertices and some root $w$.

As $n \geq 3$, the sub-root $m$ of $T$ is an internal vertex. So, the cost $C_a(T, w)$ can be written as the sum of the cost of the sub-root $m$ and costs of the sub-trees $T_1, ..., T_{d_T(m) - 1}$ with $n_1, ..., n_{d_T(m) - 1}$ pendent vertices respectively, attached to $m$:

$$C_a(T, w) = c(d_T(m)) + \sum_{i=1}^{d_T(m) - 1} C_a(T_i, m).$$

As $n_i < n$, by induction hypothesis

$$C_a(T, w) \geq c(d_T(m)) + \sum_{i=1}^{d_T(m) - 1} \left( (n_i - 1)c(1) + (n_i - 2)\frac{c(\Delta(n_i))}{\Delta(n_i) - 2} \right).$$

Note that from (5) follows that

$$\frac{c(\Delta(n_i))}{\Delta(n_i) - 2} \geq \frac{c(\Delta(n))}{\Delta(n) - 2},$$
and also that $n_1 + \ldots + n_{d_T(m)-1} = n + d_T(m) - 2$. Thus,

$$
C_a(T, w) \geq c(d_T(m)) + \sum_{i=1}^{d_T(m)-1} \left\{ (n_i - 1)c(1) + (n_i - 2)\frac{c(\Delta(n))}{\Delta(n) - 2} \right\} =
$$

$$
= (n - 1)c(1) + c(d_T(m)) + (n - d_T(m))\frac{c(\Delta(n))}{\Delta(n) - 2}. 
$$

(7)

Obviously, $3 \leq d_T(m) \leq n$, so

$$
C_a(T, w) \geq (n - 1)c(1) + \min_{d=3,\ldots,n} \left\{ c(d) + (n - d)\frac{c(\Delta(n))}{\Delta(n) - 2} \right\} =
$$

$$
(n - 1)c(1) + (n - 2)\frac{c(\Delta(n))}{\Delta(n) - 2} + \min_{d=3,\ldots,n} (d - 2) \left[ \frac{c(d)}{d - 2} - \frac{c(\Delta(n))}{\Delta(n) - 2} \right]. 
$$

(8)

From (5) we know that the expression in square brackets achieves its minimum (which is equal to zero) at $d = \Delta(n)$. So, the minimum of the product $(d - 2) \left[ \frac{c(d)}{d - 2} - \frac{c(\Delta(n))}{\Delta(n) - 2} \right]$ is also zero, and

$$
C_a(T, w) \geq (n - 1)c(1) + (n - 2)\frac{c(\Delta(n))}{\Delta(n) - 2}.
$$

So, inequality (4) is proved.

When $q(n) = \frac{n - 2}{\Delta(n) - 2}$ is integer, there exists a $\Delta(n)$-tree $T^*$ with $n$ pendant and $q(n)$ internal vertices, which has the cost $C(T^*) = nc(1) + q(n)c(\Delta(n)) = nc(1) + (n - 2)\frac{c(\Delta(n))}{\Delta(n) - 2} = C(n)$.

This completes the proof.

Example 1 The above theorem covers the first Zagreb index with $c(k) = k^2$ and the zeroth order general Randić index $c(k) = k^\alpha$ as special cases. In particular, using (4) one can show that for $\alpha \geq \ln 2/\ln(4/3)$ a 3-tree is optimal (and exists for all $n \geq 2$), while for

$$
\alpha \in \left[ \ln \left( \frac{d-1}{d-2} \right)/\ln \left( \frac{d+1}{d} \right), \ln \left( \frac{d-2}{d-3} \right)/\ln \left( \frac{d}{d-1} \right) \right]
$$

the optimal degree $\Delta(n) = d$, where $d = 4, 5, \ldots, \text{for } n \geq d$ (this means that $d$-tree is optimal for $n \geq d$ when such a tree exists). For $\alpha \leq 1$ the optimal tree is a star $K_{1,n}$, as $\frac{d^\alpha}{d-2}$ in (5) is monotone decreasing for $d \geq 3$.

\footnote{We use the scheme of the proof from [7], where the similar result was obtained for directed trees under a more general cost function.}
Example 2 The first and the second multiplicative Zagreb indices were defined in [11] as

\[ \Pi_1(G) := \prod_{v \in V(G)} d_G(v)^2, \]

\[ \Pi_2(G) := \prod_{uv \in E(G)} d_G(u)d_G(v). \]

Instead of summation, as in (1) and (2), contributions of vertices here (in the case of the first index) or edges (in the case of the second index) are multiplied.

Minimization of \( \Pi_1(G) \) reduces to minimization of

\[ C(G) := \ln \Pi_1(G) = 2 \sum_{v \in V(G)} \ln d_G(v). \]

From Theorem 2, as \( \frac{\ln d}{d-2} \) is monotone decreasing for \( d \geq 3 \), the tree with \( n \) pendent vertices minimizing \( \Pi_1 \) is a star \( K_{1,n} \).

It is shown in [11] that for an arbitrary tree \( T \)

\[ \Pi_2(T) = \prod_{v \in V(T)} d_T(v)^{d_T(v)}. \]

So, minimization of \( \Pi_2(T) \) for all trees with \( n \) pendent vertices is equivalent to minimization of \( C(T) := \ln \Pi_2(T) = \sum_{v \in V(T)} d_T(v) \ln d_T(v) \). Set \( c(d) = d \ln d \ln d \) in (5) and obtain \( \Delta(n) = \min[n, 5] \). Then, from (4) we see that \( \Pi_2(T) = \exp(C(T)) \geq \exp \left( \frac{5 \ln 5}{3} (n-2) \right) \) for \( n \geq 5 \) with equality at any 5-tree when \( (n-2)/3 \) is integer.

When \( \frac{n-2}{\Delta(n)-2} \) is not integer, there exists no \( \Delta(n) \)-tree with \( n \) pendent vertices, and the lower bound (4) is not sharp. Nevertheless, for every specific function \( c(d) \) one often can prove the optimal tree to be a some minimal perturbation of the \( \Delta(n) \)-tree. Typically the optimal tree is a bidegree tree, where almost all internal vertices have degree \( \Delta(n) \), while several vertices have degree \( \Delta(n) + 1 \) or \( \Delta(n) - 1 \) (like in Theorem 1).

## 2 The Second Zagreb Index

An internal vertex in a tree is called a stem vertex if it has incident pendent vertices (see [3]). The edge connecting a stem with a pendent vertex will be referred to as a stem edge.
Theorem 3. For any tree $T$ with $n \geq 8$ pendent vertices $M_2(T) \geq 11n - 27$. The equality holds if each stem vertex in $T$ has degree 4 or 5 while other internal vertices having degree 3. At least one such tree exits for any $n \geq 9$. □

Proof. Let us employ again the idea of an attached tree from Theorem 2. Below we suggest a suitable generalization of the concept of an attached tree, then we interrelate its cost with $M_2$, and, finally, use induction on $n$ to prove the lower bound. The cost of trees, which minimize $M_2$, is found by a direct calculation.

Let us allow the root of an attached tree to have arbitrary degree $p \geq 1$. Actually we do not add vertices incident to the root – it is still incident only to the sub-root – but the degree of the root is substituted to the contribution of the edge $wm$ connecting the root $w$ with the sub-root $m$ to the index $M_2$. For the attached tree $T$ with the root $w$ of degree $p$ and the sub-root $m$ of degree $d$ define its cost as

$$C_a(T, w, p) := pd + \sum_{uv \in E(T)\setminus\{wm\}} d_T(u)d_T(v). \quad (9)$$

We will consider the root as a pendent vertex only when its degree $p = 1$. Note that it implies the following interrelation between $M_2(T)$ and the cost of the attached tree $T$ with an arbitrary root $w \in W(T)$: $M_2(T) = C_a(T, w, 1)$. So, the problem of minimization of $M_2$ over the set of all trees with $n$ pendent vertices is equivalent to the problem of minimization of the cost of an attached tree with $n$ vertices and the root of degree 1.

First we use induction to show that for any attached tree $T$ with $n$ pendent vertices and some root $w$ of degree $p \geq 3$

$$C_a(T, w, p) \geq \begin{cases} p, & \text{if } n = 1, \\ 11n + 3p - 18, & \text{if } n \geq 2. \end{cases} \quad (10)$$

Note, that, as before, we can restrict attention to the trees where all internal vertices (including the root) have degree at least 3. For $n = 1$ the inequality (10) trivially holds as the only attached tree has only one edge. From (9), its cost is $p$.

Suppose inequality (10) holds for all $n' < n$. Let us prove that it also holds for $n$. As $n \geq 2$, the sub-root of any attached tree is an internal vertex. Consider a tree $T$ with some root $w$ of degree $p \geq 3$ and the sub-root $m$ of degree $d \geq 3$ having $\delta \geq 0$ incident pendent vertices and $\Delta \geq 0$ incident
internal vertices. Note that $d = \delta + \Delta + 1$ and $3 \leq d \leq n+1$. The cost of the attached tree $T$ consists of the cost $pd$ of the edge $mw$, the total cost $\delta d$ of $\delta$ pendent vertices being incident to $m$, and the sum of costs of $\Delta$ sub-trees $T_1, \ldots, T_\Delta$ attached to $m$: $C_a(T, w, p) = pd + \delta d + \sum_{i=1}^{\Delta} C_a(T_i, m, d)$.

To estimate $C_a(T, w, p)$ consider separately the case of $\Delta = 0$ and that of $\Delta > 0$:

1. If $\Delta = 0$ then $T = K_{1,n+1}$ with $\delta = n$ and $d = n+1$, so $C_a(K_{1,n+1}, w, p) = (p + n)(n + 1)$. Denote $C_1 := (p + n)(n + 1)$ for short.

2. Suppose $\Delta \geq 1$ and let the tree $T_i$ have $n_i \geq 2$ pendent vertices, $i = 1, \ldots, \Delta$. As $2 \leq n_i < n$, by induction hypothesis $C_a(T_i, m, d) \geq 11n_i + 3d - 18$. Taking into account the balance equation $\sum_{i=1}^{\Delta} n_i = n - \delta$, we can estimate the cost of the attached tree from below:

$$C_a(T, w, p) \geq pd + \delta d + 11n - 11\delta + 3(d - \delta - 1)(d - 6) = 11n + pd + \delta(7 - 2d) + 3(d - 1)(d - 6). \quad (11)$$

As $n_i \geq 2$, it follows that $3 \leq d \leq n$. Also, from $\Delta \geq 1$ and from $d = \delta + \Delta + 1$ it follows that $0 \leq \delta \leq d - 2$. Let us find $d$ and $\delta$ which minimize the right-hand side (r.h.s.) in (11). Below we consider separately the case of $d = 3$ and that of $d \geq 4$:

- If $d = 3$ then $7 - 2d > 0$, and r.h.s in (11) achieves minimum at $\delta = 0$ and equals $11n + 3p + 3(d - 1)(d - 6)$, which reduces to $C_2 := 11n + 3p - 18$.

- If $d \geq 4$ then $7 - 2d < 0$, so r.h.s. in (11) achieves its minimum at $\delta = d - 2$, and equals $11n + pd + d^2 - 10d + 4$. For $p \geq 3$ and $d \geq 4$ this expression is monotone in $d$ and, thus, r.h.s in (11) is not less than $11n + 4p - 20$, which is greater than $C_2$ for $p \geq 3$.

So, we conclude that if $\Delta \geq 1$, then $C_a(T, w, p) \geq C_2 = 11n + 3p - 18$.

Let us compare cases 1 and 2 and prove that $C_1$ is never less than $C_2$ for $n \geq 2$ and $p \geq 3$. Actually, the difference $C_1 - C_2 = p(n - 2) - 10n + n^2 + 18$ is monotone in $p$, and, thus, achieves its minimum at $p = 3$. Substituting $p = 3$ we find that $C_1 - C_2 \geq n^2 - 7n + 12$, which is non-negative for all integer $n$. 

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So, we proved inequality (10). Let us use it now to prove that for $p = 1$ and $n \geq 9 \ C_a(T, w, 1) \geq 11n - 27$.

For $n \geq 3$ in the attached tree $T$ with $n$ pendent vertices (including the root $w$, as $p = 1$) the sub-root $m$ is an internal vertex. Let the sub-root $m$ have degree $d \geq 3$ which adds up from $\delta \geq 1$ incident pendent vertices (including the root) and $\Delta \geq 0$ internal vertices.

The cost of the attached tree $T$ consists of the total cost $\delta d$ of $\delta$ pendent vertices incident to $m$ and the sum of costs of $\Delta$ sub-trees $T_1, \ldots, T_\Delta$ attached to the sub-root $m$: $C_a(T, w, 1) = \delta d + \sum_{i=1}^{\Delta} C_a(T_i, m, d)$.

1. If $\Delta = 0$, then $T = K_{1,n}$ with $\delta = d = n$, so $C_a(K_{1,n}, w, 1) = n^2$.

2. Suppose $\Delta \geq 1$ and let the tree $T_i$ have $n_i \geq 2$ pendent vertices, $i = 1, \ldots, \Delta$. As $n_i \geq 2$ and $d \geq 3$, from (10) $C_a(T_i, m, d) \geq 11n_i + 3d - 18$.

Accounting for the balance equalities $\sum_{i=1}^{\Delta} n_i = n - \delta$ and $\delta + \Delta = d$, we estimate the cost of the attached tree as

$$C_a(T, w, 1) \geq \delta d + 11n - 11\delta + 3(d - \delta)(d - 6) =$$

$$= 11n + \delta(7 - 2d) + 3d(d - 6) \quad (12)$$

As $n_i \geq 2$, it follows that $3 \leq d \leq n - 1$. Also recall that $1 \leq \delta \leq d - 1$. Let us minimize r.h.s. in (12) over all $d \geq 3, n - 1$ and $\delta = 1, d - 1$.

The arguments are similar to that in the case of $p \geq 3$:

- If $d = 3$, then $7 - 2d > 0$ and r.h.s. in (12) achieves its minimum $11n - 26$ at $\delta = 1$.
- If $d \geq 4$, then $7 - 2d < 0$ and r.h.s. in (12) achieves minimum $11n + (d - 1)(7 - 2d) + 3d(d - 6) = 11n + d^2 - 9d - 7$ at $\delta = d - 1$.

Minimum of $11n + d^2 - 9d - 7$ over all integer $d$ is achieved at $d = 4$ and $d = 5$ and is equal to $11n - 27$. This is one less than $11n - 26$ which we had in the previous case of $d = 3$.\footnote{This point in the proof is mentioned below in the discussion as a clue to the result for chemical graphs.}

So, finally we conclude that if $\Delta \geq 1$, then $C_a(T, w, 1) \geq 11n - 27$.\footnote{This point in the proof is mentioned below in the discussion as a clue to the result for chemical graphs.}
Combining cases 1 and 2 we obtain the estimate $C_a(T, w, 1) \geq \min\{n^2, 11n - 27\}$. For $n \geq 8$ $n^2 > 11n - 27$, so the inequality $M_2(T) = C_a(T, w, 1) \geq 11n - 27$ holds.

For $n < 8$ $n^2 < 11n - 27$ and, thus, the optimal tree is a star $K_{1,n}$. Let us prove that for any tree $T_{4,5}$ with $n \geq 9$ pendent vertices, in which stem vertices have degrees 4 or 5 while the rest internal vertices having degree 3, $M_2(T_{4,5}) = 11n - 27$. Consider such a tree with $s_4$ stem vertices of degree 4 and $s_5$ stem vertices of degree 5. Each pendent vertex is assigned to some stem, so the balance equation $3s_4 + 4s_5 = n$ holds. Note that for any $n \geq 9$ $s_4 \geq 0$ and $s_5 \geq 0$ can be chosen to fulfill the balance, so the tree $T_{4,5}$ does exist for $n \geq 9$.

The edge set $E(T_{4,5}) = S_4 \cup S_5 \cup E_4 \cup E_5 \cup E_I$, where:

- $S_4$ is the set of stem edges incident to stem vertices of degree 4,
- $S_5$ is the set of stem edges incident to stem vertices of degree 5,
- $E_4$ is the set of edges connecting stem vertices of degree 4 to internal vertices,
- $E_5$ is the set of edges connecting stem vertices of degree 5 to internal vertices,
- $E_I$ is the set of edges connecting non-stem internal vertices.

Obviously, $|S_4| = 3s_4$ and, according to (2), each edge makes the contribution of 4 to the index $M_2(T_{4,5})$, $|S_5| = 3s_4$ and each edge from $S_5$ makes the contribution of 5. $|E_4| = s_4$ and, as any edge from $E_4$ connects the stem vertex of degree 4 with an internal vertex of degree 3, its contribution is 12. Similarly, the contribution of each of $s_5$ edges from $E_5$ is 15.

Finally, consider a “defoliated” tree $T_b$ obtained from $T_{4,5}$ by deleting all pendent vertices and stem edges. Stem vertices of $T_{4,5}$ become leaves in $T_b$ and $E(T_b) = E_4 \cup E_5 \cup E_I$. By construction, $T_b$ is a 3-tree with $s_4 + s_5$ pendent vertices, so it consists of $|V(T_b)| = 2s_4 + 2s_5 - 2$ vertices and $|E(T_b)| = 2s_4 + 2s_5 - 3$ edges. Thus, $|E_I| = |E(T_b)| - |E_4| - |E_5| = s_4 + s_5 - 3$. Each edge from $E_I$ connects two vertices of degree 3 and, thus, makes the contribution of 9 to $M_2(T_{4,5})$. Summing up all contributions we have:

$$M_2(T_{4,5}) = 4|S_4| + 5|S_5| + 12|E_4| + 15|S_5| + 9|E_I| = 33s_4 + 44s_5 - 27.$$  

Taking into account the balance equation $3s_4 + 4s_5 = n$ we finally obtain $M_2(T_{4,5}) = 11n - 27$ irrespective of the values of $s_4$ and $s_5$. ■
Theorem 3 provides trees which minimize $M_2$ over all trees with $n \geq 9$ pendent vertices. From the proof of Theorem 3 we know that for $n < 8$ the optimal tree is a star $K_{1,n}$. The optimal tree for $n = 8$ is shown in Fig. 1a.$^3$

![Image of trees](image-url)

Figure 1: The $M_2$-minimal tree and the second-best tree for $n = 8$

Theorem 3 says that for some $n$ the trees, which minimize $M_2$, are not chemical graphs. An example is shown in Fig. 1a. The optimal chemical tree for $n = 8$ is shown in Fig. 1b. This tree corresponds to trans-2-butene $C_4H_8$ if hydrogen atoms are not suppressed from the diagram or to triisobutylene $C_{12}H_{24}$ otherwise.

Actually, if $n \mod 3 = 1$, there should be at least one stem vertex of degree 5 in the optimal tree $T_{4,5}$, if $n \mod 3 = 2$, then at least two stem vertices of degree 5 are required to build the optimal tree $T_{4,5}$. From the proof of Theorem 3 one can conclude that the lower bound $11n - 27$ is not achievable with chemical graphs in these cases.

At the same time, for $n \mod 3 = 1$ replacement of the subtree rooted in the stem vertex of degree 5 with the subtree enclosed in a dashed circle in Fig. 1b gives a chemical graph with the value $M_2$, which is only one more than the lower bound $11n - 27$. This graph appears to be the optimal chemical graph when $n \mod 3 = 1$. Analogously, for $n \mod 3 = 2$ replacement of two stem vertices and their incident pendants with the fragment from Fig. 1b gives a chemical tree with $M_2 = 11n - 25$, yet this tree is not the best chemical tree for this $n$. The proof of Theorem 3 can be easily adopted to justify this claim (the footnote in the proof marks the place of possible adjustment) but

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$^3$We used a quasi-polynomial algorithm from [8] to enumerate attached trees.
one can better find a counterexample with direct enumeration of all optimal chemical graphs with the algorithm of complexity $n^4$ from [8]. Examples of optimal chemical trees for $n = 19$ and 20 are depicted in Fig. 2.

![Chemical trees for $n = 19, 20$](image)

Figure 2: Examples of chemical trees minimizing $M_2$ for $n = 19, 20$

### 3 Conclusion

Above we suggested an optimization framework for degree-based indices of undirected trees. Using the discussed approach one can calculate lower bounds for Zagreb-like indices and find the graphs minimizing these indices over the set of trees (or chemical trees) with the fixed number of pendent vertices.

Theorem 1 provides a tight lower-bound estimate for $M_1$ and shows that it is achieved at 4-trees. Theorem 2 gives a high-quality lower-bound estimate for the generalized $M_1$-like index. Theorem 3 proves the tight lower-bound estimate for $M_2$ and characterizes $M_2$-minimal trees.

Although one can surely suggest a simpler reasoning for theorems 2 and 3, the above proofs have an advantage, as they are open for generalization to other degree-based graph indices, e.g., to the general Randić index, which
is defined as \( R_\alpha(G) := \sum_{uv \in E(G)} d_G(u)^\alpha d_G(v)^\alpha \) (also known as \( \alpha \)-weight, see [2]), or even to the abstract degree-based topological index

\[
C(G) := \sum_{v \in V(G)} c_1(d_G(v)) + \sum_{uv \in E(G)} c_2(d_G(u), d_G(v)),
\]

where \( c_1(d) \) is a non-negative function of a natural argument and \( c_2(d_1, d_2) \) is a non-negative symmetric function of natural arguments. This index generalizes almost all known topological graph indices based on vertex degrees. As an example, one may employ the outline of the proof of Theorem 3 to justify the lower-bound estimate \( 61n/3 - 46 \) for the sum \( M_1 + M_2 \). This estimate holds for trees with the number of pendent vertices \( n \geq 6 \).

The proofs of theorems 2 and 3, in fact, appeal to the technique developed in [6, 7, 8] for directed trees with the fixed set of leaves. As the framework developed there is not limited to the case of degree-based topological indices, it seems promising to apply this approach to analyze trees with the fixed number of pendent vertices, which minimize complex topological indices: distance-based ones (like the Wiener index), or linear combinations of distance- and degree-based indices (some settings are provided in [13, 17]).

**References**


Erratum: Minimizing Degree-based Topological Indices for Trees with Given Number of Pendent Vertices

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Abstract

Theorem 3 in [1] says that the second Zagreb index $M_2$ cannot be less than $11n - 27$ for a tree with $n \geq 8$ pendent vertices. Yet the tree exists with $n = 8$ vertices (the two-sided broom) violating this inequality. The reason is that the proof of Theorem 3 relays on a tacit assumption that an index-minimizing tree contains no vertices of degree 2. This assumption appears to be invalid in general. In this erratum we show that the inequality $M_2 \geq 11n - 27$ still holds for trees with $n \geq 9$ vertices and provide the valid proof of the (corrected) Theorem 3.

Let $G$ be a simple connected undirected graph with the vertex set $V(G)$ and the edge set $E(G)$. Denote by $d_G(v)$ the degree of a vertex $v \in V(G)$ in the graph $G$, i.e., the number of vertices being incident to $v$ in $G$. The second Zagreb index is defined as

$$M_2(G) := \sum_{uv \in E(G)} d_G(u) d_G(v). \quad (1)$$

The vertex $v \in V(G)$ with $d_G(v) = 1$ is called a pendent vertex. All others are internal vertices. A connected graph $T$ with $N$ vertices and $N - 1$ edges is called a tree. An internal vertex in a tree is called a stem vertex if it has at most one incident internal vertex.

In [1] the following theorem was stated.

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Theorem 3 For any tree $T$ with $n \geq 8$ pendent vertices $M_2(T) \geq 11n - 27$. The equality holds if each stem vertex in $T$ has degree 4 or 5 while the other internal vertices have degree 3. At least one such tree exists for any $n \geq 9$.

However later a tree was found with $n = 8$ pendent vertices (the two-sided broom $D(4; 3; 4)$, see Fig. 1a) with $M_2(D(4; 3; 4)) = 60 < 11n - 27$. The inaccuracy in the proof of theorem 3 is originated from the following statement: “...as before, we can restrict attention to the trees where all internal vertices ... have degree at least 3...”. This assumption is not valid in general. For example, for 8 pendent vertices the $M_2$-minimizing tree is presented in Fig. 1a.

![Figure 1: Two-sided brooms](image)

Below we show that the statement of Theorem 3 is still valid for trees with $n \geq 9$ pendent vertices by proving the following corrected version of Theorem 3.

**Theorem 3** For any tree $T$ with $n \geq 9$ pendent vertices $M_2(T) \geq 11n - 27$. The equality holds if each stem vertex in $T$ has degree 4 or 5 while other internal vertices having degree 3. At least one such tree exists for any $n \geq 9$.

We will need the following auxiliary results. Below any tree minimizing $M_2$ over the set of all trees with $n$ pendent vertices is called optimal for short.

**Lemma 1** For any edge $vv' \in E(T)$ in an optimal tree $T$ with $n \geq 3$ pendent vertices either $d_T(v) \geq 3$ or $d_T(v') \geq 3$.

**Proof** Assume that, by contradiction, $d_T(v) = d \leq 2$ and $d_T(v') = d' \leq 2$. Either $d = 2$ or $d' = 2$, as otherwise $T = K_2$ and, thus, the tree $T$ cannot have $n \geq 3$ pendent vertices. With no loss of generality suppose that $d' = 2$, and, thus, $d \leq d'$. Let $v'' \in V(T)$ be the second vertex incident to $v'$, and define $d' := d_T(v'')$. Let us consider the tree $T'$
obtained from $T$ by deleting the internal vertex $v'$ with its incident edges and adding the edge $vv''$. Obviously, $M_2(T') - M_2(T) = dd'' - dd' - d'd''$, and from $d \leq d'$ we find that $M_2(T') - M_2(T) \leq -dd' < 0$. The trees $T$ and $T'$ have the same number of pendent vertices, so $T$ cannot be optimal. This contradiction completes the proof.

Lemma 2 In an optimal tree with $n \geq 8$ pendent vertices any internal vertex has at least one incident internal vertex.

Proof If the lemma is not valid, an optimal tree is a star $K_{1,n}$ with $M_2(K_{1,n}) = n^2$. Consider a two-sided broom $D(4;3;n-4)$ (see Fig. 1b) with $n$ pendent vertices and $M_2(D(4;3;n-4)) = n^2 - 5n + 36$. For $n \geq 8$ $M_2(D(4;3;n-4)) < M_2(K_{1,n})$, so $K_{1,n}$ cannot be optimal. This contradiction completes the proof.

Lemma 3 Any vertex degree is at most 6 in an optimal tree with $n \geq 8$ pendent vertices.

Proof Assume, by contradiction, that in an optimal tree $T$ some vertex $v \in V(T)$ has degree $d_T(v) = p > 6$. Let $v_1, \ldots, v_p$ be its incident vertices with degrees $d_1 \geq \ldots \geq d_p$ respectively. From Lemma 2 we know that $d_1 \geq 2$.

Let $T'$ be a tree obtained from $T$ by adding vertices $v'$ and $v''$, edges $vv'$ and $v'v''$, and redirecting edges $vv_i$, $i = 4, \ldots, p$, to the vertex $v''$ instead of $v$ (see Fig. 2).

Figure 2: Transformation of the vertex with degree $d \geq 6$

\[
\Delta := M_2(T') - M_2(T) = \sum_{i=1}^{3} 4d_i + 2 \cdot 4 + 2(p-2) + \sum_{i=4}^{p} (p-2)d_i - \sum_{i=1}^{p} pd_i = \\
= 2p + 4 - 2 \sum_{i=4}^{p} d_i - (p-4) \sum_{i=1}^{3} d_i. \quad (2)
\]

If $p \geq 7$ then $p-4 > 0$ in (2). From $d_1 \geq 2$, $d_i \geq 1$, $i = 2, \ldots, p$, it follows that $\sum_{i=1}^{3} d_i \geq 4$.

Thus, $\Delta \leq 2p + 4 - 2(p-3) - 4(p-4) = 26 - 4p < 0$. The trees $T$ and $T'$ have the same number of pendent vertices, so $T$ cannot be optimal. This contradiction completes the proof.
An attached tree is a rooted tree with a root being a pendent vertex parameterized with some “virtual degree” (degree of the vertex this tree is “attached” to). The vertex incident to the root is called a sub-root, and if the sub-root has degree 2, its incident vertex other than root is called a sub-sub-root. It will be convenient to consider the root as a non-pendent vertex.

The cost of an attached tree $T$ with some root $w$ of “virtual degree” $p$ and a sub-root $m$ of degree $d$ is defined as

$$C_a(T, w, p) := pd + \sum_{uv \in E(T) \setminus \{wm\}} d_T(u) d_T(v). \quad (3)$$

Consider a tree $T$ and fix any vertex $v \in V(T)$. If it has degree $p$ and incident vertices $v_1, ..., v_p$, then $T$ is a union of $p$ attached trees $T_1, ..., T_p$ with the common root $v$ and sub-roots $v_1, ..., v_p$, so $M_2(T) = \sum_{i=1}^{p} C_a(T_i, v, p)$. Below we limit attention to the attached trees, which can be met in optimal trees, so Lemmas 1, 2, and 3 are supposed to be valid for every attached tree in hand.

Let $T_a(n, p)$ be the collection of all attached trees with $n$ pendent vertices where the root (denoted with $w$) has degree $p \geq 2$ (remember the root is considered non-pendent), and introduce the cost of an optimal attached tree $C^*_a(n, p) = \min_{T \in T_a(n, p)} C_a(T, w, p)$.

**Lemma 4** For $n = 1$ $C^*_a(n, p) = p$, while for $n \geq 2$

$$C^*_a(n, p) = \min_{d=2, ..., 6, n_1, ..., n_{d-1}} \left\{ pd + \sum_{i=1}^{d-1} C^*_a(n_i, d) | n_i \geq 1, \sum_{i=1}^{d-1} n_i = n \right\}. \quad (4)$$

**Proof** The case of $n = 1$ is obvious. For $n \geq 2$ each combination of $d$ and $n_1, ..., n_{d-1}$ in the right-hand side of (4) gives rise to an attached tree with $n$ pendent vertices, the sub-root enjoying degree $d$ and being a root of $d - 1$ optimal attached trees with $n_1, ..., n_{d-1}$ pendent vertices respectively. So, $C^*_a(n, p)$ cannot exceed the right-hand side in (4).

Let an optimal attached tree $T$ with $n$ pendent vertices have a root $w$ and a sub-root $m$ of some degree $d^*$. Then $T$ is a union of the edge $wm$ and $d^* - 1 \geq 1$ attached sub-trees $T_1, ..., T_{d^* - 1}$ with the common root $m$. Let the trees $T_1, ..., T_{d^* - 1}$ have $n^*_1, ..., n^*_{d^* - 1}$ pendent vertices respectively. By definition, $C_a(T_i, m, d^*) \geq C_a(n^*_i, d^*)$. So,

$$C^*_a(n, p) = pd^* + \sum_{i=1}^{d^* - 1} C_a(T^*_i, m, d^*) \geq pd^* + \sum_{i=1}^{d^* - 1} C_a(n^*_i, d^*),$$

which is obviously not less than the right-hand side in (4).
Let us rewrite (4) as $C^*_a(n, p) = \min [C_{>2}(n, p), C_2(n, p)]$, where

$$C_{>2}(n, p) := \min_{d = 3, \ldots, 6, n_1, \ldots, n_{d-1}} \left\{ pd + \sum_{i=1}^{d-1} C^*_a(n_i, d) | n_i \geq 1, \sum_{i=1}^{d-1} n_i = n \right\},$$

(5)

$$C_2(n, p) := 2p + C^*_a(n, 2).$$

(6)

From Lemma 1, vertices of degree 2 cannot be incident in an optimal tree. So, if the root has degree 2 in an optimal attached tree, the sub-root must have some degree $d \geq 3$, and, thus, $C^*_a(n, 2) = C_{>2}(n, 2)$.

Now we are ready to prove Theorem 3$^*$.  

PROOF Let us prove the following estimate for the cost of an optimal attached tree:

$$C^*_a(n, p) \geq C_a(n, p) = \begin{cases} p & \text{if } n = 1, \\ 40 & \text{if } p = 5 \text{ and } n = 4, \\ 32 & \text{if } p = 6 \text{ and } n = 3, \\ 42 & \text{if } p = 6 \text{ and } n = 4, \\ 54 & \text{if } p = 6 \text{ and } n = 5, \\ 11n + 3p - 18 & \text{otherwise}, \end{cases}$$

(7)

which is valid for $p = 3, \ldots, 6$.

For $n = 1$ inequality (7) trivially holds. Assume it holds for all $n' < n$. Let us prove that it also holds for $n$. As $d \geq 3$ in (5), so $n_i < n$, $i = 1, \ldots, d - 1$, and, by induction hypothesis, $C^*_a(n_i, d) \geq C_a(n_i, d)$ in (5). Thus, from (5), (6), we are enough to prove that

$$\min_{d = 3, \ldots, 6, n_1, \ldots, n_{d-1}} \left\{ pd + \sum_{i=1}^{d-1} C^*_a(n_i, d) | n_i \geq 1, \sum_{i=1}^{d-1} n_i = n \right\} \geq C_a(n, p),$$

(8)

and

$$2p + \min_{d = 3, \ldots, 6, n_1, \ldots, n_{d-1}} \left\{ 2d + \sum_{i=1}^{d-1} C_a(n_i, d) | n_i \geq 1, \sum_{i=1}^{d-1} n_i = n \right\} \geq C_a(n, p).$$

(9)

For $n = 2, \ldots, 25$ inequalities (8) and (9) are validated by exhaustive enumeration in their left sides. Lines 2-5 in (7) correspond to the situations when the optimal attached tree is a broom $B(3, n)$, in which a sub-root has degree 2.

Consider $n \geq 26$ and an arbitrary vector $(n_1, \ldots, n_{d-1})$ such that $n_i \geq 1, \sum_{i=1}^{d-1} n_i = n$. Let us define $\delta_i := \# \{ j : n_j = i, j = 1, \ldots, d - 1 \}$ and $I_d := \{ i : C_i(i, d) \neq 11n + 3d - 18 \}$. 
For $n \geq 26$ at least one $\delta_i \geq 1$ for $i \geq 6$, so $\sum_{i \in I_d} \delta_i \leq d - 2$, and (8) can be written as

$$\min_{d=3,\ldots,6} \min_{\delta_i \in I_d} \left\{pd + \sum_{i \in I_d} \delta_i C_{n}(i, d) + 11 \left(n - \sum_{i \in I_d} \delta_i\right) + (3d - 11) \left(d - 1 - \sum_{i \in I_d} i\right) \mid \delta_i \geq 0, \sum_{i \in I_d} \delta_i \leq d - 2\right\} \geq C_n(n, p). \quad (10)$$

For (9) we can perform a similar transformation.

1. Consider $d = 3$. As $I_3 = \{1\}$, substituting (7) into the left-hand side of (10) obtain

$$\min_{\delta_1 = 0,1} \left\{pd + \delta_1 d + 11(n - \delta_1) + (d - 1 - \delta_1)(3d - 18)\right\} = \min_{\delta_1 = 0,1} \{11n + 3p + \delta_1 - 18\} = 11n + 3p - 18,$$

which is equal to $C_n(n, p)$, so (8) holds.

In the same way, substituting (7) into the left-hand side of (9) we obtain

$$\min_{\delta_1 = 0,1} \{2p + 2d + \delta_1 d + 11(n - \delta_1) + (d - 1 - \delta_1)(3d - 18)\} = 11n + 2p - 12,$$

which is not less than $C_n(n, p) = 11n + 3p - 18$ for $p \leq 6$, so (9) also holds.

2. For $d = 4$ $I_4 = \{1\}$, and substitution of (7) into the left-hand side of (10) gives

$$\min_{\delta_1 = 0,1,2} \left\{pd + \delta_1 d + 11(n - \delta_1) + (d - 1 - \delta_1)(3d - 18)\right\} = \min_{\delta_1 = 0,1,2} \{11n + 4p + \delta_1 - 18\} = 11n + 4p - 20,$$

which is greater than $C_n(n, p) = 11n + 3p - 18$ for $p \geq 3$, so (8) holds.

In the same way for (9) we obtain

$$\min_{\delta_1 = 0,1,2} \{2p + 2d + \delta_1 d + 11(n - \delta_1) + (d - 1 - \delta_1)(3d - 18)\} = 11n + 2p - 12,$$

which is not less than $C_n(n, p) = 11n + 3p - 18$ for $p \leq 6$, so (9) holds.

3. For $d = 5$ $I_5 = \{1, 4\}$, so, substituting (7) into the left-hand side of (10), we obtain

$$\min_{\delta_1, \delta_4 \geq 0} \left\{pd + \delta_1 d + 40\delta_4 + 11(n - \delta_1 - 4\delta_4) + (d - 1 - \delta_1 - \delta_4)(3d - 18)\right\} | \delta_1 + \delta_4 \leq d - 2 = \min_{\delta_1, \delta_4 \geq 0} \{11n + 5p - 3\delta_1 - \delta_4 - 12|\delta_1 + \delta_4 \leq 3\}.$$

The latter minimum is attained at $\delta_1 = 3, \delta_4 = 0$ and is equal to $11n + 5p - 21$, which is greater than $C_n(n, p) = 11n + 3p - 18$ for $p \geq 2$, so (8) holds.
Analogously for (9) we obtain
\[
\min_{\delta_1, \delta_4 \geq 0} \{2p + 2d + \delta_1 d + 40 \delta_4 + 11(n - \delta_1 - 4 \delta_4) + (d - 1 - \delta_1 - \delta_4)(3d - 18)\}
\]
\[
|\delta_1 + \delta_4 \leq d - 2\} = \min_{\delta_1, \delta_4 \geq 0} \{11n + 2p - 3\delta_1 - \delta_4 - 2|\delta_1 + \delta_4 \leq 3\} = 11n + 2p - 11,
\]
which is always greater than \(C_a(n, p) = 11n + 3p - 18\) for \(p \leq 6\). Thus, (9) holds.

4. For \(d = 6\) \(I_6 = \{1, 3, 4, 5\}\), so we write the left-hand side of (10) as
\[
\min_{\delta_1, \delta_3, \delta_4, \delta_5 \geq 0} \{pd + \delta_1 d + 32 \delta_3 + 42 \delta_4 + 54 \delta_5 + 11(n - \delta_1 - 3 \delta_3 - 4 \delta_4 - 5 \delta_5) +
\]
\[
+(d - 1 - \delta_1 - \delta_3 - \delta_4 - \delta_5)(3d - 18)|\delta_1 + \delta_3 + \delta_4 + \delta_5 \leq d - 2\} =
\]
\[
\min_{\delta_1, \delta_3, \delta_4, \delta_5 \geq 0} \{11n + 6p - 5 \delta_1 - \delta_3 - 2 \delta_4 - \delta_5|\delta_1 + \delta_3 + \delta_4 + \delta_5 \leq 4\}.
\]
The minimum is attained at \(\delta_1 = 4, \delta_3 = \delta_4 = \delta_5 = 0\) and is equal to \(11n + 6p - 20\), which is greater than \(C_a(n, p) = 11n + 3p - 18\) for \(p \geq 1\), so (8) holds.

In the same way we prove that the left-hand side in (9) is equal to \(11n + 2p - 8\), which is greater than \(C_a(n, p) = 11n + 3p - 18\) for \(p \leq 6\), so (9) holds.

Thus, we proved inequality (7). Let us prove that \(M_2(T) \geq 11n - 27\) for every tree with \(n\) pendent vertices. By Lemma 2, the optimal tree \(T\) is not a star for \(n \geq 9\), so every internal vertex in an optimal tree has an incident internal vertex. At least one of them must be a stem vertex \(m\) of some degree \(d\), which has has \(d - 1\) incident pendent vertices and one incident internal vertex. From Lemmas 1 and 3, \(d \in \{3, \ldots, 6\}\).

So, the value of the index \(M_2(T)\) adds up from the total contribution \((d - 1)d\) of \(d - 1\) pendent vertices and the cost of an attached sub-tree \(T_1\):
\[
M_2(T) = (d - 1)d + C_a(T_1, m, d) \geq (d - 1)d + C_a(n - d + 1, d).
\]

Consider \(n \geq 11\), so that \(n - d + 1 \geq 6\) and \(C_a(n - d + 1, d)\) is always equal to \(11(n - d + 1) + 3d - 18\). In this case \(M_2(T) \geq 11n + (d - 9)d - 7\). The minimum in the right-hand side is attained at \(d = 4, 5\) and is equal to \(11n - 27\).

For \(n = 9, 10\) we also need to check that double brooms \(D(d - 1, 3, n - d + 1)\), originated from the lines 2-5 in (7), do not violate inequality \(M_2(D(d - 1, 3, n - d + 1)) \geq 11n - 27\). For example, \(M_2(D(5, 3, 4)) > 5 \cdot 6 + C_a(4, 6) = 11n - 27 = 72\), \(M_2(D(5, 3, 5)) \geq 5 \cdot 6 + C_a(5, 6) = 84 > 11n - 27 = 83\).

The existence of the optimal tree is proved as in Theorem 3 in [1].
References