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

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(Received May 21, 2014)

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]

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

(1)

The vertex $v \in V(G)$ with $d_{G}(v) = 1$ is called a pendant 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.

![Two-sided brooms](image)

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 $d \geq 6$](image)

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

If $p \geq 7$, then $p - 4 > 0$ in (2). From $d_1 \geq 2$, $d_i \geq 1$, $i = 2, \cdots, p$, 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. 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

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

Consider a tree $T$ and fix any vertex $v \in V(T)$. If it has degree $p$ and incident vertices $v_1, \ldots, v_p$, 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 $T_a(n, p)$ 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

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

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

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

**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 $wm$ 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,

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

which is obviously not less than the right-hand side in (4).

Let us rewrite (4) as

$$C_a^*(n, p) = \min[C_a^*(n, p), C_2(n, p)]$$

where

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

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 $p = 3,\ldots,6$:

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

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, $C_a^*(n_i, d) \geq C_a(n_i, d)$ 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 $C_a(n_i, d)$. Rewriting (5) and (6) using the shorthand notation

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

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

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

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

$$ C(n, p, d) = \min_{\delta_1, \ldots, \delta_{n-1}} \left\{ pd + \sum_{i=1}^{n-1} \delta_i C_n(i, d) \right\} $$

$$ = \min_{\delta_1, \ldots, \delta_{n-1}} \left\{ pd + \sum_{i=1}^{n-1} \delta_i (11i + 3d - 18 + E(i, d)) \right\} $$

$$ = \min_{\delta_1, \ldots, \delta_{n-1}} \left\{ pd + 11n + (7-2p)\delta_1 + (3p-18)(d-1) + \sum_{i=1}^{n-1} \delta_i E(i, d) \right\}. \quad (11) $$

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

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

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 $T_1$:

$$M_2(T) = (d - 1)d + C_a(T_1, m, d) \geq (d - 1)d + C_a(n - d + 1, d).$$

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 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,

$$M_2(D(5, 3, 4)) \geq 5 \cdot 6 + C_a(4, 6) = 11n - 27 = 72$$

$$M_2(D(5, 3, 5)) \geq 5 \cdot 6 + C_a(5, 6) = 84 > 11n - 27 = 83.$$

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

References
