

Trees of Given Order and Independence Number with Minimal First Zagreb Index

Alexander Vasilyev^a, Ratko Darda^b, Dragan Stevanović^{a,c}

^a University of Primorska, Institute Andrej Marušič, Muzejski trg 2, Koper, Slovenia

^b University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technology, Glagoljaška 8, Koper, Slovenia

^c Mathematical Institute, Serbian Academy of Science and Arts, Knez Mihajlova 36, Belgrade, Serbia

alexander.vasilyev@upr.si, draso.darda@gmail.com, dragance106@yahoo.com

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Abstract

We characterize extremal trees with minimal first Zagreb index among trees of order n and the independence number α , solving one of open problems of Das, Xu and Gutman from [*MATCH Commun. Math. Comput. Chem.* **70** (2013), 301–314].

1 Introduction

Let G be a simple graph with the vertex set $V(G)$, $n = |V(G)|$, and the edge set $E(G)$, $m = |E(G)|$. The degree d_v of a vertex $v \in V(G)$ is the number of vertices in G adjacent to v . A subset $S \subseteq V(G)$ of mutually non-adjacent vertices is said to be an independent set in G , and the independence number $\alpha(G)$ is the maximum cardinality of an independent set in G .

The first and the second Zagreb indices, defined as

$$M_1 = M_1(G) = \sum_{u \in V(G)} d_u^2,$$
$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

are widely studied degree-based topological indices, that were introduced by Gutman and Trinajstić [1] in 1972. Gutman provides an overview of recent developments among degree-based topological indices in [2], while further mathematical properties of M_1 and M_2 are

surveyed in [3, 4]. Das, Xu and Gutman [5] have recently established upper bounds on M_1 and M_2 of trees in terms of the order n and the independence number α . They posed three open problems, one of which is characterization of extremal trees with minimal (first or second) Zagreb index among trees of order n and the independence number α . We solve this problem for the first Zagreb index in Theorem 1 below.

The use of MathChem [6], an open source Python package for calculating topological indices, has been beneficial in studying the structure of extremal trees with minimal first Zagreb index among trees of small order n , $4 \leq n \leq 20$, and the independence number α , $\lceil n/2 \rceil \leq \alpha \leq n - 1$. These extremal trees are available at <http://osebje.famnit.upr.si/~alexander.vasilyev/independent/M1.html>. The extremal tree is the path P_n for $\alpha = \lceil n/2 \rceil$, and the star S_n for $\alpha = n - 1$, while for $\lceil n/2 \rceil < \alpha < n - 1$ extremal trees consist of coalescence of stars having almost equal orders (i.e., differing by at most one), with a pair of leaves identified in neighboring stars. Extremal trees are illustrated in Figs. 1 and 2 for two particular choices $(n, \alpha) = (10, 6)$ and $(n, \alpha) = (11, 8)$. Trees in Fig. 1 consist of three stars of order three and a star of order four, while trees in Fig. 2 consist of two stars of order four and a star of order five. In principle, extremal trees are not unique and they can be characterized more formally as follows.

Definition 1 *The set $\mathcal{T}_{n,\alpha}$ consists of all trees $T = (V, E)$ with n vertices and the independence number α such that the degrees of vertices in its maximum independent set S differ by at most one among each other, and such that the complement $\bar{S} = V \setminus S$ is also an independent set whose vertex degrees differ by at most one among each other.*

With respect to Figs. 1 and 2, the set S is formed by black vertices of degree one (leaves of stars) and degree two (vertices belonging to two stars), while \bar{S} is formed by centers of the stars (represented by white vertices). The fact that vertices in \bar{S} have degrees that differ by at most one means that the orders of stars differ by at most one.

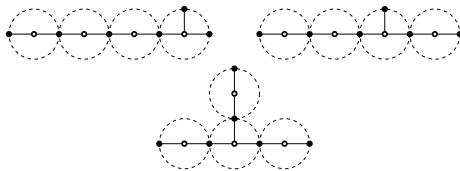


Figure 1: Three non-isomorphic trees with $n = 10$, $\alpha = 6$ and minimum value of $M_1 = 36$.



Figure 2: Two non-isomorphic trees with $n = 11$, $\alpha = 8$ and minimum value of $M_1 = 48$.

The main result of this note is the following

Theorem 1 *If T is a tree with n vertices and the independence number α , then*

$$M_1(T) \geq 2(n-1) + \left\lfloor \frac{n-1}{\alpha} \right\rfloor (2n-2-\alpha) + \left\lceil \frac{n-1}{n-\alpha} \right\rceil (n-2+\alpha) - \left\lfloor \frac{n-1}{\alpha} \right\rfloor^2 \alpha - \left\lceil \frac{n-1}{n-\alpha} \right\rceil^2 (n-\alpha) \quad (1)$$

with equality if and only if $T \in \mathcal{T}_{n,\alpha}$.

2 Proof of Theorem 1

Let T be a tree with n vertices and the independence number α . Let S be an independent set containing α vertices of T , and let $\bar{S} = V(T) \setminus S$ be the set of the remaining vertices of T . Denote by l the number of edges $uv \in E(T)$ such that $u \in S, v \in \bar{S}$, and by k the number of edges between vertices in \bar{S} . As there are no edges between vertices of S , and T has $n-1$ edges in total, we have that

$$k + l = n - 1, \quad (2)$$

$$\sum_{u \in S} d_u = l, \quad (3)$$

$$\sum_{v \in \bar{S}} d_v = l + 2k. \quad (4)$$

Write the first Zagreb index of T as

$$M_1(T) = \sum_{u \in S} d_u^2 + \sum_{v \in \bar{S}} d_v^2.$$

Let us, for the moment being, forget that the values d_u represent the actual degrees of vertices in S , and treat them just as a sequence of integers satisfying the condition (3). It is easy to see that, in such setting, the minimal value of $\sum_{u \in S} d_u^2$ is attained if $d_u \in \{\lfloor \frac{l}{\alpha} \rfloor, \lceil \frac{l}{\alpha} \rceil\}$ for each $u \in S$. Namely, if there exist $u', u'' \in S$ such that $d_{u'} - d_{u''} \geq 2$, then we obtain smaller sum of squares if we replace $d_{u'}$ and $d_{u''}$ by $d_{u'} - 1$ and $d_{u''} + 1$:

$$(d_{u'} - 1)^2 + (d_{u''} + 1)^2 = d_{u'}^2 + d_{u''}^2 - 2(d_{u'} - d_{u''} - 1) < d_{u'}^2 + d_{u''}^2.$$

Replacing in this way the pairs of integers $d_{u'}, d_{u''}$ that differ by at least two as long as they exist, we see that the minimal value of $\sum_{u \in S} d_u^2$ is necessarily attained if all numbers d_u , $u \in S$, differ by at most one among each other, and therefore, are equal to either $\lfloor \frac{l}{\alpha} \rfloor$ or $\lceil \frac{l}{\alpha} \rceil$. (This argument for minimizing the first Zagreb index was used several times earlier—see, for example, [7, 8].)

Analogously, the minimal value of $\sum_{v \in \bar{S}} d_v^2$ is attained if $d_v \in \{ \lfloor \frac{l+2k}{n-\alpha} \rfloor, \lceil \frac{l+2k}{n-\alpha} \rceil \}$.

We can now bound the sum $\sum_{u \in S} d_u^2$ from below in terms of n, α and l (or, due to (2), in terms of n, α and k).

If $l = \alpha q$ for $q \in Z$, then all degrees d_u , $u \in S$, are equal to $\frac{l}{\alpha} = q$, so that

$$\sum_{u \in S} d_u^2 = \alpha \cdot \frac{l^2}{\alpha^2} = \frac{l^2}{\alpha} = \alpha \cdot q^2.$$

Suppose now that $l = \alpha q + r$ for $q \in Z$ and $0 < r < \alpha$. Then the minimal value of M_1 is attained if $d_u = q$ or $d_u = q + 1$ for each $u \in S$. From (3) we see that then r vertices have degree $q + 1$, while $\alpha - r$ vertices have degree q , so that

$$\sum_{u \in S} d_u^2 \geq (\alpha - r)q^2 + r(q + 1)^2 = \alpha q^2 + r(2q + 1). \tag{5}$$

Having in mind that $q = \lfloor \frac{l}{\alpha} \rfloor$ and $r = l - \alpha \lfloor \frac{l}{\alpha} \rfloor$, we have that

$$\alpha q^2 + r(2q + 1) = \alpha \left\lfloor \frac{l}{\alpha} \right\rfloor^2 + \left(l - \alpha \left\lfloor \frac{l}{\alpha} \right\rfloor \right) \left(2 \left\lfloor \frac{l}{\alpha} \right\rfloor + 1 \right) = (2l - \alpha) \left\lfloor \frac{l}{\alpha} \right\rfloor - \alpha \left\lfloor \frac{l}{\alpha} \right\rfloor^2 + l. \tag{6}$$

Combining (5) and (6) with (2) we get

$$\sum_{u \in S} d_u^2 \geq (2(n - 1 - k) - \alpha) \left\lfloor \frac{n - 1 - k}{\alpha} \right\rfloor - \alpha \left\lfloor \frac{n - 1 - k}{\alpha} \right\rfloor^2 + n - 1 - k. \tag{7}$$

Analogous approach applied to \bar{S} yields

$$\sum_{v \in \bar{S}} d_v^2 \geq (2(n - 1 + k) - (n - \alpha)) \left\lfloor \frac{n - 1 + k}{n - \alpha} \right\rfloor - (n - \alpha) \left\lfloor \frac{n - 1 + k}{n - \alpha} \right\rfloor^2 + n - 1 + k. \tag{8}$$

By summing inequalities (7) and (8) we obtain

$$\begin{aligned} M_1(T) \geq & 2(n - 1) + (2n - 2k - \alpha - 2) \left\lfloor \frac{n - 1 - k}{\alpha} \right\rfloor - \alpha \left\lfloor \frac{n - 1 - k}{\alpha} \right\rfloor^2 \\ & + (n + 2k + \alpha - 2) \left\lfloor \frac{n - 1 + k}{n - \alpha} \right\rfloor - (n - \alpha) \left\lfloor \frac{n - 1 + k}{n - \alpha} \right\rfloor^2. \end{aligned} \tag{9}$$

Denote the expression on the right hand side of (9) as the function $f(k)$ for fixed n and α . As the lower bound (1) is equal to $f(0)$, in order to prove Theorem 1 it is enough to show that the minimum of $f(k)$ for feasible values of k is obtained exactly for $k = 0$.

Let us deal with $\lfloor \frac{n-1-k}{\alpha} \rfloor$ first. The conditions that there are no edges between vertices in the independent set S and that T is connected imply that the number $l = n - 1 - k$ of edges between S and \bar{S} is at least $|S| = \alpha$, so that

$$\frac{n-1-k}{\alpha} \geq \frac{\alpha}{\alpha} = 1.$$

On the other hand, the independence number of trees, as instances of bipartite graphs, satisfies $\alpha \geq \frac{n}{2}$, so that

$$\frac{n-1-k}{\alpha} \leq \frac{n-1}{n/2} < 2.$$

Hence, $\lfloor \frac{n-1-k}{\alpha} \rfloor = 1$ and $f(n, \alpha, k)$ can be written as

$$f(k) = 4(n-1) - 2(\alpha+k) + (n+2k+\alpha-2) \left\lfloor \frac{n-1+k}{n-\alpha} \right\rfloor - (n-\alpha) \left\lfloor \frac{n-1+k}{n-\alpha} \right\rfloor^2. \quad (10)$$

Next, consider $\lfloor \frac{n-1+k}{n-\alpha} \rfloor$. Since $0 \leq k \leq n-1-\alpha$, we have that

$$\frac{n-1}{n-\alpha} \leq \frac{n-1+k}{n-\alpha} < \frac{n-1}{n-\alpha} + 1,$$

so that

$$\left\lfloor \frac{n-1+k}{n-\alpha} \right\rfloor = \left\lfloor \frac{n-1}{n-\alpha} \right\rfloor \quad \text{for } 0 \leq k \leq (n-\alpha) \left\lfloor \frac{n-1}{n-\alpha} \right\rfloor - \alpha, \quad (11)$$

and

$$\left\lfloor \frac{n-1+k}{n-\alpha} \right\rfloor = \left\lfloor \frac{n-1}{n-\alpha} \right\rfloor + 1 \quad \text{for } (n-\alpha) \left\lfloor \frac{n-1}{n-\alpha} \right\rfloor - \alpha + 1 \leq k \leq n-\alpha-1. \quad (12)$$

Let $t = \lfloor \frac{n-1+k}{n-\alpha} \rfloor$. The function f then becomes

$$f(k) = 4(n-1) - 2\alpha + 2k(t-1) + (n+\alpha-2)t - (n-\alpha)t^2. \quad (13)$$

From $k \geq 0$ and $\alpha \geq \lfloor \frac{n}{2} \rfloor$ we have that

$$\frac{n-1+k}{n-\alpha} \geq \frac{n-1}{\lfloor \frac{n}{2} \rfloor} = \begin{cases} 2, & \text{if } n \text{ is odd,} \\ 2 - \frac{2}{n}, & \text{if } n \text{ is even,} \end{cases}$$

showing that $t = 1$ is possible if and only if $k = 0$, n is even, and $\alpha = n/2$. The only tree satisfying these conditions is the path $P_{2\alpha}$, and $P_{2\alpha}$ is the unique element of the set $H_{2\alpha, \alpha}$, hence Theorem 1 holds in this case.

For all other cases $t \geq 2$ holds. We can note then from (13) that f becomes the linear function in k , with constant positive coefficient $2(t-1)$, when k belongs to one of the two intervals given in (11) and (12). The minimum of f on these intervals is, therefore, attained at the respective minimal values of k , i.e., at

$$k = 0 \text{ and } k = k' = (n-\alpha) \left\lfloor \frac{n-1}{n-\alpha} \right\rfloor - \alpha + 1,$$

while the minimum of f on the union of these intervals is obtained at either 0 or k' . The difference of the values of f at 0 and k' is equal to

$$f(k') - f(0) = 2(n - \alpha) \left[\frac{n - 1}{n - \alpha} \right]^2 - 2(n - 1) \left[\frac{n - 1}{n - \alpha} \right] + 2(\alpha - 1). \quad (14)$$

The roots of the quadratic function $2(n - \alpha)x^2 - 2(n - 1)x + 2(\alpha - 1)$ are equal to 1 and $\frac{\alpha - 1}{n - \alpha}$. Since the case $2\alpha = n$ has been dealt with already (see the preceding paragraph), we have that $2\alpha \geq n + 1$, so that $\frac{\alpha - 1}{n - \alpha} \geq 1$ is the larger of two roots. Further, let q and r be the quotient and the remainder of the division of $n - 1$ by $n - \alpha$:

$$n - 1 = q(n - \alpha) + r, \quad q \in Z, \quad 0 \leq r < n - \alpha.$$

From the condition $r < n - \alpha$ we obtain that

$$n - r - 1 < \alpha - 1 \quad \Rightarrow \quad q(n - \alpha) > \alpha - 1 \quad \Rightarrow \quad \left[\frac{n - 1}{n - \alpha} \right] = q > \frac{\alpha - 1}{n - \alpha},$$

so that the value of the quadratic function on the right hand side of (14) is strictly positive, as its argument $\left[\frac{n - 1}{n - \alpha} \right]$ is strictly larger than the larger of its two roots. Hence $f(k') > f(0)$ and the minimum of the function $f(k)$ for all feasible k is attained exactly at $k = 0$. This proves inequality (1) in Theorem 1.

Equality holds in (1) if and only if $k = 0$, i.e., \bar{S} is also an independent set of T , vertices in S have degrees that differ by at most one, and vertices in \bar{S} have degrees that differ by at most one among each other. Hence, equality holds in (1) if and only if $T \in \mathcal{T}_{n,\alpha}$. ■

3 Further remarks

Theorem 1 extends more-or-less directly to unicyclic graphs. In particular, let $\mathcal{U}_{n,\alpha}$ denote the set consisting of all unicyclic graphs G with n vertices and the independence number α , such that the degrees of vertices in its maximum independent set S differ by at most one among each other, and such that the complement $\bar{S} = V \setminus S$ is also an independent set whose vertex degrees differ by at most one among each other. The graphs in $\mathcal{U}_{n,\alpha}$ consist of coalescence of stars, whose orders differ by at most one, with pairs of leaves identified in neighboring stars (see Fig. 3 for an example of $\mathcal{U}_{10,7}$).

Note that the basic ingredients of the proof of Theorem 1 were the facts $k + l = n - 1$ and $\alpha \geq \frac{n}{2}$, which, in the case of unicyclic graphs, become $k + l = n$ and $\alpha \geq \lfloor \frac{n}{2} \rfloor$. Following closely the proof of Theorem 1, and taking care of the special case $\alpha = \frac{n - 1}{2}$, one can prove the following

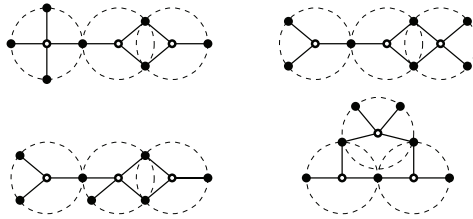


Figure 3: Four non-isomorphic unicyclic graphs with $n = 10$, $\alpha = 7$ and minimum value of $M_1 = 50$.

Theorem 2 *If G is a unicyclic graph with n vertices and the independence number α , then*

$$M_1(G) \geq 4n - 2\alpha + (n + \alpha) \left\lfloor \frac{n}{n - \alpha} \right\rfloor - (n - \alpha) \left\lfloor \frac{n}{n - \alpha} \right\rfloor^2,$$

with equality if and only if $G \in \mathcal{U}_{n,\alpha}$ when $\alpha \geq \frac{n}{2}$ and $G \cong C_{2\alpha+1}$ when $\alpha = \frac{n-1}{2}$.

As a matter of fact, this result could further be extended to bicyclic and graphs with more cycles, provided that $\alpha \geq \frac{n}{2}$. However, an increasing number of graphs having $\alpha < \frac{n}{2}$ has to be treated separately then, making this task more and more laborious.

On the other hand, it appears that the problem of characterization of extremal trees with minimal second Zagreb index among trees of order n and the independence number α cannot be solved as easily as it was the case with the first Zagreb index. The main obstacle is that we can no longer rely on the arguments of Das [7] and Gutman [8] to conclude that the degrees of vertices in S have to differ by at most one, simply because the second Zagreb index is no longer a sum of terms over the set of vertices, but over the set of edges. Although by inspecting the extremal trees with minimal second Zagreb index of small order n , $4 \leq n \leq 20$, and the independence number α , $\lceil n/2 \rceil \leq \alpha \leq n - 1$, which are available at <http://osebje.famnit.upr.si/~alexander.vasilyev/independent/M2.html>, one can conclude that the extremal trees are once again coalescence of stars, these stars no longer have to be of almost equal orders. This is exemplified by the case $n = 19$, $\alpha = 15$, in which case one of the extremal trees represents a coalescence of three stars of order six and one star of order four (see Fig. 4). Hence characterization of trees with minimal second Zagreb index remains an open problem.

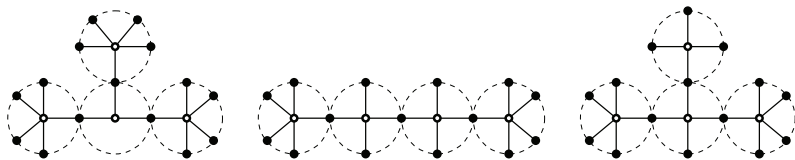


Figure 4: Three non-isomorphic trees with $n = 19$, $\alpha = 15$ and minimum value of $M_2 = 108$.

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