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# Trees with maximal second Zagreb index and prescribed number of vertices of the given degree

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## Abstract

In this paper we present a simple algorithm for calculating the maximal value of the second Zagreb index for trees with prescribed number of vertices of given degree. The user needs only to input values $n_1, n_2, ..., n_\Delta$ where $n_i$ is the number of vertices of degree $i$. The algorithm outputs the edge connectivity values $m_{ij}$ as well as the maximal value of the second Zagreb index. The complexity of the algorithm is proportional to $\Delta^3$, where $\Delta$ is maximal degree. Since complexity is independent of the number of vertices, for chemical trees that have $\Delta \leq 4$ the algorithm works in constant time no matter how large the molecule is.

## Introduction

The Zagreb Indices [4, 5] belong to the earliest molecular descriptors. They have found many practical uses and their properties have been continuously studied (see [4, 5, 7, 9, 10, 11, 13] and references therein). The second Zagreb index, denoted by $M_2$, is defined by:

$$M_2(T) = \sum_{uv \in E(T)} d(u) \cdot d(v),$$

where $E(T)$ is the set of edges of a tree $T$ and $d(u)$ is the degree of vertex $u$. Various properties of this index have been extensively studied [1, 2, 3, 6, 8, 11, 12, 14, 15, 16]. Here we report a simple approach to calculate the maximal value of $M_2$ for trees with a fixed number of vertices of a given degree.

## Main results

Let $T$ be any tree, i.e., any simple acyclic connected graph. By $E(T)$ we denote the set of edges of $T$, by $e(T)$ number of its edges and by $n(T)$ number of its vertices; and by $\Delta$ maximal degree. By $m_{ij}$, $1 \le i \le j \le \Delta$, we denote the number of edges that connect vertices of degrees $i$ and $j$ and by $n_i$, $i = 1,...,\Delta$, number of vertices of degree $i$. Let us start with the auxiliary lemma.

**Lemma 1.** Let $T$ be a tree with maximal Zagreb index with $n_i$ vertices of degree $i$ and maximal degree $\Delta$ and let $T_k$ be a subgraph induced by vertices of degree $\ge k$. Then $T_k$ is connected.

**Proof:** If $k = 1$, the claim is obvious. Hence, suppose that $k \ge 2$. Suppose to the contrary, that $T_k$ is not connected. Let $u, v \in V(T_k)$ be two vertices in different components of $T_k$ that are on the smallest distance in $T$ and let $uv_1...v_pv$ be a path (in $T$) from $u$ to $v$. Note that $v_1,...,v_p \notin V(T_k)$ Let $T(u)$ be the component of graph $T - uv_1$ that contains vertex $u$. Since, $T(u)$ is tree, it contains at least one vertex $w \ne u$ of degree 1. Let $uw_1...w_{q-1}w_q (= w)$ be a path from $u$ to $w$. Let $w_r$ be the first vertex of degree $< k$ on this path (such vertex exists, because $d(w) < k$). Let us observe path $w_rw_{r-1}...w_1uv_1...v_pv$. Let $T'$ be a graph defined by $T' = T - w_rw_{r-1} - v_pv + w_{r-1}v + v_pw_r$. Note that $T'$ is tree and that all vertices in $T'$ and $T$ have the same degree. Hence,

$$M_2(T') - M_2(T) = d(w_{r-1}) \cdot d(v) + d(v_p) \cdot d(w_r) - d(w_r) \cdot d(w_{r-1}) - d(v_p) \cdot d(v).$$

Since, $d(w_{r-1}), d(v) \geq k > d(w_r), d(w_p)$, from the Chebishev inequality it follows that $M_2(T') - M_2(T) > 0$, which is in contradiction with maximality of $T$. ■

Now, we can prove our main result.

**Theorem 2.** Let $T$ be a tree with maximal Zagreb index with $n_i$ vertices of degree $i$ and maximal degree $\Delta$. Then,

1) $m_{\Delta\Delta} = n_\Delta - 1$;

2) $m_{ij} = \min\left\{ n_i - \sum_{k=j+1}^{\Delta} m_{ik}, j \cdot n_j - \sum_{k=i+1}^{j} m_{kj} - \sum_{k=j}^{\Delta} m_{jk} \right\}$ for each $1 \leq i < j \leq \Delta$;

3) $m_{ii} = n_i - \sum_{k=i+1}^{\Delta} m_{ik}$ for each $i = 1, \dots, \Delta - 1$.

**Proof:** Suppose to the contrary. Let $T$ be a tree that contradicts the assumptions of the Theorem and let $(i, j)$ be the largest pair according to lexicographical order such that $m_{ij}$ contradicts the assumptions of the theorem. Distinguish five cases:

CASE 1: $i < j$ and $m_{ij} < \min\left\{ n_i - \sum_{k=j+1}^{\Delta} m_{ik}, j \cdot n_j - \sum_{k=i+1}^{j} m_{kj} - \sum_{k=j}^{\Delta} m_{jk} \right\}$.

It follows that there is a vertex $u_j$ of degree $j$ adjacent to vertex $u_q$ of degree $q < i$. Also, it follows that there is a vertex $u_i'$ of degree $i$ that is not adjacent to any vertex of degree $\geq j$. Lemma 1 implies that $T_i$ and $T_j$ are trees. Note that $T_i - T_j$ is a forest and each component has exactly one vertex incident to $T_j$. Note that component of $T_i - T_j$ that contains $u_i'$ is not an isolated vertex and hence it has at least two leaves. Let $u_i$ be a leaf that is not adjacent to any vertex in $T_j$. Hence, $u_i$ is a leaf in $T_i$ without neighbors of degree $\geq j$. Denote by $u_i''$ its only neighbor in $T_i$ (which is in $T_i - T_j$, hence of degree $< j$). Note that $T_i - u_i$ is connected and it contains vertices $u_j$ and $u_i''$. Hence, $T' = T - u_i''u_i - u_ju_q + u_i''u_q + u_ju_i$ is also a tree and has all degrees equal as $T$, but

$$M_2(T') - M_2(T) = d(u_i'')\cdot d(u_q) + d(u_j)\cdot d(u_i) - d(u_i'')\cdot d(u_i) - d(u_j)\cdot d(u_q).$$

Since, $d(u_q) < d(u_i)$ and $d(u_i'') < d(u_j)$, from Cebishev inequality it follows that $M_2(T') - M_2(T) > 0$, which is in contradiction with maximality of $T$.

CASE 2: $i = j < \Delta$ and $m_{ii} \neq n_i - \sum_{k=i+1}^{\Delta} m_{ik}$.

From Lemma 1, it follows that $T_i$ is tree and $T_{i+1}$ is its subtree. Hence, $m_{ii} + \sum_{k=i+1}^{\Delta} m_{ik} = e(T_i) - e(T_{i+1}) = n(T_i) - n(T_{i+1}) = n_i$ which is a contradiction.

CASE 3: $i = j = \Delta$ and $m_{\Delta\Delta} \neq n_{\Delta-1}$.

This is in contradiction with the fact that $T_\Delta$ is a tree.

CASE 4: $i < j$ and $m_{ij} > j \cdot n_j - \sum_{k=i+1}^{j} m_{kj} - \sum_{k=j}^{\Delta} m_{jk}$.

In this case, we have $\sum_{k=1}^{i} m_{kj} + \sum_{k=i+1}^{j} m_{kj} + \sum_{k=j}^{\Delta} m_{jk} = j \cdot n_j < m_{ij} + \sum_{k=i+1}^{j} m_{kj} + \sum_{k=j}^{\Delta} m_{jk}$ which is an obvious contradiction.

CASE 5: $i < j$ and $m_{ij} > n_i - \sum_{k=j+1}^{\Delta} m_{ik}$.

Let $T'$ be a subgraph of $T$ induced by vertices of degree $i$ and vertices of degree $\geq j$. Note that $T'$ is acyclic and contains tree $T_j$. Hence, $m_{ij} + \sum_{k=j+1}^{\Delta} m_{ik} = e(T_i) - e(T_{i+1}) \leq n(T') - n(T_j) = n_i$, which is a contradiction.

All the cases are exhausted and the Theorem is proved. ■

Theorem 2 gives explicit formulas for calculation of $m_{ij}$ for $1 \leq i \leq j \leq \Delta$ by the following algorithm:

Put $i = j = \Delta$

Calculate $m_{\Delta\Delta}$

While $i \geq 1$

    While $j \geq i$

        Calculate $m_{ij}$

    End While

End While

This double loop is executed $\Delta \cdot (\Delta + 1)/2$ times and in each calculation there are at most $3\Delta$ operations that gives the algorithm of the complexity□ $\Delta^3$. After that $M_2(T)$ can be easily calculated as: $M_2(T) = \sum_{1 \leq i \leq j \leq \Delta} m_{ij} \cdot i \cdot j$, which can be done in □ $\Delta^2$ operations. Note that the algorithm gives not only value of $M_2$ but also all connectivities $m_{ij}$. By small modifications, one could easily generate the algorithm that also produces one tree with the maximal Zagreb index. Of course, it may be the case that more than one graph obtain the maximal Zagreb index (moreover, it can be shown that their number is non-polynomial in the number of vertices), hence generation of all graphs with the maximal Zagreb index is a much more complex task.

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