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Note on Minimizing Degree–Based Topological Indices of Trees with Given Number of Pendent Vertices

Mikhail Goubko[1], **Tamás Réti**[2]

[1]*Institute of Control Sciences of RAS, Moscow, Russia*
mgoubko@mail.ru

[2]*Óbuda University, Budapest, Hungary*
reti.tamas@bgk.uni-obuda.hu

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Abstract

Theorem 3 in [2] claims that the second Zagreb index M_2 cannot be less than $11n - 27$ for a tree with $n \geq 8$ pendent vertices. Yet, a 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 note 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 [1]

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

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

In [2] the following theorem was stated.

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. In particular, for 8 pendent vertices the M_2-minimizing tree is depicted in Fig. 1a.

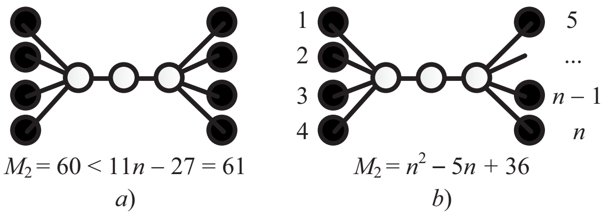

Figure 1: Two-sided brooms

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 below auxiliary results. In what follows, any tree with n pendent vertices, which minimizes M_2 over the set of all trees with n pendent vertices, is called *optimal.*

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, consequently, $d \leq d'$. 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, then the 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 $M_2(D(4;3;n-4)) = n^2 - 5n + 36$. As $n^2 - 5n + 36 < n^2$ for $n \geq 8$, 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 $d_1 \geq \cdots \geq d_p$, 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).

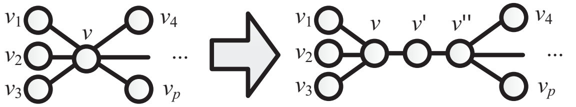

Figure 2: Transformation of vertex v with degree $d \geq 6$

$$\begin{aligned}\Delta := M_2(T') - M_2(T) &= \sum_{i=1}^{3} 4\, d_i + 2 \cdot 4 + 2\,(p-2) + \sum_{i=4}^{p} (p-2)\, d_i - \sum_{i=1}^{p} p\, d_i \\ &= 2\,p + 4 - 2 \sum_{i=4}^{p} d_i - (p-4) \sum_{i=1}^{3} d_i\ . \qquad (2)\end{aligned}$$

If $p \geq 7$, then $p - 4 > 0$ in (2). From $d_1 \geq 2$, $d_i \geq 1$, $i = 2, \cdots, p$, it follows that $\sum_{i=1}^{3} d_i \geq 4$. Thus, $\Delta \leq 2\,p + 4 - 2\,(p-3) - 4\,(p-4) = 26 - 4\,p < 0$. 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*. 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

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

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

Let $\mathcal{T}_a(n, p)$ 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 not considered pendent), and introduce the cost of an optimal attached tree

$$C_a^*(n, p) = \min_{T \in \mathcal{T}_a(n,p)} C_a(T, w, p)\ .$$

Lemma 4. *$C_a^*(1, p) = p$, while for $n \geq 2$*

$$C_a^*(n, p) = \min_{d=2,\ldots,6}\ \min_{n_1,\ldots,n_{d-1}} \left\{ pd + \sum_{i=1}^{d-1} C_a^*(n_i, d) | n_i \in \mathbb{N}\ ,\ \sum_{i=1}^{d-1} n_i = n \right\}. \tag{4}$$

Proof. The case of $n = 1$ is obvious. For $n \geq 2$ each combination of d and $n_1, \ldots, n_{d-1}$ on 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 $n_1, \ldots, n_{d-1}$ 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 $w\,m$ and $d^* - 1 \geq 1$ attached sub-trees $T_1, \ldots, T_{d^*-1}$ with the common root m. Let the trees $T_1, \ldots, T_{d^*-1}$ have $n_1^*, \ldots, n_{d^*-1}^*$

pendent vertices respectively. By definition, $C_a(T_i, m, d^*) \geq C_a^*(n_i^*, d^*)$. So,

$$C_a^*(n,p) = p\,d^* + \sum_{i=1}^{d^*-1} C_a(T_i^*, m, d^*) \geq p\,d^* + \sum_{i=1}^{d^*-1} C_a^*(n_i^*, d^*)$$

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

$$C_{>2}(n,p) := \min_{d=3,\ldots,6}\ \min_{n_1,\ldots,n_{d-1}} \left\{ pd + \sum_{i=1}^{d-1} C_a^*(n_i, d) | n_i \in \mathbb{N}\ ,\ \sum_{i=1}^{d-1} n_i = n \right\} \tag{5}$$

and

$$C_2(n,p) := 2p + C_a^*(n,2)\ . \tag{6}$$

From Lemma 1, the 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 justify the following lower bound estimate for the cost of an optimal attached tree, which is valid for $p = 3,\ldots,6$:

$$C_a^*(n,p) \geq \underline{C}_a(n,p) := \begin{cases} p & \text{if } n = 1 \\ 11n + 3p - 18 + E(n,p) & \text{if } n \geq 2 \end{cases} \tag{7}$$

where $E(4,6) = -2$, $E(4,5) = E(3,6) = E(5,6) = -1$, and $E(n,p) = 0$ otherwise.

The inequality (7) trivially holds for $n = 1$. Assume it holds for all $n' < n$. Let us prove that it also holds for n. As $d \geq 3$ and $n_i \geq 1$ in (5), we have $n_i < n$, $i = 1,\ldots,d-1$, and, by the induction hypothesis, $C_a^*(n_i,d) \geq \underline{C}_a(n_i,d)$ in (5). Thus, we can estimate $C_2(n,p)$ and $C_{>2}(n,p)$ from below by replacing $C_a^*(n_i,d)$ with $\underline{C}_a(n_i,d)$. Rewriting (5) and (6) using the shorthand notation

$$C(n,p,d) := \min_{n_1,\ldots,n_{d-1}} \left\{ pd + \sum_{i=1}^{d-1} \underline{C}_a(n_i,d) | n_i \in \mathbb{N}\ ,\ \sum_{i=1}^{d-1} n_i = n \right\} \tag{8}$$

we see, that justifying inequality (7) is equivalent to proving that for $p = 3,\ldots,6$:

$$\min_{d=3,\ldots,6} C(n,p,d) \geq \underline{C}_a(n,p) \tag{9}$$

$$2p + \min_{d=3,\ldots,6} C(n,2,d) \geq \underline{C}_a(n,p)\ . \tag{10}$$

For $n = 2, \ldots, 7$, $p = 2, \ldots, 6$, we use (8) to calculate numerically $C(n,p,d)$, so inequalities (9) and (10) are directly validated. $E(n,p) \neq 0$ when the optimal attached tree with n pendent vertices and degree p of a root is a *broom* $B(3,n)$ with sub-root of degree 2.

Consider $n \geq 8$ and an arbitrary natural vector $(n_1, \ldots, n_{d-1})$, such that $\sum_{i=1}^{d-1} n_i = n$. Define $\delta_i := \#\{j : n_j = i, j = 1, \ldots, d-1\}$ and rewrite (8) as

$$\begin{aligned} C(n,p,d) &= \min_{\delta_1,\ldots,\delta_{n-1}} \left\{ pd + \sum_{i=1}^{n-1} \delta_i \underline{C}_a(i,d) \right\} \\ &= \min_{\delta_1,\ldots,\delta_{n-1}} \left\{ pd + \sum_{i=1}^{n-1} \delta_i (11i + 3d - 18 + E(i,d)) \right\} \\ &= \min_{\delta_1,\ldots,\delta_{n-1}} \left\{ pd + 11n + (7-2p)\delta_1 + (3p-18)(d-1) + \sum_{i=1}^{n-1} \delta_i E(i,d) \right\}. \qquad (11) \end{aligned}$$

We minimize here over all $\delta_1, \ldots, \delta_{n-1} \in \mathbb{N}_0$, such that

$$\sum_{i=1}^{n-1} \delta_i = d-1, \sum_{i=1}^{n-1} i\,\delta_i = n\ . \qquad (12)$$

Let us estimate $C(n,p,3)$ from below. Substituting $d = 3$ into (11), we have

$$C(n,p,3) = \min_{\delta_1,\ldots,\delta_{n-1}} \{11n + 3p - 18 + \delta_1\}$$

which is never less than $11n + 3p - 18$.

For $d = 4$, expression (11) gives

$$C(n,p,4) = \min_{\delta_1,\ldots,\delta_{n-1}} \{11n + 4p - 18 - \delta_1\}$$

As we consider only $p \geq 2$, inequality $11n + 4p - 18 - \delta_1 < 11n + 3p - 18$ holds only for $\delta_1 \geq 3$. From (12), it implies $n = 3$. Thus, for $n \geq 8$, $C(n,p,4) \geq 11n + 3p - 18$.

For $d = 5$, we write (11) as

$$C(n,p,5) = \min_{\delta_1,\ldots,\delta_{n-1}} \{11n + 5p - 12 - 3\delta_1 - \delta_4\}\ .$$

Inequality $11n + 5p - 12 - 3\delta_1 - \delta_4 < 11n + 3p - 18$ holds only when $3\delta_1 + \delta_4 > 2p + 6 \geq 10$. From (12), the latter implies $\delta_1 = 4, \delta_4 = 0$, and, thus, $n = 4$. Consequently, for $n \geq 8$, $C(n,p,5) \geq 11n + 3p - 18$.

For $d = 6$, expression (11) gives

$$C(n,p,6) = \min_{\delta_1,\ldots,\delta_{n-1}} \{11n + 6p - 5\delta_1 - \delta_3 2\delta_4 - \delta_5\}\ .$$

Inequality $11n+6p-5\delta_1-\delta_3 2\delta_4-\delta_5 < 11n+3p-18$ holds only when $5\delta_1+\delta_3+2\delta_4+\delta_5 > 3p+18 \geq 24$. From (12), the latter implies $\delta_1 = 5, \delta_3 = \delta_4 = \delta_5 = 0$, and, thus, $n = 5$. Consequently, for $n \geq 8$, $C(n,p,6) \geq 11n+3p-18$.

The obtained estimates for $C(n,p,d)$ justify inequality (9). Then we write

$$2p + \min_{d=3,\ldots,6} C(n,2,d) \geq 2p + 11n + 2\cdot 3 - 18 = 11n + 2p - 12 \geq 11n + 3p - 18$$

for $p \leq 6$, so, inequality (10) also holds for $n \geq 8$. Thus, we proved inequality (7).

Let us prove that $M_2 \geq 11n - 27$ for every tree with $n \geq 9$ pendent vertices. By Lemma 2, any internal vertex in an optimal tree T has an incident internal vertex. At least one internal vertex is a stem vertex m. Let its degree be d. From Lemmas 1 and 3, $d \in \{3,\ldots,6\}$.

The vertex m has $d-1$ incident pendent vertices and one incident internal vertex. So, the value of $M_2(T)$ adds up from the total contribution $(d-1)d$ of $d-1$ pendent vertices and the cost of an attached sub-tree T_1:

$$M_2(T) = (d-1)d + C_a(T_1,m,d) \geq (d-1)d + \underline{C}_a(n-d+1,d)\ .$$

Consider $n \geq 11$, so that $n-d+1 \geq 6$ and $\underline{C}_a(n-d+1,d)$ 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 the double brooms $D(d-1,3,n-d+1)$ (they originate from the cases when $E(n,p) \neq 0$ in (7)) do not violate inequality $M_2(D(d-1,3,n-d+1)) \geq 11n - 27$. For example,

$$M_2(D(5,3,4)) \geq 5\cdot 6 + \underline{C}_a(4,6) = 11n - 27 = 72$$

$$M_2(D(5,3,5)) \geq 5\cdot 6 + \underline{C}_a(5,6) = 84 > 11n - 27 = 83\ .$$

The existence of the optimal tree is proved as in Theorem 3 in [2]. ■

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