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 and chemical 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]. 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

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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 pendent vertex) minimizes M_2 over the set of trees with the fixed maximum degree Δ (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 pendent vertices. If hydrogen atoms are not suppressed from the molecular graphs [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, pendent vertices stand for methyl groups 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 pendent 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 pendent 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 Π_1 and Π_2.

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

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

while the second Zagreb index – as

$$M_2(G) := \sum_{uv \in E(G)} d_G(u)\, d_G(v) \ . \tag{2}$$

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 $n \geqslant 2$ pendent vertices $M_1(T) \geqslant 9n - 16$ if n is even. The equality holds if T is a 4-tree (with $d_T(m) = 4$ for all $m \in V(G) \backslash W(G)$). If n is odd, then $M_1(T) \geqslant 9n - 15$, 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 $d_1, \ldots, d_q$ the following identity holds:

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

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 $d_i = 3, 4, \ldots,$ $i = 1, \ldots, q$ 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, $M_1(T) \geqslant n + 16(n-2)/2 = 9n - 16$. It follows from (3) that the tree T_{even} with $q = (n-2)/2$ internal vertices of degree 4 exists for even n. An obvious calculation gives $M_1(T_{even}) = 9n - 16$. 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_{odd} with all internal vertices having degree 4 except the one of degree 3 with $M_1(T_{odd}) = 9n - 15$. As the index M_1 is integer-valued, T_{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 CH_3 (in hydrogen-suppressed diagrams) in terms of minimization of the first Zagreb index. In both cases M_1 is minimized by alkanes $C_m H_{2m+2}$.

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 $n \geqslant 2$*

$$C(T) \geqslant \underline{C}(n) := nc(1) + (n-2)\frac{c(\Delta(n))}{\Delta(n) - 2} \tag{4}$$

for an arbitrary tree T with n pendent vertices, where

$$\Delta(2) = 3 \quad, \quad \Delta(n) \in \underset{d=3,\dots,n}{\operatorname{argmin}} \frac{c(d)}{d-2} \quad \text{for } n > 2 . \tag{5}$$

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 in an attached tree 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 $n \geqslant 2$ pendent vertices

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

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 $n \geqslant 3$, 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 $T_1, \ldots, T_{d_T(m)-1}$ with $n_1, \ldots, n_{d_T(m)-1}$ 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 the induction hypothesis

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

Note that from (5) follows that

$$\frac{c(\Delta(n_i))}{\Delta(n_i) - 2} \geqslant \frac{c(\Delta(n))}{\Delta(n) - 2}$$

and also that $n_1 + \cdots + n_{d_T(m)-1} = n + d_T(m) - 2$. Thus,

$$
\begin{aligned}
C_a(T, w) &\geqslant c(d_T(m)) + \sum_{i=1}^{d_T(m)-1} \left[(n_i - 1)c(1) + (n_i - 2)\frac{c(\Delta(n))}{\Delta(n) - 2}\right] \\
&= (n-1)c(1) + c(d_T(m)) + (n - d_T(m))\frac{c(\Delta(n))}{\Delta(n) - 2} . \tag{7}
\end{aligned}
$$

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

$$
\begin{aligned}
C_a(T, w) &\geqslant (n-1)c(1) + \min_{d=3,\ldots,n} \left\{c(d) + (n-d)\frac{c(\Delta(n))}{\Delta(n) - 2}\right\} \\
&= (n-1)c(1) + (n-2)\frac{c(\Delta(n))}{\Delta(n) - 2} + \min_{d=3,\ldots,n}(d-2)\left[\frac{c(d)}{d-2} - \frac{c(\Delta(n))}{\Delta(n) - 2}\right] . \tag{8}
\end{aligned}
$$

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

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

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 pendent and $q(n)$ internal vertices, which has the cost

$$C(T^*) = nc(1) + q(n)c(\Delta(n)) = nc(1) + (n-2)\frac{c(\Delta(n))}{\Delta(n) - 2} = \underline{C}(n) \; .$$

This completes the proof[1]. $\blacksquare$

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 $\alpha \geqslant \ln 2/\ln(4/3)$ a 3-tree is optimal (and exists for all $n \geqslant 2$), while for

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

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

Example 2 The first and the second multiplicative Zagreb indices were defined in [11] as

$$\Pi_1(G) := \prod_{v \in V(G)} d_G(v)^2 \; , \quad \Pi_2(G) := \prod_{uv \in E(G)} d_G(u)d_G(v) \; .$$

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 $d \geqslant 3$, the tree with n pendent vertices minimizing Π_1 is a star $K_{1,n}$.

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[1]We use the scheme of the proof from [7], where the similar result was obtained for directed trees under a more general cost function.

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 $c(d) = d \ln d$ in (5) and obtain $\Delta(n) = \min[n, 5]$. Then, from (4) we see that $\Pi_2(T) = \exp(C(T)) \geqslant \exp\left(\frac{5 \ln 5}{3}(n - 2)\right)$ for $n \geqslant 5$ with equality at any 5-tree when $(n - 2)/3$ is integer. $\qquad \square$

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 $n \geqslant 8$ pendent vertices $M_2(T) \geqslant 11n - 27$. 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 $n \geqslant 9$.* $\qquad \square$

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 $p \geqslant 1$. 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

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

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 $p \geqslant 3$

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

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 $n \geqslant 2$, the sub-root of any attached tree is an internal vertex. Consider a tree T with some root w of degree $p \geqslant 3$ and the sub-root m of degree $d \geqslant 3$ having $\delta \geqslant 0$ incident pendent vertices and $\Delta \geqslant 0$ incident internal vertices. Note that $d = \delta + \Delta + 1$ and $3 \leqslant d \leqslant n + 1$. The cost of the attached tree T consists of the cost pd of the edge mw, the total cost δd of δ pendent vertices being incident to m, and the sum of costs of Δ sub-trees $T_1, \dots, T_\Delta$ 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 $\Delta \geqslant 1$ and let the tree T_i have $n_i \geqslant 2$ pendent vertices, $i = 1, \dots, \Delta$. As $2 \leqslant n_i < n$, by induction hypothesis $C_a(T_i, m, d) \geqslant 11n_i + 3d - 18$. 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:

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

$$11n + pd + \delta(7 - 2d) + 3(d - 1)(d - 6). \tag{11}$$

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

- 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 $d \geqslant 4$ 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 $p \geqslant 3$ and $d \geqslant 4$ 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 $p \geqslant 3$.

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

Let us compare cases 1 and 2 and prove that C_1 is never less than C_2 for $n \geqslant 2$ and $p \geqslant 3$. 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 $C_1 - C_2 \geqslant n^2 - 7n + 12$, which is non-negative for all integer n.

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

For $n \geqslant 3$ 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 $d \geqslant 3$ which adds up from $\delta \geqslant 1$ incident pendent vertices (including the root) and $\Delta \geqslant 0$ internal vertices.

The cost of the attached tree T consists of the total cost δd of δ pendent vertices incident to m and the sum of costs of Δ 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 $\Delta \geqslant 1$ and let the tree T_i have $n_i \geqslant 2$ pendent vertices, $i = 1, \ldots, \Delta$. As $n_i \geqslant 2$ and $d \geqslant 3$, from (10) $C_a(T_i, m, d) \geqslant 11n_i + 3d - 18$. 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

$$
\begin{aligned}
C_a(T, w, 1) &\geqslant \delta d + 11n - 11\delta + 3(d - \delta)(d - 6) \\
&= 11n + \delta(7 - 2d) + 3d(d - 6) .
\end{aligned}
\tag{12}
$$

As $n_i \geqslant 2$, it follows that $3 \leqslant d \leqslant n - 1$. Also recall that $1 \leqslant \delta \leqslant d - 1$. Let us minimize r.h.s. in (12) over all $d = \overline{3, n-1}$ and $\delta = \overline{1, d-1}$. The arguments are similar to that in the case of $p \geqslant 3$:

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

- If $d \geqslant 4$, 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 $d = 3$.

So, finally we conclude that if $\Delta \geqslant 1$, then $C_a(T, w, 1) \geqslant 11n - 27$.

Combining cases 1 and 2 we obtain the estimate $C_a(T, w, 1) \geqslant \min[n^2, 11n - 27]$. For $n \geqslant 8$ $n^2 > 11n - 27$, so the inequality $M_2(T) = C_a(T, w, 1) \geqslant 11n - 27$ 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 $n \geqslant 9$ 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 $n \geqslant 9$ $s_4 \geqslant 0$ and $s_5 \geqslant 0$ can be chosen to fulfill the balance, so the tree $T_{4,5}$ does exist for $n \geqslant 9$.

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 $n \geqslant 9$ 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.[2]
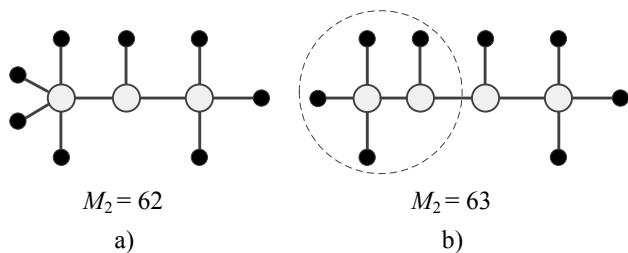

$M_2 = 62$ $M_2 = 63$

a) b)

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 $n \bmod 3 = 1$, there should be at least one stem vertex of degree 5 in the optimal tree $T_{4,5}$, if $n \bmod 3 = 2$, 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 $n \bmod 3 = 1$ 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

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[2]We used a quasi-polynomial algorithm from [8] to enumerate attached trees.

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 $n \bmod 3 = 1$. Analogously, for $n \bmod 3 = 2$ replacement of two stem vertices and their incident pendents 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. We used the algorithm of complexity n^4 from [8] to build a counterexample. Examples of optimal chemical trees for $n = 19$ and 20 are depicted in Fig. 2. One can easily check with direct calculation that when $n \bmod 3 = 2$, attaching a fragment in a dashed circle from Fig. 2b to any "standard tree" with stem vertices of degree 4 and internal vertices of degree 3 gives the optimal chemical tree with $M_2 = 11n - 26$.

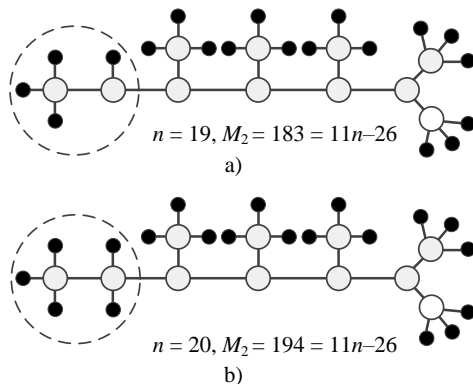$n = 19, M_2 = 183 = 11n–26$

a)

$n = 20, M_2 = 194 = 11n–26$

b)

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 α-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 $n \geqslant 6$.

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]).

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