Discrete Mathematics Letters
www.dmlett.com

Discrete Math. Lett. **2** (2019) 10–17

Some properties of the neighborhood first Zagreb index

Tamás Réti[1,*], Akbar Ali[2], Péter Varga[1], Enikő Bitay[3]

[1]*Óbuda University, Bécsiút, 96/B, H-1034 Budapest, Hungary*
[2]*Knowledge Unit of Science, University of Management and Technology, Sialkot 51310, Pakistan*
[3]*Sapientia Hungarian University of Transylvania, 540485 Târgu-Mureş, Op.9., Cp.4, Romania*

(Received: 26 November 2018. Received in revised form: 20 March 2019. Accepted: 8 July 2019. Published online: 12 July 2019.)

© 2019 the authors. This is an open access article under the CC BY (International 4.0) license (https://creativecommons.org/licenses/by/4.0/).

Abstract

The neighborhood first Zagreb index (NM_1) has been recently introduced for characterizing the topological structure of molecular graphs. In this study, we present some sharp bounds on the index NM_1 and establish its relations with the first and second Zagreb indices in case of some special graphs. It is verified and demonstrated on examples that in several cases, the index NM_1 outperforms the discriminating performance of the majority of traditional degree-based molecular descriptors (for example, Randić connectivity index, the sum-connectivity index, the harmonic index, the geometric-arithmetic index, etc.).

Keywords: chemical graph theory; first Zagreb index; second Zagreb index; neighborhood topological indices; neighborhood first Zagreb index.

2010 Mathematics Subject Classification: 05C07, 05C35, 92E10.

1. Introduction

All the graphs considered in this paper are simple, finite and connected. Notation and terminology that are not defined here can be found in the standard books [17, 35]. For a graph G, $V(G)$ and $E(G)$ denote the set of vertices and edges, and n and m the numbers of vertices and edges, respectively. An edge of G connecting vertices u and v is denoted by uv, and the degree $d(u)$ of a vertex $u \in V(G)$ is the number of edges incident with u.

The first Zagreb index M_1 (firstly appeared in [25]) and the second Zagreb index M_2 (introduced in [23]) for a graph G can be defined as

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

Theory of these Zagreb indices is well established, see for example the papers [2, 20, 21, 24, 25, 28, 29, 31], recent surveys [2, 4, 6, 22] and related references listed therein.

For a vertex $u \in V(G)$, there are several notation for representing the "sum of degrees of the vertices adjacent to u" in literature - for example, Cao [8] and Yu *et al.* [41] used the notation $t(u)$ (and called it 2-degree), Abdo *et al.* [1] used the notation $d_{2,u}$ and Hagos [26] used $S(u)$ - however, we suggest the notation $S_G(u)$ or simply $S(u)$ or S_u (due to the obvious reason, as S stands for sum) for future use. The *average-degree* [41] (also known as *dual degree* [14]) of a vertex $u \in V(G)$ is the number $\frac{S(u)}{d(u)}$ and we denote it by $a(u)$. Consider the following two general graph invariants

$$I_1(G) = \sum_{u\in V(G)} f_1(S(u)) \quad \text{and} \quad I_2(G) = \sum_{uv\in E(G)} f_2(S(u),S(v))\,.$$

Some special cases of the above invariants I_1 and I_2 have already been appeared in mathematical chemistry. For example, if we take $f_1(S(u)) = S(u)$ or $\frac{1}{\sqrt{S(u)}}$ then I_1 gives the first Zagreb index M_1 (see the proof of Lemma 2.4 in [9]) or first extended zeroth-order connectivity index [5, 36, 40, 42], respectively and if we take $f_2(S(u),S(v)) = S(u)+S(v)$, $\frac{1}{\sqrt{S(u)S(v)}}$, $\sqrt{\frac{S(u)+S(v)-2}{S(u)S(v)}}$ or $\frac{2\sqrt{S(u)S(v)}}{S(u)+S(v)}$ then I_2 gives $2M_2$ (see Lemma 2.6 in [9]), the first extended first-order connectivity index [5], fourth atom-bond connectivity index [16] or fifth geometric-arithmetic index [18], respectively. On the same lines, it is natural to consider the following variants of the first and second Zagreb indices:

$$NM_1(G) = \sum_{v\in V(G)} (S(v))^2 \quad \text{and} \quad NM_2(G) = \sum_{uv\in E(G)} S(u)S(v)\,.$$

*Corresponding author (tamas.reti@bkg.uni-obuda.hu)

We refer the invariants NM_1 and NM_2 as the neighborhood first Zagreb index and neighborhood second Zagreb index. In this paper, we are concerned with the neighborhood first Zagreb index NM_1, which was initially appeared in Refs. [11,30] and referred as the neighborhood Zagreb index [30]. Clearly, the invariant NM_1 can rewritten [11] as

$$NM_1(G) = \sum_{v \in V(G)} (d(v)a(v))^2 .$$

The main purpose of the present paper is to establish some properties of NM_1.

Now, we recall some notation and definitions which will be used in the remaining paper. Denote by $\Delta = \Delta(G)$ and $\delta = \delta(G)$ the maximum and the minimum degrees of a graph G. Let $A = A(G)$ be the adjacency matrix of G. We denote by $\rho(G)$ (or simply ρ) the largest eigenvalue of $A(G)$ and call it the spectral radius of G.

A graph is called *r-regular* if all its vertices have the degree r. A graph is called *irregular* if it contains at least two vertices with different degrees. An irregular graph G is said to be *bidegreed* graph if $\delta \neq \Delta$ and $d(u) \in \{\delta, \Delta\}$ for every $u \in V(G)$. A *semiregular* graph G is a bipartite bidegreed graph in which every edge of G joins a vertex of degree δ to a vertex of degree Δ [41]. For example, the complete bipartite graphs form a subset of semiregular graphs.

A graph G is said to be *harmonic* (or *pseudo-regular*) [13] (see also [1,7,32,41]) if every vertex of G has the same average-degree. It can be easily observed that the average-degree of any vertex of a harmonic graph must be a positive integer [19]. The spectral radius ρ of a harmonic graph G is equal to the average-degree of any vertex of G. It is obvious that every regular graph is a harmonic graph. It should be noted that a harmonic graph can be bipartite or non-bipartite. A bipartite graph G is called *pseudo-semiregular* [41] if each vertex in the same part of bipartition has the same average-degree. From these definitions it follows that semiregular graphs form a subset of pseudo-semiregular graphs. If (V_1, V_2) is a bipartition of a pseudo-semiregular graph G such that p_1 and p_2 are the average-degrees of vertices in V_1 and V_2, respectively, then the spectral radius of G can be calculated as $\rho = \sqrt{p_1 p_2}$, see [41]. It is worth noting that the 5-vertex path graph P_5 is the smallest pseudo-semiregular graph.

2. Some bounds on the graph invariant NM_1

We start with the following obvious but important result concerning NM_1:

Lemma 2.1. *If G is an n-vertex graph such that $uv \notin E(G)$, $u \neq v$, then*

$$NM_1(G + uv) > NM_1(G).$$

If G is an n-vertex r-regular graph then $NM_1(G) = nr^4$. Particularly, $NM_1(K_n) = n(n-1)^4$ where K_n is the n-vertex complete graph.

Proposition 2.2. *For $n \geq 3$, if G is a connected graph of order n then*

$$NM_1(P_n) \leq NM_1(G) \leq NM_1(K_n)$$

with left (respectively, right) equality if and only if G is isomorphic to the n-vertex path graph P_n (respectively, complete graph K_n), where

$$NM_1(K_n) = n(n-1)^4 \quad \text{and} \quad NM_1(P_n) = \begin{cases} 12 & \text{if } n = 3, \\ 26 & \text{if } n = 4, \\ 16n - 38 & \text{if } n \geq 5. \end{cases}$$

Proof. From Lemma 2.1, it follows that among all the n-vertex graphs, $n \geq 3$, the graph with maximal NM_1 value is the complete graph K_n and the graph with minimal NM_1 value must be a tree (obviously path graph P_3 if $n = 3$). In what follows, we prove the lower bound, that is $NM_1(P_n) \leq NM_1(G)$ by assuming that G is an n-vertex tree where $n \geq 4$.

For the path P_4 we obtain $NM_1(P_4) = 26$. If $n \geq 5$, there exist two vertices u_1 and u_2 for which $\left(S(u_1)\right)^2 = \left(S(u_2)\right)^2 = 4$, two vertices v_1 and v_2 for which $\left(S(v_1)\right)^2 = \left(S(v_2)\right)^2 = 9$ and $n-4$ vertices $w_1, w_2, \cdots, w_{n-4}$ with $\left(S(w_i)\right)^2 = 16$ for $i = 1, 2, \cdots, n-4$. Consequently, for $n \geq 5$, it follows that $NM_1(P_n) = 16n - 38$. For $n \geq 4$, routine computation gives $NM_1(P_n) < NM_1(S_n)$ where S_n is the n-vertex star graph. In the remaining proof, we assume that $G \ncong S_n$. We use induction on n. For $n = 5$, the desired result can be easily verified. Suppose that the result holds for all trees of order $k-1$, where $k \geq 6$. Let T be a k-vertex tree, $k \geq 6$, different from S_k and let $u_0 \in V(T)$ be a pendant vertex adjacent to the vertex v. Let $d(v) = x$ and $N(v) = \{u_0, u_1, u_2, ..., u_{r-1}, u_r, ..., u_{x-1}\}$ where $d_{u_i} = 1$ for $i = 0, 1, \ldots, r-1$ and $d_{u_i} \geq 2$ for $i = r, r+1, \ldots, x-1$ (since $N(v)$ contains at least one non-pendant vertex because T is different from S_k). Let T^* be the tree obtained from T by removing the vertex u_0. Bearing in mind the inequalities $\sum_{i=1}^{x-1} d(u_i) \geq 2$ and $\sum_{w\in N(u_i)} d(w) \geq 4$ for $i = r, r+1, \ldots, x-1$, we have

$$NM_1(T) - NM_1(T^*) = x^2 + \left(\sum_{i=1}^{x-1} d(u_i) + 1\right)^2 - \left(\sum_{i=1}^{x-1} d(u_i)\right)^2 + (r-1)[x^2 - (x-1)^2]$$
$$+\sum_{i=1}^{x-1}\left[\left(\sum_{w\in N(u_i)} d(w)\right)^2 - \left(\sum_{w\in N(u_i)} d(w) - 1\right)^2\right] \geq 16.$$

By using the induction hypothesis in the above inequality, we get $NM_1(T) \geq 16k - 38$ with equality if and only if T is isomorphic to P_k. This completes the induction and hence the proof.

□

Lemma 2.3. [9] *For a graph G, it holds that*

$$M_1(G) = \sum_{u\in V(G)} \big(d(u)\big)^2 = \sum_{u\in V(G)} d(u)a(u)$$

and

$$M_2(G) = \sum_{uv\in E(G)} d(u)d(v) = \frac{1}{2}\sum_{u\in V(G)} \big(d(u)\big)^2 a(u).$$

Proposition 2.4. *If G is a graph with minimum degree δ and maximum degree Δ then*

$$2\delta M_2(G) \leq NM_1(G) \leq 2\Delta M_2(G)\,. \tag{1}$$

The equality sign in (1) holds if and only if G is a regular graph.

Proof. By using Lemma 2.3, one obtains

$$NM_1(G) = \sum_{u\in V(G)} [d(u)a(u)]^2 \leq \Delta \sum_{u\in V(G)} \big(d(u)\big)^2 a(u) = 2\Delta M_2(G)$$

and similarly

$$2\delta M_2(G) = \delta \sum_{u\in V(G)} \big(d(u)\big)^2 a(u) \leq \sum_{u\in V(G)} \big(d(u)\big)^2 \big(a(u)\big)^2 = NM_1(G).$$

□

Lemma 2.5. *(Cauchy-Schwarz inequality) If $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ and $\boldsymbol{x} = (y_1, y_2, \ldots, y_n)$ are two sequences of real numbers then*

$$\left(\sum_{j=1}^{n} x_j y_j\right)^2 \leq \left(\sum_{j=1}^{n} x_j^2\right)\left(\sum_{j=1}^{n} y_j^2\right)$$

with equality if and only if the sequences $\boldsymbol{x}$ and $\boldsymbol{y}$ are proportional, that is, there is a constant c such that $x_j = cy_j$ for each j, $1 \leq j \leq n$.

Proposition 2.6. *Let G be a non-trivial n-vertex graph. It holds that*

$$NM_1(G) \geq \frac{\big(M_1(G)\big)^2}{n} \tag{2}$$

with equality if and only if there exist a positive integer b such that $S(u) = b$ for every vertex $u \in V(G)$ (note that equality in (2) holds for regular graphs and semiregular graphs). Also, it holds that

$$NM_1(G) \geq \frac{4\big(M_2(G)\big)^2}{M_1(G)}. \tag{3}$$

with equality if and only if G is a harmonic graph.

Proof. Let $V(G) = \{u_1, u_2, \ldots, u_n\}$, $d(u_j) = d_j$ and $a(u_j) = a_j$ for $j = 1, 2, \ldots, n$.

Firstly, we prove (2). If we take $x_j = 1$ and $y_j = d_j a_j$ then by using Lemmas 2.3 and 2.5, we obtain

$$\big(M_1(G)\big)^2 = \left(\sum_{j=1}^{n} d_j a_j\right)^2 \leq \left(\sum_{j=1}^{n} 1\right)\sum_{j=1}^{n} (d_j a_j)^2 = n \cdot NM_1(G),$$

where the equation $\big(M_1(G)\big)^2 = n \cdot NM_1(G)$ holds if and only if there exist a positive integer b such that $d_1 a_1 = a_2 d_2 = \cdots = a_n d_n = b$.

Now, we prove (3). If we take $x_j = d_j$ and $y_j = d_j a_j$ then again by using Lemmas 2.3 and 2.5, we get

$$4\big(M_2(G)\big)^2 = \left(\sum_{j=1}^{n} (d_j)^2 a_j\right)^2 \le \left(\sum_{j=1}^{n} (d_j)^2\right) \sum_{j=1}^{n} (d_j a_j)^2 = M_1(G) \cdot NM_1(G),$$

where the equation $4\big(M_2(G)\big)^2 = M_1(G) \cdot NM_1(G)$ holds if and only if there exist a positive number c such that $a_1 = a_2 = \cdots = a_n = c$.

□

In literature, there exist many lower and upper bounds on the Zagreb indices M_1 and M_2. By using Propositions 2.4, 2.6 and some existing bounds on M_1 and M_2, we can easily establish new bounds on the invariant NM_1. For example, by using the following existing result and Proposition 2.4, we obtain Proposition 2.8.

Theorem 2.7. [10] *If G is a graph with order n, size m, minimum degree δ, maximum degree Δ and second maximum degree Δ_2 then*

$$M_2(G) \ge 2m^2 - \Delta m(n-1) + \frac{\Delta - 1}{2}\left(\Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(\Delta_2 - \delta)^2(n-2)}{(n-1)^2}\right) \tag{4}$$

and

$$M_2(G) \le 2m^2 - \delta m(n-1) + \frac{\delta - 1}{2}\left(m(n+1) + \Delta(\Delta - n) + \frac{2(m-\Delta)^2}{n-2}\right) \tag{5}$$

where the equality sign in (4) holds if and only if G is a regular graph and the equality sign in (5) holds if and only if either $G \cong K_n$ or $G \cong K^*_{2,n-2}$ (that is, a graph obtained from the complete bipartite graph $K_{2,n-2}$ by adding an edge between the vertices of degree $n-2$).

Proposition 2.8. *If G is a graph with order n, size m, minimum degree δ, maximum degree Δ and second maximum degree Δ_2 then*

$$NM_1(G) \ge 2\delta\left(2m^2 - \Delta m(n-1) + \frac{\Delta - 1}{2}\left(\Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(\Delta_2 - \delta)^2(n-2)}{(n-1)^2}\right)\right) \tag{6}$$

and

$$NM_1(G) \le 2\Delta\left(2m^2 - \delta m(n-1) + \frac{\delta - 1}{2}\left(m(n+1) + \Delta(\Delta - n) + \frac{2(m-\Delta)^2}{n-2}\right)\right) \tag{7}$$

where the equality sign in (6) holds if and only if G is a regular graph and the equality sign in (7) holds if and only if $G \cong K_n$.

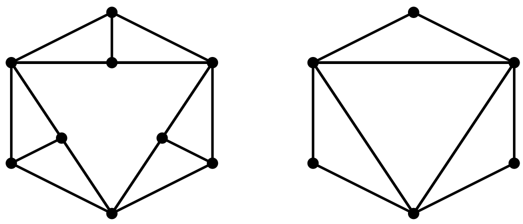

Figure 1: Bidegreed graphs used in Example 2.9.

Example 2.9. *In this example, we compare the lower bounds on the invariant NM_1 given in (1), (2) and (3). We consider the bidegreed graphs H_1 and H_2 depicted in Figure 1. The graph H_1, taken from Ref. [27], is a 9-vertex distance-balanced graph with $\delta = 3$, $\Delta = 4$, $M_1(H_1) = 102$, $M_2(H_1) = 171$ and $NM_1(H_1) = 1158$. For Inequality (1), we have*

$$1158 = NM_1(H_1) > 2\delta M_2(H_1) = 1026\,.$$

For Inequalities (2) and (3), we obtain

$$1158 = NM_1(H_1) > \frac{\big(M_1(H_1)\big)^2}{n} = 1156\,,$$

$$1158 = NM_1(H_1) > \frac{4\big(M_2(H_1)\big)^2}{M_1(H_1)} = 1146.7\,.$$

For the 6-vertex bidegreed graph H_2, it holds that $\delta = 3$, $\Delta = 4$, $M_1(H_2) = 60$, $M_2(H_2) = 96$, $NM_1(H_2) = 624$ and hence

$$624 = NM_1(H_2) > 2\delta M_2(H_2) > 384\,,$$

$$624 = NM_1(H_2) > \frac{\big(M_1(H_2)\big)^2}{n} = 600\,,$$

$$624 = NM_1(H_2) > \frac{4\big(M_2(H_2)\big)^2}{M_1(H_2)} = 614.4\,.$$

Therefore, the lower bounds on the invariant NM_1 given in (2) and (3) seem to be very good estimates. But, as it is demonstrated in this example, they are incomparable.

3. Relation between NM_1 and Zagreb indices

Proposition 3.1. *If G is an n-vertex semiregular graph with size m then*

$$\frac{M_1(G)}{n} = \frac{M_2(G)}{m} \quad \textit{and} \quad NM_1(G) = \frac{\big(M_1(G)\big)^2}{n} = \frac{M_1(G)\cdot M_2(G)}{m}\,.$$

Proof. Let δ and Δ be the minimum and maximum degrees of G. From the assumption that G is a semiregular graph, it follows that $S(u) = \Delta\delta$ for every vertex $u \in V(G)$ and $d(u)d(v) = \Delta\delta$ for every edge $uv \in E(G)$, which imply the desired result. □

Lemma 3.2. [33] *Let G be an n-vertex irregular harmonic graph with size m and spectral radius ρ. Then $a(u) = \rho$ for every vertex $u \in V(G)$, $M_1(G) = 2m\rho$ and $M_2(G) = m\rho^2$.*

Proposition 3.3. *If G is an irregular harmonic graph then*

$$NM_1(G) = \frac{M_1(G)\cdot M_2(G)}{m} = \frac{4\big(M_2(G)\big)^2}{M_1(G)}\,.$$

Proof. By using the definition of NM_1 and bearing in mind Lemma 3.2, we have

$$\begin{aligned} NM_1(G) &= \sum_{u\in V(G)} [d(u)a(u)]^2 = \rho^2 \sum_{u\in V(G)} \big(d(u)\big)^2 = \rho^2\cdot M_1(G) = \frac{M_1(G)\cdot M_2(G)}{m} \\ &= \frac{2m\rho(m\rho^2)}{m} = \frac{2m^2\rho^4}{\rho m} = \frac{4\big(M_2(G)\big)^2}{2\rho m} = \frac{4\big(M_2(G)\big)^2}{M_1(G)}\,. \end{aligned}$$

□

Lemma 3.4. [1] *If G is a pseudo-semiregular graph with size m and spectral radius ρ then $M_2(G) = m\rho^2$.*

Lemma 3.5. [41] *If G is a pseudo-semiregular graph with spectral radius ρ then*

$$NM_1(G) = \sum_{u\in V(G)} \big(S(u)\big)^2 = M_1(G)\cdot\rho^2.$$

Proposition 3.6. *If G is a pseudo-semiregular graph then*

$$NM_1(G) = \frac{M_1(G)\cdot M_2(G)}{m}\,.$$

Proof. The result directly follows from Lemmas 3.4 and 3.5. □

4. The discriminating performance of NM_1

Denote by $m_{r,s}(G)$ (or $m_{r,s}$, when there is no confusion) the number of edges in G with end-vertex degrees r and s. Two graphs G_1 and G_2 satisfying $m_{r,s}(G_1) = m_{r,s}(G_2)$ for all r and s with $1 \le r \le s \le \Delta$, are called *edge-equivalent* graphs. A topological index TI satisfying $TI(G_1) = TI(G_2)$ for every pair of edge-equivalent graphs G_1 and G_2, is called *edge-equivalent* topological index. We remark that the bond incident degree indices [38, 39] (BID indices for short [3]) are edge-equivalent topological indices – general form of the BID indices is

$$\mathrm{BID}(G) = \sum_{uv\in E(G)} f(d(u), d(v)) = \sum_{r\le s} m_{r,s} f(r,s) \tag{8}$$

where $f(r, s)$ is a bivariate symmetric function. It should be emphasized that the majority of degree-based topological indices used in mathematical chemistry are BID indices. These indices can be generated from (8) depending on the choice of $f(r, s)$. Well-known examples [20, 24, 29, 38, 39] are the first Zagreb index, second Zagreb index, Randić/connectivity index, atom-bond connectivity index, sum-connectivity index, harmonic index, augmented Zagreb index and geometric-arithmetic index.

For investigating the discriminatory performance of the topological index NM_1, we consider the 8-vertex trees representing the octane isomers. These 18 molecular graphs of octane isomers are depicted in Figure 2.

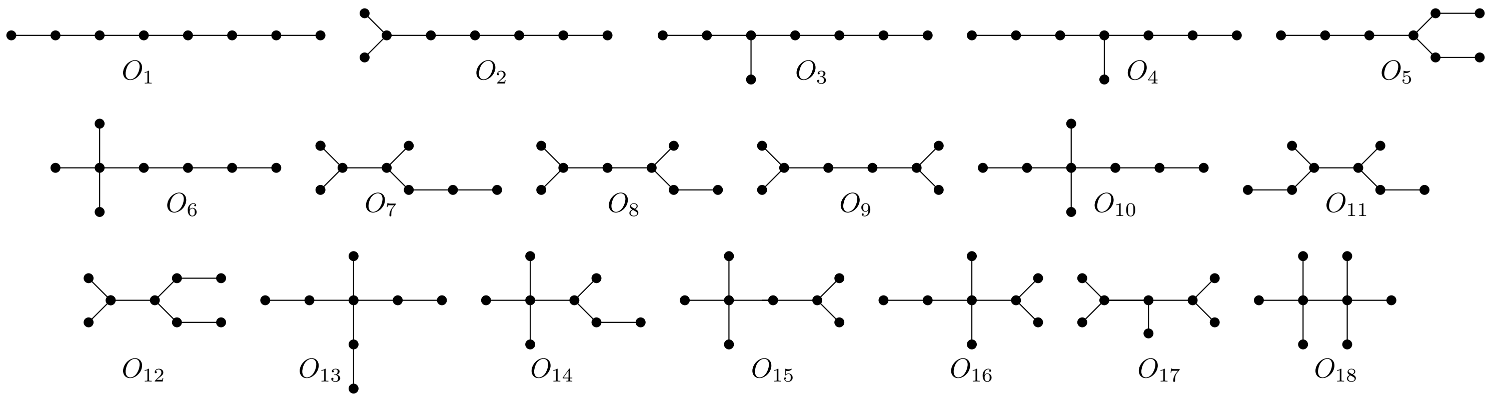

Figure 2: Molecular graphs of 18 octane isomers.

From Figure 2, it can be easily seen that the trees O_3 and O_4 are edge-equivalent, but their corresponding neighborhood first Zagreb indices are different: $NM_1(O_3) = 108$ and $NM_1(O_4) = 110$. Similarly, the trees O_{11} and O_{12} are edge-equivalent graphs possessing different neighborhood first Zagreb indices: $NM_1(O_{11}) = 130$ and $NM_1(O_{12}) = 132$. Thus, the topological index NM_1 does not belong to the class of edge-equivalent topological indices. Consequently, we can conclude that the topological index NM_1 is characterized by a better discriminatory power than the traditional BID indices. This observation has been confirmed in [30]. Particularly, Mondal *et al.* [30] proved that all the molecular graphs of 18 octane isomers have different NM_1 values.

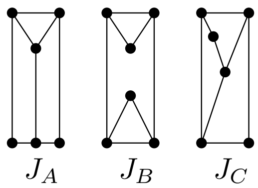

Figure 3: Three small 6-vertex edge-equivalent graphs.

It should be noted that in some particular cases, the discrimination ability of NM_1 is limited but always better than that of the BID indices. This phenomenon can be explained by considering the edge-equivalent graphs depicted in Figure 3: we have $NM_1(J_A) = 330$, but $NM_1(J_B) = NM_1(J_C) = 328$ (needless to say that all these three graphs have the same value of any arbitrary BID index; that is, using an arbitrary BID index, it is impossible to discriminate between the graphs J_A, J_B and J_C).

5. Final remarks

There exists a broad class of irregular graphs called 2-walk linear graphs for which the neighborhood first Zagreb index can be easily computed. An irregular graph G is called 2-walk linear (more precisely, 2-walk (a, b)-linear) if there exists a unique integer pair (a, b) such that

$$S(u) = d(u)a(u) = ad(u) + b$$

holds for every vertex u of G, see [26]. As it is known, for a 2-walk (a, b) linear graph G, the corresponding spectral radius ρ can be calculated as

$$\rho = \frac{a + \sqrt{a^2 + 4b}}{2}.$$

It is important to note that semiregular and irregular harmonic graphs form subsets of 2-walk linear graphs, and in these particular cases, $a = 0$ for semiregular graphs, while $b = 0$ for irregular harmonic graphs. Based on the previous considerations, the neighborhood first Zagreb index of a 2-walk linear graph G is calculated as

$$NM_1(G) = \sum_{u \in V(G)} [ad(u) + b]^2 = a^2 M_1(G) + 4abm + nb^2. \tag{9}$$

Graphs H_1 and H_2 depicted in Figure 1 are 2-walk linear graphs with parameters $a = 1, b = 8$ and $a = 2, b = 4$, respectively. Using Equation (9), it is easy to check that $NM_1(H_1) = 1158$ and $NM_1(H_2) = 624$.

We close this paper by mentioning the following graph invariants which depend on the average degrees of a graph's vertices.

$$I_3(G) = \sum_{u \in V(G)} f_3(S(u), d(u)) \quad \text{and} \quad I_4(G) = \sum_{uv \in E(G)} f_4(a(u), a(v)).$$

It is noted that the invariants $I_3^*(G) = \sum_{u \in V(G)} f_3^*(a(u))$ and $I_3^{**}(G) = \sum_{u \in V(G)} f_3^{**}(d(u), a(u))$ are special cases of I_3. Initial observation on the invariants I_3 and I_4 gives us a hope that some choices of the functions f_3 and f_4 may correspond to some good predictors of certain properties of chemical compounds. It needs to be mentioned here that some special cases of I_3 and I_4 have already been appeared in literature: for example, if $f_3(a(u)) = \frac{1}{a(u)}$, $a(u)$ or $\frac{a(u)}{n}$ then I_3 gives the inverse dual degree [15, 34], symmetric division deg index [12, 37], average neighbor degree number [12, 33], where n is order of the graph under consideration, and if $f_4(a(u), a(v)) = a(u) + a(v)$ then I_4 is the first Zagreb index M_1 because

$$\sum_{u \in V(G)} h(u) = \sum_{uv \in E(G)} \left(\frac{h(u)}{d(u)} + \frac{h(v)}{d(v)} \right) \quad \text{(see [12])}$$

and hence

$$M_1(G) = \sum_{u \in V(G)} S(u) = \sum_{u \in V(G)} d(u)a(u) = \sum_{uv \in E(G)} [a(u) + a(v)].$$

References

[1] H. Abdo, D. Dimitrov, T. Reti, D. Stevanović, Estimation of the spectral radius of graph by the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 741–751.
[2] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 5–84.
[3] A. Ali, Z. Raza, A. A. Bhatti, Bond incident degree (BID) indices of polyomino chains: a unified approach, *Appl. Math. Comput.* **287-288** (2016) 28–37.
[4] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalizations: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 249–311.
[5] D. Bonchev, L. B. Kier, Topological atomic indices and the electronic changes in alkanes, *J. Math. Chem.* **9** (1992) 75–85.
[6] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.
[7] B. Borovićanin, S. Grünewald, I. Gutman, M. Petrović, Harmonic graphs with a small number of cycles, *Discrete Math.* **26** (2003) 31–44.
[8] D. S. Cao, Bounds on eigenvalues and chromatic numbers, *Linear Algebra Appl.* **270** (1998) 1–13.
[9] K. C. Das, Maximizing the sum of the squares of the degrees, *Discrete Math.* **285** (2004) 57–66.
[10] K. C. Das, K. Xu, J. Nam, Zagreb indices of graphs, *Front. Math. China* **10** (2015) 567–582.
[11] T. Došlić, T. Réti, Novel degree-based molecular descriptors with increased discriminating power, *Acta Polytech. Hung.* **9** (2012) 17–30.
[12] T. Došlić, T. Réti, D. Vukičević, On the vertex degree indices of connected graphs, *Chem. Phys. Lett.* **512** (2011) 283–286.
[13] A. Dress, I. Gutman, The number of walks in graphs, *Appl. Math. Left.* **16** (2003) 797–801.
[14] S. Fajtlowicz, On conjectures of Graffiti. II, *Congr. Numer.* **60** (1987) 187–197.
[15] S. Fajtlowicz, Written on the wall, a list of conjectures of Graffiti, University of Houston, Preprint.
[16] M. Ghorbani, M. A. Hosseinzadeh, Computing ABC_4 index of nanostar dendrimers, *Optoelectron. Adv. Mater. Rapid Commun.* **4** (2010) 1419–1422.
[17] C. Godsil, G. Royle, *Algebraic Graph Theory*, Springer-Verlag, New York, 2001.
[18] A. Graovac, M. Ghorbani, M. A. Hosseinzadeh, Computing fifth geometric-arithmetic index for nanostar dendrimers, *J. Math. Nanosci.* **1** (2011) 33–42.
[19] S. Grünewald, Harmonic trees, *Appl. Math. Lett.* **15** (2002) 1001–1004.
[20] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.
[21] I. Gutman, K. C. Das, The first Zagreb indices 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
[22] I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graph. Comb.*, DOI:10.1016/j.akcej.2018.05.002, In press.
[23] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.
[24] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors. Vertex-degree-based topological indices, *J. Serb. Chem. Soc.* **78** (2013) 805–810.
[25] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
[26] E. M. Hagos, Some results on graph spectra, *Linear Algebra Appl.* **356** (2002) 103–111.
[27] A. Ilić, S. Klavžar, M. Milanović, On distance-balanced graphs, *Eur. J. Comb.* **31** (2010) 733–737.
[28] B. Liu, Z. You, A survey on comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 581–593.
[29] I. Ž. Milovanović, V. M. Ćirić, I. Z. Milentijević, E. I. Milovanović. On some spectral, vertex and edge degree-based graph invariants, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 177–188.
[30] S. Mondal, N. De, A. Pal, On neighbourhood Zagreb index of product graphs, *arXiv*:1805.05273v1 [math.CO] (2018).
[31] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
[32] M. Petrović, B. Borovićanin, Z. Radosavljević, The integral 3-harmonic graphs, *Linear Algebra Appl.* **416** (2006) 298–312.
[33] T. Réti, I. Gutman, D. Vukičević, On Zagreb indices of pseudo-regular graphs, *J. Math. Nanosci.* **1** (2011) 1–12.
[34] M. K. Siu, Z. Zhang, S. Zhou, An inequality between the diameter and the inverse dual degree of a tree, *Discrete Math.* **259** (2002) 351–358.
[35] D. Stevanović, *Spectral Radius of Graphs,* Academic Press, Amsterdam, 2015.

[36] A. A. Toropov, A. P. Toropova, T. T. Ismailov, N. L. Voropaeva, I. N. Ruban, Extended molecular connectivity: predication of boiling points of alkanes, *J. Struct. Chem.* **38** (1997) 965–969.
[37] D. Vukičević, M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta* **83** (2010) 243–260.
[38] D. Vukičević, Bond additive modeling 4. QSPR and QSQR studies of the variable adriatic indices, *Croat. Chem. Acta* **84** (2011) 87–91.
[39] D. Vukičević, J. Durdević, Bond additive modelling 10. Upper and lower bounds of bond incident degree indices of catacondensed flouranthenes, *Chem. Phys. Lett.* **515** (2011) 186–189.
[40] S. Wang, B. Zhou, On the first extended zeroth-order connectivity index of trees, *Iran. J. Sci. Tech. A* **38** (2014) 213–219.
[41] A. Yu, M. Lu, F. Tian, On the spectral radius of graphs, *Linear Algebra Appl.* **387** (2004) 41–49.
[42] B. Zhou, N. Trinajstić, On extended connectivity indices, *J. Math. Chem.* **46** (2009) 1172–1180.