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On the Constant Difference of Zagreb Indices[1]

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Abstract

Let $\Phi(z)$, $z \in \mathbb{Z}$, be the set of all connected graphs whose difference of the second and the first Zagreb index is equal to z. We show that $\Phi(z)$ contains exactly one element, a star, for $z < -2$, while it is infinite for $z \geq -2$. Moreover, all elements of $\Phi(-2)$ and $\Phi(-1)$ are trees, while $\Phi(0)$, besides trees, contains the cycles only. Constructions of new elements of $\Phi(z)$ from the existing ones are based on the existence of vertices of degree two. We further show that the only elements of $\cup_{z \leq 0} \Phi(z)$, which do not contain vertices of degree two, are stars and the molecular graphs of 2,3–dimethylbutane and 2,2,3–trimethylbutane.

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1 Introduction

Let G be a connected simple graph with the vertex set $V(G)$, $n = |V(G)|$, and the edge set $E(G)$, $m = |E(G)|$. The first and the second Zagreb index of G are defined as

$$M_1(G) = \sum_{u \in V(G)} d^2(u) \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

where $d(u)$ denotes the degree of a vertex $u \in V(G)$. The Zagreb indices are among the oldest and most famous topological indices—they were introduced by Gutman and Trinajstić in 1972, while the recent surveys of their chemical importance and mathematical properties appear in [1, 2].

Comparing the values of the Zagreb indices of the same graph, Hansen and Vukičević initially conjectured in [3] that

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \tag{1}$$

with equality attained for complete graphs. This conjecture generated a lot of research, and for a survey on its developments the reader is referred to [4]. While the conjecture does not hold in general, it does hold for chemically important classes of trees, unicyclic graphs and graphs with maximum vertex degree four. In the case of trees, the inequality (1) has been proved first by Vukičević and Graovac [5], and new proofs has been found recently by Andova, Cohen and Škrekovski [6], and by Stevanović and Milanič [7].

We pursue here a direct approach to comparing the Zagreb indices of the same graph. Let

$$ZD(G) = M_2(G) - M_1(G)$$

and define the set $\Phi(z)$, for $z \in \mathbb{Z}$, as

$$\Phi(z) = \{G : G \text{ is connected and } ZD(G) = z\}.$$

If $G \in \Phi(z)$, we will also say that G is *z-Zagreb-balanced.*

Basic examples and constructions of new elements of $\Phi(z)$ from the existing ones, based on the existence of vertices of degree two, are given in Section 2. While $\Phi(z)$ is infinite for $z \geq -2$, in Section 3 we show that, for $z < -2$, $\Phi(z)$ contains exactly one element, a star. Further, in Section 4 all elements of $\Phi(-2)$ and $\Phi(-1)$ are shown to be trees, while $\Phi(0)$, besides trees, contains the cycles only. Some further properties of the elements of $\Phi(-2)$, $\Phi(-1)$ and $\Phi(0)$ also given in this section. Finally, in Section 5 we show that, for $-2 \leq z \leq 0$, each element of $\Phi(z)$ has vertices of degree two, except for two molecular graphs (of 2,3-dimethylbutane and of 2,2,3-trimethylbutane) that do not have vertices of degree two.

This direct approach to comparing Zagreb indices has been pursued in [8] previously, where Caporossi, Hansen and Vukičević showed that:

(i) if $m \leq 6n/5$ then $ZD(G) \geq 6(m-n)$, with equality attained if and only if G is a graph with vertices of degree 2 and 3 only and the vertices of degree 3 form an independent set, and

(ii) if $m \geq n$ then $ZD(G) \geq 11m - 12n$, with equality attained if G is a graph with vertices of degree 2 and 3 only and, when $m \geq 6n/5$, no pair of vertices of degree 2 are adjacent.

2 Basic examples and construction

We start with two examples which, together, show that $\Phi(z)$ is nonempty for each $z \in \mathbb{Z}$.

Example 1 *For a star $K_{1,z}$, $z \geq 1$, we have that $M_1(K_{1,z}) = z^2 + z$ and $M_2(K_{1,z}) = z^2$, so that $ZD(K_{1,z}) = -z$.*

Example 2 *For $z \geq 0$, let P_{2z+3} be a path on $2z+3$ vertices, having the vertex set $V(P_{2z+3}) = \{v_1, \dots, v_{2z+3}\}$. We construct the graph $PC(z)$ on $n = 3z+3$ vertices by adding a pendant edge to vertices v_3, v_5, …, v_{2z+1} (Fig. 1). From $M_1(PC(z)) = 14z+6$ and $M_2(PC(z)) = 15z+4$, we have $ZD(PC(z)) = z-2$.*

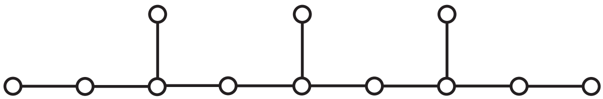

Figure 1: Graph $PC(3)$.

Hence, $\Phi(z)$ contains a star $K_{1,-z}$ for $z \leq -1$, while it contains $PC(z+2)$ for $z \geq -2$. Next, we present two constructions of new elements of $\Phi(z)$ from the existing ones.

Proposition 3 *Let G be a graph with vertex w of degree two, and let G_k be the graph obtained from G by replacing w with the path on k vertices, as in Fig. 2. Then $ZD(G_k) = ZD(G)$.*

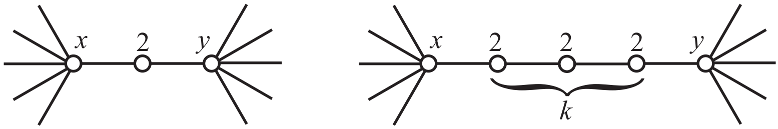

Figure 2: Graphs G (left) and G_k (right).

Proof Note that the first Zagreb index may be written in an alternative form:

$$M_1(G) = \sum_{v \in V(G)} d^2(v) = \sum_{uv \in E(G)} (d(u) + d(v))\,. \tag{2}$$

Hence,

$$ZD(G) = M_2(G) - M_1(G) = \sum_{uv \in E(G)} (d(u)d(v) - d(u) - d(v))\,. \tag{3}$$

Now, let x and y denote the degrees of the neighbors of w, and let E' denote the edges of G which are not incident with w. Then

$$\begin{aligned} ZD(G) &= (2x - x - 2) + (2y - y - 2) + \sum_{uv \in E'} (d(u)d(v) - d(u) - d(v)) \\ &= (x-2) + (y-2) + (k-1)(2 \cdot 2 - 2 - 2) + \sum_{uv \in E'} (d(u)d(v) - d(u) - d(v)) \\ &= ZD(G_k)\,. \qquad \blacksquare \end{aligned}$$

Proposition 4 *Let G be a graph with vertex w of degree two, adjacent to vertex z of degree one, and let G^k be the graph obtained by G by attaching k pendant vertices to z, as in Fig. 3. Then $ZD(G^k) = ZD(G)$.*

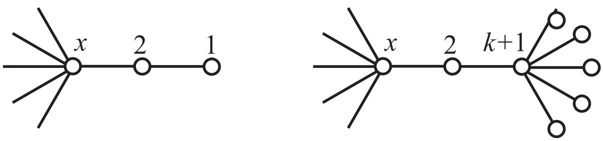

Figure 3: Graphs G (left) and G^k (right).

Proof Let x denote the degree of the other neighbor of w, and let E' denote the edges of G which are not incident with w. Then

$$\begin{aligned} ZD(G^k) &= (2x - x - 2) + [2(k+1) - (k+1) - 2] + k[(k+1) \cdot 1 - (k+1) - 1] \\ &+ \sum_{uv \in E'} (d(u)d(v) - d(u) - d(v)) \end{aligned}$$

$$= (x-2) - 1 + \sum_{uv \in E'} (d(u)d(v) - d(u) - d(v))$$
$$= ZD(G). \qquad \blacksquare$$

Apparently, both Propositions 3 and 4 may be applied to the graph $PC(z+2) \in \Phi(z)$ for $z \geq -2$. Since the numbers of new vertices added to an existing graph in $\Phi(z)$ by these propositions are arbitrary, we conclude that each set $\Phi(z)$, $z \geq -2$, is infinite.

3 $\Phi(z)$ contains a unique element for $z < -2$

Unlike the case for $z \geq -2$, here we show that $\Phi(z)$ for $z < -2$ contains the star $K_{1,-z}$ only. The following useful lemma was proved by Vukičević and Pisanski in [9].

Lemma 5 ([9]) *If G is a simple connected graph, then*

$$ZD(G) = p_3(G) + 3t(G) - m \tag{4}$$

where $p_3(G)$ is the number of 3–paths and $t(G)$ is the number of triangles in G.

The next lemma establishes the monotonicity of ZD under particular conditions.

Lemma 6 *Let $H_0, \ldots, H_k$ be the sequence of connected graphs, such that $H_i = H_{i-1} + e_i$ for $i = 1, \ldots, k$. If H_0 is not a star, then*

$$ZD(H_0) \leq \ldots \leq ZD(H_k).$$

Proof We show that $ZD(H_{i-1}) \leq ZD(H_i)$ for each $i = 1, \ldots, k$. From Lemma 5 we have

$$ZD(H_i) - ZD(H_{i-1}) = [p_3(H_i) - p_3(H_{i-1})] + 3[t(H_i) - t(H_{i-1})] - 1.$$

Suppose first that the edge $e_i = H_i - H_{i-1}$ joins two vertices p and q of H_{i-1}. The degrees of p and q in H_{i-1} are at least one, as H_{i-1} is connected. Thus, e_i forms in H_i either at least one new 3-path in which it is a middle edge or at least one new triangle; in either case, $ZD(H_{i-1}) \leq ZD(H_i)$.

Otherwise, suppose that e_i joins a vertex p that does not belong to H_{i-1} with a vertex q of H_{i-1}. The degree of q in H_{i-1} is at least one, and since H_{i-1} is not a star (with a center at q), at least one neighbor r of q in H_{i-1} has degree at least two. If s is a neighbor of r different from q, then e_i forms a new 3-path $pqrs$ in H_i, hence $ZD(H_{i-1}) \leq ZD(H_i)$. $\blacksquare$

Proposition 7 *If a connected graph G is not a star, then*

$$ZD(G) \geq -2 \ .$$

Proof Let u be the vertex of G having maximal degree $d(u) = \Delta$, and let $N(u) = \{v_1, \ldots, v_\Delta\}$ be the set of neighbors of u. Since G is not a star, there exists a neighbor of u with degree at least two. Suppose, without loss of generality, that $d(v_1) \geq 2$ and let $w \in N(v_1) \setminus \{u\}$. Let H be the subgraph of G on the subset of vertices $\{u, v_1, \ldots, v_\Delta, w\}$, with the subset of edges $\{uv_1, uv_2, \ldots, uv_\Delta, v_1w\}$. There are two possible cases for H, depending on whether or not $w \in \{v_2, \ldots, v_k\}$, as shown in Fig. 4. In the former case $ZD(H) = \Delta - 2 > -2$, while in the latter case $ZD(H) = -2$.

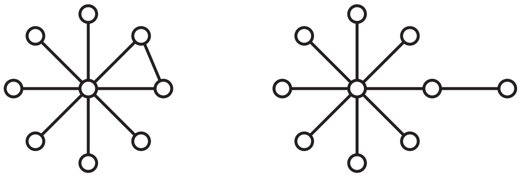

Figure 4: Subgraph H: case $w \in \{v_2, \ldots, v_k\}$ at the left, case $w \notin \{v_2, \ldots, v_k\}$ at the right.

Next, note that the edges of $E(G) \setminus E(H)$ can be ordered as $\{e_1, \ldots, e_{m-\Delta-1}\}$ in such a way that all subgraphs in the sequence

$$H_0 = H, \qquad H_i = H_{i-1} + e_i \quad \text{for } i = 1, \ldots, m - \Delta - 1$$

are connected. For example, such ordering can be obtained by choosing as e_i an edge from $E(G) \setminus E(H_{i-1})$ which joins two vertices of H_{i-1}, whenever such edge exists; otherwise, by choosing as e_i an edge which joins a vertex of H_{i-1} with a vertex from $V(G) \setminus V(H_{i-1})$.

From Lemma 6 we now have

$$-2 \leq ZD(H) = ZD(H_0) \leq \ldots \leq ZD(H_{m-\Delta-1}) = ZD(G) \, . \qquad \blacksquare$$

The previous proposition shows that $\Phi(z)$, for $z < -2$, cannot contain any element other than the star $K_{1,-z}$. Moreover, this proposition improves the inequality

$$M_2(G) - M_1(G) \geq -\delta_2(G)$$

where $\delta_2(G)$ is the second smallest vertex degree of G, which has appeared earlier in [5, 7]. This inequality is valid only for trees.

4 Elements of $\Phi(-2)$, $\Phi(-1)$ and $\Phi(0)$ and their properties

From the previous section, we see that the first nontrivial sets $\Phi(z)$ are $\Phi(-2)$, $\Phi(-1)$ and $\Phi(0)$. They share further property that all of their elements are trees, with the exception of the cycles C_n being the sole nontree elements of $\Phi(0)$.

Proposition 8 *If G is a connected graph that is neither a tree nor a cycle, then*

$$ZD(G) \geq 1 \,.$$

Proof Since G is not a tree, it contains a cycle $C = \{v_1, \ldots, v_k\}$, $3 \leq k \leq n$, as a subgraph. Further, since G is not a cycle, at least one vertex from C has degree at least three. Suppose, without loss of generality, that $d(v_1) \geq 3$ and let w be a neighbor of u different from v_2 and v_k. Let H be the subgraph of G on the subset of vertices $\{v_1, \ldots, v_k, w\}$. The possible cases for H are shown in Fig. 5, where e denotes the edge $v_1 w$. It is straightforward to check that, in each of these cases, $ZD(H) \geq 1$ holds.

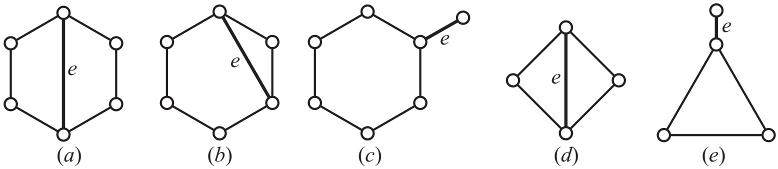

Figure 5: Ways to add an edge to a cycle.

Similarly as in the proof of Proposition 7, the edges of $E(G) \setminus E(H)$ can be ordered as $\{e_1, \ldots, e_{m-k-1}\}$ in such a way that all subgraphs in the sequence

$$H_0 = H, \qquad H_i = H_{i-1} + e_i \quad \text{for } i = 1, \ldots, m-k-1$$

are connected. From Lemma 6 we now have

$$1 \leq ZD(H) = ZD(H_0) \leq \ldots \leq ZD(H_{m-k-1}) = ZD(G) \,. \qquad \blacksquare$$

Using the computer search, we found that the smallest elements of $\Phi(-2)$, $\Phi(-1)$ and $\Phi(0)$. Up to six vertices, the set $\Phi(-2)$ contains only paths P_n, $n \geq 3$ and brooms—a path with a star attached to one of path's end vertices. The smallest tree in $\Phi(-2)$ that is neither a path nor a broom is shown in Fig. 6.

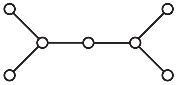

Figure 6: The smallest tree (the graph of 2,4-dimethylpentane) in $\Phi(-2)$, which is neither a path nor a broom.

Other than K_2, the set $\Phi(-1)$ does not contain other trees up to five vertices, while it contains two trees on six vertices, representing 2,3–dimethylbutane and 3–methylpentane (Fig. 7).

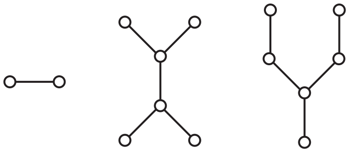

Figure 7: The trees with at most 6 vertices in $\Phi(-1)$.

The set $\Phi(0)$ does not contain trees up to six vertices, while it contains four trees on seven vertices, representing 3–ethylpentane, 2,3–dimethylpentane, 3,3–dimethylpentane and 2,2,3–trimethylbutane (Fig. 8).

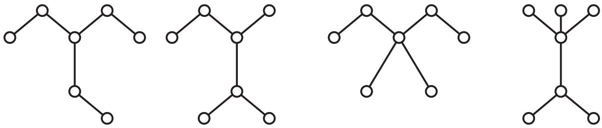

Figure 8: The trees with at most 7 vertices in $\Phi(0)$.

Some further properties of the elements of $\Phi(-2)$, $\Phi(-1)$ and $\Phi(0)$ are given in the following paragraphs.

All cycles C_n belong to $\Phi(0)$, as $M_1(C_n) = M_2(C_n) = 4n$. It is interesting that the trees in $\Phi(-2) \cup \Phi(-1) \cup \Phi(0)$, other than paths, also satisfy that the value of their first Zagreb index is at least four times the number of edges: Horoldagva proved in his thesis [10, Theorem 2.5] that, for a connected graph G with n vertices and maximum vertex degree Δ holds

$$M_1(G) \geq 4n + (\Delta - 1)(\Delta - 2) - 6$$

with equality if and only if G is a starlike tree or a path. For any tree T holds $m = n-1$, so that

$$M_1(T) \geq 4m + \Delta(\Delta - 3)\,.$$

If $\Delta \geq 3$ then $M_1(T) \geq 4m$. if $\Delta = 1$ or $\Delta = 2$, then T is a path (on two vertices if $\Delta = 1$), in which case $M_1(T) = 4m - 2$.

Next, the sets $\Phi(-2)$, $\Phi(-1)$ and $\Phi(0)$ contain only paths and 2,3-dimethylbutane as bidegreed graphs, in which the degree of each vertex $v \in V(G)$ is either δ or Δ, $\delta < \Delta$. Namely, if $G \in \Phi(-2) \cup \Phi(-1) \cup \Phi(0)$ and it is not regular, then G cannot be a cycle and it has to be a tree, hence $\delta = 1$. Now, if there are k vertices of degree one and $n-k$ vertices of degree Δ, then

$$M_1(G) = k + (n-k)\Delta^2 \qquad\qquad M_2(G) = k\Delta + (m-k)\Delta^2 = k\Delta + (n-1-k)\Delta^2\,.$$

From $M_2(G) - M_1(G) \in \{-2,-1,0\}$ we get

$$k(\Delta - 1) - \Delta^2 \in \{-2,-1,0\}.$$

In the first case, $k = \Delta + 1 - \frac{1}{\Delta - 1}$ is an integer, and this is possible if and only if $\Delta = 2$ and $k = 2$, i.e., if and only if G is a path. In the second case, $k = \Delta + 1$ and let v be a vertex of degree Δ. Obviously, $\Delta \geq 3$, as paths are only trees with $\Delta = 2$ and do not have three leaves. Each of Δ branches of tree G attached at v contains at least one leaf, and since the number of leaves is $\Delta + 1$, then exactly one of these branches has to contain two leaves. However, that branch must also contain at least one further vertex of degree Δ, which shows that the number of leaves in this branch is at least $\Delta - 1$. Since this branch contains exactly two leaves, we get $\Delta = 3$ and the only 3,1-bidegreed tree with four leaves is that of 2,3-dimethylbutane. In the third case, $k = \Delta + 1 + \frac{1}{\Delta - 1}$ is an integer, which is possible if and only if $\Delta = 2$ and $k = 4$, however, this is impossible as paths do not have four leaves.

Recently, Vukičević, Gutman, Furtula, Andova and Dimitrov [11] considered the sets of graphs for which strict inequality holds in (1). The trees in $\Phi(-2) \cup \Phi(-1) \cup \Phi(0)$, other than the paths P_2 and P_3, provide further examples of such graphs (having arbitrarily large maximum vertex degree). Namely, if $T \in \Phi(0)$ then from $M_1(T) = M_2(T)$ and $n > m$, the strict inequality in (1) follows immediately. If $T \in \Phi(-1)$, the strict inequality in (1) reduces to $n < M_1(T)$, which is satisfied by any tree having at least three vertices. If

$T \in \Phi(-2)$, the strict inequality in (1) reduces to $2n < M_1(T)$. However, the inequality between arithmetic and quadratic means

$$\frac{2m}{n} = \frac{\sum_{u \in V(T)} d(u)}{n} \leq \sqrt{\frac{\sum_{u \in V(T)} d^2(u)}{n}} = \sqrt{\frac{M_1(T)}{n}}$$

implies that $M_1(T) \geq \frac{4(n-1)^2}{n} > 2n$ whenever $n \geq 4$ (and the only tree in $\Phi(-2)$ with less than four vertices is P_3).

5 Trees with no vertices of degree two in $\Phi(z)$, $z \leq 0$

Constructions given by Propositions 3 and 4 exploit the existence of degree two vertices to provide new examples of elements in $\Phi(z)$. Here we show that, for each $z \leq 0$, at most one element of $\Phi(z)$ does not contain degree two vertices. This is trivially satisfied for one-element sets $\Phi(z)$ containing the star $K_{1,-z}$ for $z < -2$, so we concentrate on nonstars.

Proposition 9 *If $T \in \Phi(z)$ for $z \leq 0$ is not a star and does not contain degree two vertices, then T is a molecular graph of either 2,3–dimethylbutane or 2,2,3–trimethylbutane.*

Proof From Proposition 8 we conclude that T is a tree. As it is not a star, there exists an edge $e = uv \in E(T)$, such that $d(u) = s+1$ and $d(v) = t+1$ with $s, t \geq 2$. Assume that $s \leq t$. Denote the neighbors of u by $v, u_1, \ldots, u_s$, and the neighbors of v by $u, v_1, \ldots, v_t$, and let H be the subgraph of T induced by the subset $\{u, v,\ u_1, \ldots, u_s,\ v_1, \ldots, v_t\}$ (Fig. 9). It holds $ZD(H) = st - s - t - 1$.

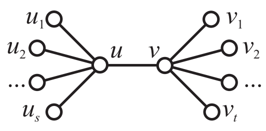

Figure 9: An induced subgraph of T.

Similarly as in the proof of Proposition 7, the edges of $E(T) \setminus E(H)$ can be ordered as $\{e_1, \ldots, e_{m-s-t-1}\}$ in such a way that all subgraphs in the sequence

$$H_0 = H, \qquad H_i = H_{i-1} + e_i \quad \text{for } i = 1, \ldots, m-s-t-1$$

are connected. For example, such ordering can be obtained by choosing as e_i an edge which joins a vertex of H_{i-1} with a vertex from $V(T) \setminus V(H_{i-1})$. From Lemma 6, we have

$$0 \geq z = ZD(T) = ZD(H_{m-s-t-1}) \geq \ldots \geq ZD(H_0) = ZD(H) = st - s - t - 1 \ .$$

Since $2 \leq s \leq t$, the inequality $0 \geq st - s - t - 1$ holds only if

$$(s,t) \in \{(2,2),(2,3)\} \ .$$

Now suppose that $d(u_i) \geq 3$ for some $1 \leq i \leq s$. Let u'_1 and u'_2 be two neighbors of u_i different from u, and let H' be the induced tree of T obtained by adding edges $u_iu'_1$ and $u_iu'_2$ to H. It is easy to see that $ZD(H') = st + s - t - 3$, and $ZD(H') > 0$ holds for both cases $(s,t) = (2,2)$ and $(s,t) = (2,3)$. Using the same argument as above, we then conclude that $ZD(T) \geq ZD(H') > 0$, a contradiction. Hence, $d(u_i) = 1$ for each $1 \leq i \leq s$.

Analogous argument shows that $d(v_j) = 1$ for each $1 \leq j \leq t$.

Thus, T is in fact equal to H, and it is the molecular graph of 2,3–dimethylbutane in case $(s,t) = (2,2)$ and the molecular graph of 2,2,3–trimethylbutane in case $(s,t) = (2,3)$. ■

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