MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **53** (2005) 111-138

ISSN 0340 - 6253

On the discriminatory power of the Zagreb indices for molecular graphs*

Damir Vukičević[a] and Nenad Trinajstić[b]

[a]Department of Mathematics, The University of Split, Nikole Tesle 12, HR-21000 Split, Croatia (e-mail: vukicevi@pmfst.hr)
[b]The Rugjer Bošković Institute, P.O.B. 180, HR-10002 Zagreb, Croatia (e-mail: trina@irb.hr)

(Received August 20, 2004)

Abstract

An algorithm is presented for studying the discriminatory power of molecular descriptors, which is exemplified on the Zagreb M_2 index and the modified Zagreb $^*M_2$ index for molecular graphs. It is found that the Zagreb M_2 index is more discriminative quantity than the modified Zagreb $^*M_2$ index. This result is surprising since one would expect the reverse result because the Zagreb M_2 indices belong to the set of *natural* numbers whilst the modified Zagreb $^*M_2$ indices to the set of *rational* numbers.

The discriminatory power of the first two Randić connectivity indices: $^0\chi$ and $^1\chi$ was also investigated because the Randić indices are grounded in the Zagreb indices though they were obtained in quite a different way. In this case, it is obtained that $^0\chi$ and $^1\chi$ indices discriminate all graphs with up to 18 vertices. In the case of graphs with 19 vertices, it has been found a pair of graphs that cannot be discriminated by $^0\chi$ and $^1\chi$ indices.

*Dedicated to the memory of Professor Oskar E. Polansky (1919-1989).

1. Introduction

A pair of graph-theoretical invariants [1], denoted by symbols M_1 and M_2, have been introduced in 1972 by the Zagreb Mathematical Chemistry Group [2]. These invariants were soon used to study branching in (molecular) graphs [3] and were given name the Zagreb (group) indices [4]. The Zagreb indices belong to a family of molecular descriptors (also called topological indices [5]) that have found use in modeling properties of molecules [6,7] and are included in most computer programs used for routine computation of these descriptors [8,9].

The Zagreb M_1 index is the sum of squared vertex-degrees, whilst the M_2 index is the sum of edge-weights given as the products of degrees of incident vertices. The Zagreb indices were modified by summing up the inverse values of the squared vertex-degrees ($^*M_1$) and the inverse values of the edge-weights ($^*M_2$) [10]. In the present report we will consider only the Zagreb M_2 and $^*M_2$ indices since they possess unexpected properties [11], some of which will be discussed here. We considered their discriminatory power on the set of molecular graphs, that is, on a set of simple connected graphs with maximal vertex-degree 4. In order to do that, we developed a general algorithm for studying the discriminatory power on molecular descriptors that was first applied to Zagreb indices and then to the first two Randić connectivity indices: ${}^0\chi$ and ${}^1\chi$.

2. Main results

Let us define basic notation that we shall need in the sequel. Let G be any simple connected graph. By $\Delta(G)$ we denote maximal degree in graph G; by $\delta(G)$ minimal degree in G; by $V(G)$ the set of vertices of G; and by $E(G)$ the set of edges of G. Let X be any set of vertices in G. By $G[X]$ we denote graph induced by set X, i.e. graph which set of vertices is X and which edges are those edges of G that have both end-vertices in X. Let Y be any set of vertices of G disjoint from X. By $G[X,Y]$, we denote a graph such that $V(G[X,Y]) = X \cup Y$ and edges of $G[X,Y]$ are edges of G that have one incident vertex in X and other in Y.

We start with a several Lemmas:

Lemma 1. Let C_n be the cycle with n vertices and let e be number such that $1 \le e \le n$. Then there is a spanning subgraph G of C_n such that $\Delta(G)-\delta(G)\le 1$.

Lemma 2. Let $n \ge 5$ and let K_n be a complete graph with n vertices. Then it is possible to pack to cycles with n vertices in K_n.

Proof: Denote $V(K_n)=\{v_1,v_2,\dots,v_n\}$. Denote cycles with required properties by C' and C''. It is sufficient to take $E(C_1)=\{v_1v_2,v_2v_3,\dots,v_{n-1}v_n,v_nv_1\}$ and

$$E(C_2)=\begin{cases}\{v_1v_3,v_3v_5,\dots,v_{n-2}v_n,v_nv_2,v_2v_4,\dots,v_{n-3}v_{n-1}v_{n-1}v_1\}, & n \text{ is odd}\\ \{v_1v_3,v_3v_5,\dots,v_{n-3}v_{n-1},v_{n-1}v_2,v_2v_n,v_nv_{n-2},v_{n-2}v_{n-4},\dots,v_6v_4,v_4v_1\}, & n \text{ is even}\end{cases}$$

From these two Lemmas and simple analyses of cases when $n \le 4$, it follows:

Lemma 3. Let n_3 be any natural number and let p', p'' be any nonnegative integers such that $p' \le \frac{n_3\cdot(n_3-1)}{2}$ and $p'+p'' \le \frac{3n_3}{2}$, then there is a graph G with n_3 vertices and $p'+p''$ edges such that $\Delta(G)-\delta(G)\le 1$, and there is a simple subgraph of G with p' edges, and also if $p'+p''\ge n_3-1$, then G is connected and if $n_3 \ge 2$ there are no loops in G.

Lemma 4. Let n_4 be any natural number and let r', r'' be any nonnegative integers such that $r' \le \frac{n_4\cdot(n_4-1)}{2}$ and $r'+r''\le 2n_4$, then there is a graph G with n_4 vertices and $r'+r''$ edges such that $\Delta(G)-\delta(G)\le 1$ and there is a simple subgraph of G with r' edges, and also if $r'+r''\ge n_4-1$, then G is connected and if $n_4 \ge 2$ there are no loops in G.

We also prove:

Lemma 5. Let k,l be a natural numbers and let $a_1,a_2,\dots,a_l,b_1,\dots,b_k$ be a nonnegative integers and let

$$\max\{b_1,\dots,b_l\}\le \min\{b_1,\dots,b_l\}+1$$

$$q \le \min\left\{\sum_{i=1}^{k}\min\{a_i,l\},\sum_{i=1}^{l}b_i\right\}.$$

Then there is a simple bipartite graph G with q edges and partition classes $A=\{x_1,\dots,x_k\}$ and $B=\{y_1,\dots y_l\}$ such that $d_G(x_i)\le a_i$ for each $i=1,\dots,k$ and $d_G(y_i)\le b_i$ for each $i=1,\dots,l$.

Proof: We prove the claim by induction on k. If $k = 1$, the claim is trivial. Let us prove the inductive step. Distinguish three cases:

1) $\min\left\{l, d_G(a_k), \sum_{i=1}^{l} b_i\right\} = l$.

In this case, we have $q - l \le \min\left\{\sum_{i=1}^{k-1}\min\{a_i, l\}, \sum_{i=1}^{l} b_i - 1\right\}$, therefore there is, by inductive hypothesis a bipartite graph G' with partition classes $\{a_1, \dots, a_{k-1}\}$ and B such that $d_G(x_i) \le a_i$ for each $i = 1, \dots, k-1$ and $d_G(y_i) \le b_i - 1$ for each $i = 1, \dots, l$. Graph $G = G' + \{a_k b_1, \dots, a_k b_l\}$ has the required properties.

2) $\min\left\{l, d_G(a_k), \sum_{i=1}^{l} b_i\right\} = d_G(a_k)$.

Without loss of generality, we may assume that $b_1 \ge b_2 \ge \dots \ge b_l$. In this case, we have

$$\max\left\{b_1 - 1, \dots, b_{d_G(x_k)} - 1, b_{d_G(x_k)+1}, \dots, b_l\right\} - \min\left\{b_1 - 1, \dots, b_{d_G(x_k)} - 1, b_{d_G(x_k)+1}, \dots, b_l\right\} \le 1;$$

$$\min\left\{\sum_{i=1}^{k-1}\min\{a_i, l\}, \sum_{i=1}^{d_G(x_k)}(b_i - 1) + \sum_{i=d_G(x_k)+1}^{l} b_i\right\},$$

Therefore there is, by inductive hypothesis a bipartite graph G' with partition classes $\{a_1, \dots, a_{k-1}\}$ and B such that $d_G(x_i) \le a_i$ for each $i = 1, \dots, k-1$, and $d_G(y_i) \le b_i - 1$ for each $i = 1, \dots, d_G(x_k)$, and $d_G(y_i) \le b_i$ for each $i = 1, \dots, d_G(x_k)$. Graph $G = G' + \left\{a_k b_1, \dots, a_k b_{d_G(x_k)}\right\}$ has the required properties.

3) $\min\left\{l, d_G(a_k), \sum_{i=1}^{l} b_i\right\} = \sum_{i=1}^{l} b_i$.

This case is trivial.

All the cases are exhausted and the claim is proved.

Now, we can prove:

Lemma 6. Let n_3 and n_4 be natural numbers and p', p'', q', q'', r' and r'' nonnegative integers such that:

$a)\ p+q+r \geq n_3+n_4-1;$

$b)\ 2p+q \leq n_3;$

$c)\ 2r+q \leq n_4;$

$d)\ p+q \geq n_3;$

$e)\ q+r \geq n_4;$

$f)\ q \geq 1;$

$g)\ p' \leq \dfrac{n_3 \cdot (n_3-1)}{2};$

$h)\ q' \leq n_3 \cdot n_4;$

$i)\ r' \leq \dfrac{n_4 \cdot (n_4-1)}{2},$

where $p = p'+p"$, $q = q'+q"$ and $r = r'+r"$. Then there is a connected graph G such that :

1) $V(G) = N_3 \cup N_4; |N_3| = n_3; |N_4| = n_4;$

2) $d_G(x) \leq 3,$ for each $x \in N_3$; $d_G(x) \leq 4,$ for each $x \in N_4$;

3) $e(G[N_3]) = p'+p"; e(G[N_3,N_4]) = q'+q"; e(G[N_4]) = r'+r";$

4) there is a simple subgraph of $G[N_3]$ with p' edges;

5) there is a simple subgraph of $G[N_3,N_4]$ with q' edges;

6) there is a simple subgraph of $G[N_4]$ with r' edges;

7) if $G[N_3]>1$, there are no loops in $G[N_3]$; if $G[N_4]>1$, there are no loops in $G[N_4]$.

Proof: Denote $N_3 = \{x_1,...,x_{n_3}\}$ and $N_4 = \{y_1,...,y_{n_4}\}$. First, let us prove that there is a graph G_1 with the following properties:

I) $V(G_1) = N_3 \cup N_4; |N_3| = n_3; |N_4| = n_4;$

II) $d_{G_1}(x) \leq 3,$ for each $x \in N_3$; $d_{G_1}(x) \leq 4,$ for each $x \in N_4$;

III) $e(G_1[N_3]) = p'+p"; e(G_1[N_3,N_4]) = q'; e(G_1[N_4]) = r'+r";$

IV) there is a simple subgraph of $G_1[N_3]$ with p' edges;

V) $G_1[N_3,N_4]$ is a simple subgraph;

VI) there is a simple subgraph of $G_1[N_3]$ with r' edges.

VII) if $G[N_3]>1$, there are no loops in $G[N_3]$; if $G[N_4]>1$, there are no loops in $G[N_4]$.

Since the relations b) and g) hold, it follows that requirements of Lemma 3 are fulfilled, so there is a graph $G_1[N_3]$ that satisfies the conditions described in Lemma 3. Analogously, since the relations c) and i) hold, it follows that requirements of Lemma 4 are fulfilled, so there is a graph $G_1[N_4]$ that satisfies the conditions described in Lemma 4. Note that

$$\max\left\{4-d_{G_1[N_3]}(x_1),....,3-d_{G_1[N_3]}(x_{n_3})\right\}-\min\left\{4-d_{G_1[N_4]}(y_1),....,4-d_{G_1[N_4]}(y_{n_4})\right\}\le 1.$$

So, form the previous Lemma, it follows that it is sufficient to prove that

$$q'\le \min\left\{\sum_{i=1}^{n_3}\min\left\{3-d_{G_1[N_3]}(x_i),n_4\right\},\sum_{i}^{n_4}\left(4-d_{G_1[N_4]}(y_i)\right)\right\}. \qquad (*)$$

Note, that

$$\max\left\{3-d_{G_1[N_3]}(x_1),....,3-d_{G_1[N_3]}(x_{n_3})\right\}-\min\left\{3-d_{G_1[N_3]}(x_1),....,3-d_{G_1[N_3]}(x_{n_3})\right\}\le 1.$$

Therefore, the expression (*) is equivalent to

$$q'\le \min\left\{\sum_{i=1}^{n_3}\min\left\{3-d_{G_1}(x_i)\right\},\sum_{i}^{n_4}\left(4-d_{G_1}(y_i)\right),n_3n_4\right\}.$$

Simple computation shows that this is equivalent to

$$q'\le \min\left\{3n_3-2p,4n_4-2r,n_3n_4\right\}.$$

Hence, it is sufficient to prove that $q'\le n_3n_4$. Note that $q'\le n_3+n_4-1$, so it remains to prove that $n_3+n_4-1\le n_3n_4$ or equivalently that $(n_3-1)(n_4-1)\ge 0$, which is true.

Note that $q''\le \min\left\{4n_4-2p-q',3n_3-2r-q'\right\}$ or equivalently, that

$$q''\le \min\left\{3n_3-\sum_{i=1}^{n_3}d_{G_1}(x_i),4n_4-\sum_{i=1}^{n_4}d_{G_1}(y_i)\right\},$$

so it can be easily seen that there is a supergraph G_2 of graph G_1 that satisfies properties 1)-7). Now, let us observe the family G of graphs H such that:

I) $V(H)=N_3\cup N_4$; $H[N_3]=G_2[N_3]; H[N_4]=G_2[N_4]$;

II) $e(H[N_3,N_4])=q+q'$ and there is a simple subgraph of $H[N_3,N_4]$ with q' edges.

Note that G is not empty since at least G_2 is in G. Denote by G graph with the smallest number of components in G. It is sufficient to prove that G is connected. Suppose to the contrary. Distinguish four cases:

CASE 1: $p \geq n_3 - 1$ and $r \geq n_4 - 1$.

Note that $H[N_3] = G_2[N_3]$ and $H[N_4] = G_2[N_4]$ are connected and that $q \geq 1$. Hence G is connected. Contradiction.

CASE 2: $p \geq n_3 - 1$ and $r < n_4 - 1$.

Note, $H[N_3] = G_2[N_3]$ is connected. Since $q + r \geq n_4$, it follows that q is not less then number of components in $G[N_4]$. Hence, there is a component C_1 in G that has two edges in $E(G[N_3, N_4])$. Denote one of them by $x_i y_i$. Let C_2 be any other component of G (note that $V(C_2) \subseteq N_4$) and y_j any vertex of C_2. Note that graph $G - x_i y_i + x_i y_j$ is in G and that it has a smaller number of components then G. Contradiction.

CASE 3: $p < n_3 - 1$ and $r \geq n_4 - 1$

Note, $H[N_4] = G_2[N_4]$ is connected. Since $q + p \geq n_3$, it follows that q is not less then number of components in $G[N_3]$. Hence, there is a component C_1 in G that has two edges in $E(G[N_3, N_4])$. Denote one of them by $x_i y_i$. Let C_2 be any other component of G (note that $V(C_2) \subseteq N_3$) and x_j any vertex of C_2. Note that graph $G - x_i y_i + x_j y_i$ is in G and that it has a smaller number of components then G. Contradiction.

CASE 4: $p < n_3 - 1$ and $r < n_4 - 1$.

Note that $H[N_3] = G_2[N_3]$ and $H[N_4] = G_2[N_4]$ are acyclic. Since $p + q + r \geq n_3 + n_4 - 1$, there is a component C that contains a cycle. There is at least one edge in C which is in $G[N_3, N_4]$ which is not a cut-edge of C. Denote this edge by xy such that $x \in N_3$ and $y \in N_4$. Let C' be any other component. Distinguish three cases:

1) $V(C') \subseteq N_3$.

Let $c \in V(C')$ be an arbitrary vertex. Graph $G - xy + yc$ is in G and it has a smaller number of components then G, which is contradiction.

2) $V(C') \subseteq N_4$.

Let $c \in V(C')$ be an arbitrary vertex. Graph $G - xy + xc$ is in G and it has a smaller number of components then G, which is contradiction.

3) $V(C')\cap N_3 \neq \varnothing$ and $V(C')\cap N_4 \neq \varnothing$.

There is an edge $x'y'$ such that $x'\in N_3$ and $y'\in N_4$ in C'. Graph $G-xy+x'y'+xy'+x'y$ is in G and it has a smaller number of components then G, which is contradiction.

We have obtained a contradiction in each case, so our claim is proved.

Let us prove our main theorem:

Theorem 7. Let n_1 and n_2 be any nonnegative integers and n_3 and n_4 be any natural numbers such that there is a molecular graph H such that $\nu(H)=(n_1,n_2,n_3,n_4)$ and let $m_{11},m_{12},m_{13},m_{14},m_{22},m_{23},m_{24},m_{33},m_{34}$ and m_{44} be any nonnegative integers. Then there is a molecular graph G such that $\nu(G)=(n_1,n_2,n_3,n_4)$ and that

$$\mu(H)=(m_{11},m_{12},m_{13},m_{14},m_{22},m_{23},m_{24},m_{33},m_{34},m_{44})$$

if and only if the following conditions hold:

1) $n_1 = m_{11}+m_{12}+m_{13}+m_{14}$;

2) $2n_2 = m_{12}+2m_{22}+m_{23}+m_{24}$;

3) $3n_3 = m_{13}+m_{23}+2m_{33}+m_{34}$;

4) $4n_4 = m_{14}+m_{24}+m_{34}+2m_{44}$;

5) $s=(m_{23}+m_{24}-m_{12})/2$ is nonnegative integer;

6) $s+m_{33}+m_{34}+m_{44}\geq n_3+n_4-1$;

7) $n_3 \leq s+m_{33}+m_{34}$;

8) $n_4 \leq s+m_{34}+m_{44}$;

9) $n_3 \leq m_{23}+m_{33}+m_{34}$;

10) $n_4 \leq m_{24}+m_{34}+m_{44}$;

11) $m_{34}+m_{24}\geq 1$;

12) $m_{34}+m_{23}\geq 1$;

13) $m_{34}+s\geq 1$;

14) $(n_3\geq 2)$ or $(s\leq \mathrm{m}_{22}+m_{24})$;

15) $(n_4\geq 2)$ or $(s\leq m_{23}+m_{22})$;

16) $(m_{12}+m_{23}+m_{24}>0)$ or $(m_{22}=0)$;

17) $m_{33} \le \frac{n_3 \cdot (n_3 - 1)}{2}$;

18) $m_{34} \le n_3 \cdot n_4$;

19) $m_{44} \le \frac{n_4 \cdot (n_4 - 1)}{2}$.

20) $m_{11} = 0$

Proof: First, let us prove sufficiency. The relations 1) – 4) and 17) – 20) are trivial. Since, G is connected 16) follows. Denote by S the set of all induced cycles and all induced paths of length at least two with both terminal edges of degree at least three in G. Note that $|S| = s$, hence 5) holds. Let G_1 be a graph obtained by replacing each path in S by a single edge and each cycle in S by a single loop and elimination of each vertex of degrees 1 and 2 in G and their adjacent edges. Note that G_1 has $s + m_{33} + m_{34} + m_{44}$ edges and $n_3 + n_4$ vertices. Since G_1 is connected, it follows that 6) holds. Let G_2 be a graph obtained from graph G_1 by contraction of all vertices that are in N_4 to a single vertex. Note that G_2 has $n_3 + 1$ vertices and at most $m_{33} + m_{34} + s$ edges that are not loops. Since G_2 is connected, it follows that 7) holds. Analogously, let G_3 be a graph obtained from graph G_1 by contraction of all vertices that are in N_3 to a single vertex. Note that G_3 has $n_4 + 1$ vertices and at most $m_{44} + m_{34} + s$ edges that are not loops. Since G_3 is connected, it follows that 8) holds. Let G_4 be a graph obtained from graph G by elimination of each vertex of degree 1 and its adjacent edge and contraction of all vertices of degrees 2 and 4 to a single vertex. Graph G_4 has $n_3 + 1$ vertices and at most $m_{23} + m_{33} + m_{34}$ edges that are not loops. Connectivity of G_4 implies 9). Analogously, let G_5 be a graph obtained from graph G by elimination of each vertex of degree 1 and its adjacent edge and contraction of all vertices of degrees 2 and 3 to a single vertex. Graph G_5 has $n_4 + 1$ vertices and at most $m_{24} + m_{34} + m_{44}$ edges that are not loops. Connectivity of G_5 implies 10). Since G is connected, it follows that $e(G[N_3, N_2 \cup N_4]) \ne \varnothing$ and $e(G[N_4, N_2 \cup N_3]) \ne \varnothing$, therefore 11) and 12) hold. Since G_1 is connected, it follows that $e(G_1[N_3, N_4]) \ne \varnothing$, therefore 13) holds.

Suppose that x is only vertex in N_3. Let S_x be a set of all induced cycles in G that contain vertex x. Note that $|S_x| \geq s - m_{24}$ and that each of this cycles has at least three edges, because G is simple. Therefore, each of these edges has at least one edge that connects two vertices of degree 2. It follows that $m_{22} \geq |S_x| \geq s - m_{24}$ and 14) holds. The relation 15) can be proved by a complete analogy.

Now, let us prove necessity. Denote $t = m_{33} + m_{34} + m_{44}$. Note that

$$\max\left\{\begin{matrix} t - m_{33} - m_{34} - m_{23}, \\ m_{44} \end{matrix}\right\} \leq \min\left\{\begin{matrix} t - n_3, \\ 2m_{44} + m_{34} + m_{24} - n_4, \\ (2m_{44} + m_{24})/2, \\ (2m_{44} + m_{24} + m_{34} - 1)/2, \\ t - m_{33} - m_{34}, \\ t - 1 - m_{33} \end{matrix}\right\}.$$

Hence, there is a nonnegative integer r such that

$$\max\left\{\begin{matrix} t - m_{33} - m_{34} - m_{23}, \\ m_{44} \end{matrix}\right\} \leq r \leq \min\left\{\begin{matrix} t - n_3, \\ 2m_{44} + m_{34} + m_{24} - n_4, \\ (2m_{44} + m_{24})/2, \\ (2m_{44} + m_{24} + m_{34} - 1)/2, \\ t - m_{33} - m_{34}, \\ t - 1 - m_{33} \end{matrix}\right\}.$$

Now, we have

$$\max\left\{\begin{matrix} r + t - 2m_{44} - m_{34} - m_{24}, \\ m_{44} \end{matrix}\right\} \leq \min\left\{\begin{matrix} 2m_{33} + m_{34} + m_{23} + r - t, \\ t - n_4, \\ t - m_{34} - r, \\ t - 1 - r \end{matrix}\right\}.$$

Therefrom, it follows that there is a nonnegative integer p such that

$$\max\left\{\begin{matrix} r + t - 2m_{44} - m_{34} - m_{24}, \\ m_{44} \end{matrix}\right\} \leq p \leq \min\left\{\begin{matrix} 2m_{33} + m_{34} + m_{23} + r - t, \\ t - n_4, \\ t - m_{34} - r, \\ t - 1 - r \end{matrix}\right\}.$$

Put $r = t - p - q$; $p' = m_{33}$; $p'' = p - p'$; $q' = m_{34}$; $q'' = q - q'$; $r' = m_{44}$; $r'' = r - r'$. Note that $p', p'', q', q'', r', r''$ are nonnegative integers that satisfie conditions of the Lemma 6. Therefore, there is a graph G_1 with the properties described in the Lemma 6. Denote by

H_{33}, H_{34} and H_{44} respectively simple subgraph of $G_1[N_3]$ with p' edges, simple subgraph of $G_1[N_3, N_4]$ with q' edges and simple subgraph of $G_1[N_4]$ with r' edges. Let G_2 be a graph obtained from graph G_1 by replacing each edge in the set

$$E(G)\setminus\left(E(H_{33})\cup E(H_{34})\cup E(H_{44})\right)$$

by a path of length 2 and adding to each vertex x in N_3 exactly $3-d_{G_1}(x)$ neighbors of degree 1 and to each vertex y in N_4 exactly $4-d_{G_1}(y)$ neighbors of degree 1. Note that $\mu_{23}(G_2)\le m_{23}\le \mu_{23}(G_2)+\mu_{12}(G_2)$ and that $\mu_{24}(G_2)\le m_{24}\le \mu_{24}(G_2)+\mu_{12}(G_2)$. Choose $m_{23}-\mu_{23}(G_2)$ edges that connect vertices of degree 1 and 3 in G_2 and $m_{24}-\mu_{24}(G_2)$ edges that connect vertices of degree 1 and 4 in G_2 and replace each of them by a path of length 2. Denote graph obtained in this way by G_3. If $m_{22}=0$, it is sufficient to take $G=G_3$. Otherwise, let G be a graph obtained from G_3 by replacing any edge incident to the vertex of degree 2 by a path of length m_{22}. Graph G has the required properties.

By a similar, but somewhat more simple techniques, one can prove:

Theorem 8. Let n_1 and n_2 be any nonnegative integers and let n_4 be any natural numbers such that there is a molecular graph H such that $\nu(H)=(n_1,n_2,0,n_4)$ and let $m_{11}, m_{12}, m_{14}, m_{22}, m_{24}$ and m_{44} be any nonnegative integers. Then there is a molecular graph G such that $\nu(G)=(n_1,n_2,0,n_4)$ and that

$$\mu(H)=(m_{11},m_{12},0,m_{14},m_{22},0,m_{24},0,0,m_{44})$$

if and only if the following conditions hold:

1) $n_1=m_{11}+m_{12}+m_{14}$;

2) $2n_2=m_{12}+2m_{22}+m_{24}$;

3) $4n_4=m_{14}+m_{24}+2m_{44}$;

4) $(m_{24}-m_{12})/2$ is a nonnegative integer;

5) $(m_{22}=0)$ or $(m_{12}+m_{24}>0)$;

6) $m_{44}\le\dfrac{n_4\cdot(n_4-1)}{2}$;

7) $(n_4\ge 2)$ or $(\mathrm{m}_{22}\ge(m_{24}-m_{12})/2)$

8) $m_{11} = 0$.

Theorem 9. Let n_1 and n_2 be any nonnegative integers and let n_3 be any natural numbers such that there is a molecular graph H such that $\nu(H) = (n_1, n_2, n_3, 0)$ and let $m_{11}, m_{12}, m_{13}, m_{22}, m_{23}$ and m_{33} be any nonnegative integers. Then there is a molecular graph G such that $\nu(G) = (n_1, n_2, n_3, 0)$ and that

$$\mu(H) = (m_{11}, m_{12}, m_{13}, 0, m_{22}, m_{23}, 0, m_{33}, 0, 0)$$

if and only if the following conditions hold:

1) $n_1 = m_{11} + m_{12} + m_{13}$;

2) $2n_2 = m_{12} + 2m_{22} + m_{23}$;

3) $3n_3 = m_{13} + m_{23} + 2m_{33}$;

4) $(m_{23} - m_{12})/2$ is a nonnegative integer;

5) $(m_{22} = 0)$ or $(m_{12} + m_{23} > 0)$;

6) $m_{33} \leq \dfrac{n_3 \cdot (n_3 - 1)}{2}$;

7) $(n_3 \geq 2)$ or $(\mathrm{m}_{22} \geq (m_{23} - m_{12})/2)$;

8) $m_{11} = 0$.

Theorem 10. Let n_1 and n_2 be any nonnegative numbers such that there is a molecular graph H such that $\nu(H) = (n_1, n_2, 0, 0)$ and let m_{11}, m_{12} and m_{22} be any nonnegative integers. Then there is a molecular graph G such that $\nu(G) = (n_1, n_2, 0, 0)$ and that

$$\mu(H) = (m_{11}, m_{12}, 0, 0, m_{22}, 0, 0, 0, 0, 0)$$

if and only if one of the following conditions hold:

1) $m_{11} = 1; m_{12} = 0; m_{22} = 0; n_1 = 2; n_2 = 0$;

2) $m_{11} = 0; m_{12} = 0; m_{22} = n_2; n_1 = 0; n_2 \geq 3$;

3) $m_{11} = 0; m_{12} = 2; m_{22} = n_2 - 1; n_1 = 2; n_2 = 0$.

It remains to prove:

Theorem 11. Let $n \geq 3$ and let n_1, n_2, n_3 and n_4 be nonnegative natural numbers such that $n_1 + n_2 + n_3 + n_4 = n$. There is a molecular graph G such that $\nu(G) = (n_1, n_2, n_3, n_4)$ if and only if the following conditions hold:

1) $n_3 + 2n_4 \geq n_1 - 2$

2) $\frac{3n_3 + 4n_4 - n_1}{2} - n_2 \leq \binom{n_3 + n_4}{2}$.

3) $n_1 + n_3$ is an even number.

4) If $n_3 + n_4 = 1$ then $n_2 \geq 3n_3 + 4n_4 - n_1$

Proof: First let us prove sufficiency. Since G is connected, we have

$$\frac{n_1 + 2n_2 + 3n_3 + 4n_4}{2} \geq n_1 + n_2 + n_3 + n_4 - 1,$$

which is equivalent to 1). Let G_1 be the graph obtained from graph G by elimination of each vertex of degree 1 or 2 together with its adjacent edges. Note that G_1 has $n_3 + n_4$ vertices and at least $\frac{3n_3 + 4n_4 - 2n_2 - n_1}{2}$ edges. Since G_1 is simple, it follows 2). The handshaking lemma implies 3). It remains to prove 4). Let x be the only vertex of degree 3 or 4. Note that each induced cycle in G has at least two vertices of degree 2 and that number of induced cycles is $\frac{3n_3 + 4n_4 - n_1}{2}$ which implies 4).

Now, let us prove sufficiency. If $n_3 + n_4 \leq 1$, the claim is trivial, so suppose that $n_3 + n_4 > 1$. Distinguish two cases:

CASE 1: $\frac{3n_3 + 4n_4 - n_1}{2} \leq \binom{n_3 + n_4}{2}$.

Put in Lemma 4 instead of n_4 number $n_3 + n_4$, and instead of r' number $\frac{3n_3 + 4n_4 - n_1}{2}$, and instead of r'' number 0. Now, this Lemma assures the existence of the simple connected graph H such that $\Delta(H) - \delta(H) \leq 1$. Note that at least n_3 vertices in H have degree less or equal 3. Let n_3 of this vertices form the set N_3 and let all other vertices form the set N_4. Add to each vertex x in N_3 exactly $3 - d_H(x)$ neighbors of degree 1 and add to each vertex x in

N_4 exactly $4-d_H(x)$ neighbors of degree 1. Now, replace any edge by a path of length n_2+1. Graph obtained in this way has the required properties.

CASE 2: $\frac{3n_3+4n_4-n_1}{2} > \binom{n_3+n_4}{2}$.

Put in Lemma 4 instead of n_4 number n_3+n_4, and instead of r' number $\binom{n_3+n_4}{2}$, and instead of r'' number $\frac{3n_3+4n_4-n_1}{2} - \binom{n_3+n_4}{2}$. Now, this Lemma assures the existence of the connected graph H such that $\Delta(H) \leq 4$ and $\Delta(H)-\delta(H) \leq 1$ without loops such that tit is a supergraph of complete graph H' with n_3+n_4 vertices. Note that at least n_3 vertices in H have degree less or equal 3. Let n_3 of this vertices form the set N_3 and let all other vertices form the set N_4. Add to each vertex x in N_3 exactly $3-d_H(x)$ neighbors of degree 1 and add to each vertex x in N_4 exactly $4-d_H(x)$ neighbors of degree 1. Now, replace all edges in $E(H)\setminus E(H')$ by a path of length 2. After that, choose any edge and replace it by the path of length $n_2 - \left(\frac{3n_3+4n_4-n_1}{2} - \binom{n_3+n_4}{2}\right)+1$. Graph obtained in this way has the required properties.

3. Algorithm

First, we present an algorithm that generates 4-tuples (n_1,n_2,n_3,n_4) such that $n_1+n_2+n_3+n_4=n$ and that there is a molecular graph G such that $\nu(G)=(n_1,n_2,n_3,n_4)$. The procedure x is any procedure that utilize this algorithm.

GenNumVer(n)

1) if $n=2$ then

1.1) $x(2,0,0,0)$

2) else if $n>2$

2.1) for each n_1 such that $0 \leq n_1 \leq n$

2.1.1) for each n_2 such that $0 \le n_2 \le n - n_1$

2.1.1.1) for each n_3 such that $0 \le n_3 \le n - n_1 - n_2$

2.1.1.1.1) $n_4 = n - n_1 - n_2 - n_3$

2.1.1.1.2) if $\begin{bmatrix} [n_3 + 2n_4 \ge n_1 - 2] \text{ and} \\ [(3n_3 + 4n_4 - n_1)/2 - n_2 \le (n_3 + n_4)(n_3 + n_4 - 1)/2] \text{ and} \\ [n_1 + n_3 = 0 \pmod 2] \text{ and } [(n_3 + n_4 \ne 1) \text{ or } (n_2 \ge 3n_3 + 4n_4 - n_1)] \end{bmatrix}$ then

2.1.1.1.2.1) $x(n_1, n_2, n_3, n_4)$

Now, we present an algorithm that, for each $n_1, n_2, n_3, n_4 \in \mathbb{N}_0$ such that there is a molecular graph G such that $\nu(G) = (n_1, n_2, n_3, n_4)$ generates 10-tuples

$$(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$$

such that there is a molecular graph H such that $\nu(H) = (n_1, n_2, n_3, n_4)$ and that $\mu(H) = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$. Again, procedure x is any procedure that utilize this algorithm.

GenNumEdges(n)

1) if $(n_3 = 0)$ and $(n_4 = 0)$ then

1.1) if $n_2 = 0$ then

1.1.1) $x(1,0,0,0,0,0,0,0,0,0)$

1.2) else if $n_1 = 0$ then

1.2.1) $x(0,0,0,0,n_2,0,0,0,0,0)$

1.3) else

1.3.1) $x(0,2,0,0,n_2 - 1,0,0,0,0,0)$

2) else if $n_3 = 0$ then

2.1) for each m_{12} such that $0 \le m_{12} \le \min\{n_1, 2n_2\}$

2.1.1) $m_{14} = n_1 - m_{12}$

2.1.2) if $m_{14} \le 4n_4$ then

2.1.2.1) for each m_{22} such that $0 \le m_{22} \le (2n_2 - m_{12})/2$

2.1.2.1.1) $m_{24} = 2n_2 - m_{12} - 2m_{22}$

2.1.2.1.2) $m_{44} = (4n_4 - m_{14} - m_{24})/2$

2.1.2.1.3) if $m_{44} \geq 0$ then

2.1.2.1.3.1) if $\begin{bmatrix} [m_{24} - m_{12} = 0 \pmod 2] \text{ and } [m_{24} - m_{12} \geq 0] \text{ and} \\ [(m_{22} = 0) \text{ or } (m_{12} + m_{24} > 0)] \text{ and} \\ [m_{44} \leq n_4(n_4 - 1)/2] \text{ and } [(n_4 \geq 2) \text{ or } (m_{22} \geq (m_{24} - m_{12})/2)] \end{bmatrix}$ then

2.1.2.1.3.1.1) $x(0, m_{12}, 0, m_{14}, m_{22}, 0, m_{24}, 0, 0, m_{44})$

3) if $n_4 = 0$ then

3.1) for each m_{12} such that $0 \leq m_{12} \leq \min\{n_1, 2n_2\}$

3.1.1) $m_{13} = n_1 - m_{12}$

3.1.2) if $m_{13} \leq 3n_3$ then

3.1.2.1) for each m_{22} such that $0 \leq m_{22} \leq (2n_2 - m_{12})/2$

3.1.2.1.1) $m_{23} = 2n_2 - m_{12} - 2m_{22}$

3.1.2.1.2) $m_{33} = (3n_3 - m_{13} - m_{23})/2$

3.1.2.1.3) if $m_{33} \geq 0$ then

3.1.2.1.3.1) if $\begin{bmatrix} [m_{23} - m_{12} = 0 \pmod 2] \text{ and } [m_{23} - m_{12} \geq 0] \text{ and} \\ [(m_{22} = 0) \text{ or } (m_{12} + m_{23} > 0)] \text{ and} \\ [m_{33} \leq n_3(n_3 - 1)/2] \text{ and } [(n_3 \geq 2) \text{ or } (m_{22} \geq (m_{23} - m_{12})/2)] \end{bmatrix}$ then

3.1.2.1.3.1.1) $x(0, m_{12}, 0, m_{14}, m_{22}, 0, m_{24}, 0, 0, m_{44})$

4) else

4.1) for each m_{12} such that $0 \leq m_{12} \leq \min\{n_1, 2n_2\}$

4.1.1) for each m_{13} such that $0 \leq m_{13} \leq \min\{n_1 - m_{12}, 3n_3\}$

4.1.1.1) $m_{14} = n_1 - m_{12} - m_{13}$

4.1.1.2) if $m_{14} \leq 4n_4$ then

4.1.1.2.1) for each m_{22} such that $0 \leq m_{22} \leq (2n_2 - m_{12})/2$

4.1.1.2.1.1) for each m_{23} such that $0 \leq m_{23} \leq \min\{2n_2 - m_{12} - 2m_{22}, 3n_3 - m_{13}\}$

4.1.1.2.1.1.1) $m_{24} = 2n_2 - m_{12} - 2m_{22} - m_{23}$

4.1.1.2.1.1.2) if $m_{14} + m_{24} \le 4n_4$

4.1.1.2.1.1.2.1) for each m_{33} such that $0 \le m_{33} \le (3n_3 - m_{13} - m_{23})/2$

4.1.1.2.1.1.2.1.1) $m_{34} = 3n_3 - m_{13} - m_{23} - 2m_{33}$

4.1.1.2.1.1.2.1.2) $m_{44} = (4n_4 - m_{14} - m_{24} - m_{34})/2$

4.1.1.2.1.1.2.1.3) if $m_{44} \ge 0$ then

4.1.1.2.1.1.2.1.3.1) $s = (m_{23} + m_{24} - m_{12})/2$

4.1.1.2.1.1.2.1.3.2) if $s \ge 0$

4.1.1.2.1.1.2.1.3.2.1) $t = s + m_{33} + m_{34} + m_{44}$

4.1.1.2.1.1.2.1.3.2.2) if $\left[\begin{array}{l} [t \ge n_3 + n_4 - 1] \text{ and } [n_3 \le s + m_{33} + m_{34}] \text{ and} \\ [\mathrm{n}_4 \le s + m_{34} + m_{44}] \text{ and } [\mathrm{n}_3 \le m_{23} + m_{33} + m_{34}] \text{ and} \\ [n_4 \le m_{24} + m_{34} + m_{44}] \text{ and } [\mathrm{m}_{34} + m_{24} \ge 1] \text{ and} \\ [m_{34} + m_{23} \ge 1] \text{ and } [m_{34} + s \ge 1] \text{ and} \\ [(n_3 \ge 2) \text{ or } (\mathrm{s} \le \mathrm{m}_{22} + m_{24})] \text{ and} \\ [(n_4 \ge 2) \text{ or } (\mathrm{s} \le \mathrm{m}_{22} + m_{23})] \text{ and} \\ [(m_{12} + m_{23} + m_{24} > 0) \text{ or } (m_{22} = 0)] \text{ and} \\ \left[m_{33} \le \binom{n_3}{2}\right] \text{ and } [m_{34} \le n_3 n_4] \text{ and } \left[m_{44} \le \binom{n_4}{2}\right] \end{array}\right]$ then

4.1.1.2.1.1.2.1.3.2.2.1) $x(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$

4. Discriminative properties of Zagreb M_2 Index and Modified Zagreb ${}^*M_2$ Index

The aim of this section is to utilize the developed algorithm. We compare discriminative properties of Zagreb M_2 index and modified Zagreb ${}^*M_2$ index for molecular graphs.

Let n be a natural number larger then 4. Define by A_n the set of all graphs with n vertices and define the following functions $(M_2)_n$, $(^*M_2)_n$: $\mu(A_n) \rightarrow \mathbb{R}$ by

$$(M_2)_n(\mu(G)) = M_2(G)$$
$$({}^*M_2)_n(\mu(G)) = {}^*M_2(G).$$

We also define

$$P_n = \{\{m_1, m_2\} : m_1, m_2 \in \mu_n(A_n), m_1 \neq m_2\}$$
$$D_n = \{\{m_1, m_2\} : m_1, m_2 \in \mu_n(A_n), (M_2)_n(m_1) \neq (M_2)_n(m_2)\}$$
$$^{*}D_n = \{\{m_1, m_2\} : m_1, m_2 \in \mu_n(A_n), (^{*}M_2)_n(m_1) \neq (^{*}M_2)_n(m_2)\}$$
$$I_n = \{\{m_1, m_2\} : m_1, m_2 \in \mu_n(A_n), (M_2)_n(m_1) = (M_2)_n(m_2)\}$$
$$^{*}I_n = \{\{m_1, m_2\} : m_1, m_2 \in \mu_n(A_n), (^{*}M_2)_n(m_1) = (^{*}M_2)_n(m_2)\}.$$

The probability that the pair of elements of $\mu(A_n)$ will be discriminated by Zagreb M_2 index is $|D_n|/|P_n|$ and probability that they won't be discriminated is $|I_n|/|P_n|$. Analogously, the probability that the pair of elements of $\mu(A_n)$ will be discriminated by modified Zagreb $^{*}M_2$ index is $|D_n^{*}|/|P_n|$ and probability that they won't be discriminated is $|I_n^{*}|/|P_n|$. Our findings are summarized below.

n	$\|I_n\|/\|P_n\|$	$\|D_n\|/\|P_n\|$	$\|I_n^{*}\|/\|P_n\|$	$\|D_n^{*}\|/\|P_n\|$	$\|I_n^{*}\|/\|I_n\|$
5	0.00000000	1.00000000	0.05238095	0.94761905	Not defined
6	0.00186480	0.99813520	0.01724942	0.98275058	9.25000000
7	0.00472813	0.99527187	0.01536643	0.98463357	3.25000000
8	0.00608154	0.99391846	0.01415128	0.98584872	2.32692308
9	0.00621716	0.99378284	0.01237858	0.98762142	1.99103390
10	0.00619617	0.99380383	0.01108734	0.98891266	1.78938770
11	0.00603875	0.99396125	0.00993674	0.99006326	1.64549741
12	0.00582063	0.99417937	0.00902557	0.99097443	1.55061876
13	0.00558597	0.99441403	0.00825816	0.99174184	1.47837380
14	0.00535675	0.99464325	0.00763061	0.99236939	1.42448536
15	0.00513608	0.99486392	0.00709174	0.99290826	1.38076962
16	0.00492681	0.99507319	0.00663258	0.99336742	1.34622159
17	0.00472759	0.99527241	0.00622986	0.99377014	1.31776853
18	0.00453984	0.99546016	0.00587785	0.99412215	1.29472683
19	0.00436312	0.99563688	0.00556556	0.99443444	1.27559160
20	0.00419698	0.99580302	0.00528736	0.99471264	1.25979960
21	0.00404094	0.99595906	0.00503723	0.99496277	1.24654920
22	0.00389452	0.99610548	0.00481149	0.99518851	1.23545068
23	0.00375713	0.99624287	0.00460628	0.99539372	1.22600914

24	0.00362818	0.99637182	0.00441904	0.99558096	1.21797718
25	0.00350705	0.99649295	0.00424736	0.99575264	1.21109151
26	0.00339323	0.99660677	0.00408941	0.99591059	1.20516758
27	0.00328615	0.99671385	0.00394345	0.99605655	1.20002244
28	0.00318528	0.99681472	0.00380818	0.99619182	1.19555384
29	0.00309018	0.99690982	0.00368238	0.99631762	1.19163898
30	0.00300042	0.99699958	0.00356511	0.99643489	1.18820427
31	0.00291557	0.99708443	0.00345545	0.99654455	1.18517210
32	0.00283529	0.99716471	0.00335269	0.99664731	1.18248630
33	0.00275923	0.99724077	0.00325615	0.99674385	1.18009685
34	0.00268708	0.99731292	0.00316529	0.99683471	1.17796610
35	0.00261857	0.99738143	0.00307958	0.99692042	1.17605469
36	0.00255343	0.99744657	0.00299859	0.99700141	1.17433813
37	0.00249143	0.99750857	0.00292193	0.99707807	1.17279014
38	0.00243236	0.99756764	0.00284925	0.99715075	1.17138962
39	0.00237602	0.99762398	0.00278023	0.99721977	1.17011850
40	0.00232223	0.99767777	0.00271460	0.99728540	1.16896276
41	0.00227082	0.99772918	0.00265210	0.99734790	1.16790770
42	0.00222163	0.99777837	0.00259252	0.99740748	1.16694294
43	0.00217454	0.99782546	0.00253564	0.99746436	1.16605818
44	0.00212941	0.99787059	0.00248128	0.99751872	1.16524491
45	0.00208611	0.99791389	0.00242927	0.99757073	1.16449546
46	0.00204455	0.99795545	0.00237946	0.99762054	1.16380372
47	0.00200462	0.99799538	0.00233170	0.99766830	1.16316341
48	0.00196623	0.99803377	0.00228588	0.99771412	1.16256983
49	0.00192929	0.99807071	0.00224187	0.99775813	1.16201838
50	0.00189371	0.99810629	0.00219956	0.99780044	1.16150514

We conclude that discriminative properties of Zagreb M_2 Index supersede those of modified $^*M_2$ Zagreb index for graphs with the at most 50 vertices.

5. Additional results

In this section, we shall demonstrate another utilization of our algorithm. We want to find how discriminative the Randić connectivity indices [6,12] ${}^0\chi$ and ${}^1\chi$ together are for graphs with the same number of vertices. One may think that the Zagreb $^*M_2$ index was precursor for the Randić connectivity index ${}^1\chi$. Obviously, if we have two graphs G_1 and G_2 such that $\mu(G_1)=\mu(G_2)$, then these graphs cannot be discriminated by indices ${}^0\chi$ and ${}^1\chi$. Therefore, we want to find out if the relation

$$\left[{}^0\chi(G_1)={}^0\chi(G_2) \text{ and } {}^1\chi(G_1)={}^1\chi(G_2)\right] \Rightarrow \mu(G_1)=\mu(G_2)$$

holds for all molecular graphs G_1 and G_2 with the same number of vertices and if not so to find a smallest n such that there is a pair of graphs with n vertices such that

$${}^0\chi(G_1)={}^0\chi(G_2) \text{ and } {}^1\chi(G_1)={}^1\chi(G_2) \text{ and } \mu(G_1)\neq\mu(G_2).$$

First, we shall need few lemmas. It can be easily proved that:

Lemma 12. Let $a,b,c,d\in\mathbb{Q}$. If $a+b\sqrt{2}+c\sqrt{3}+d\sqrt{6}=0$, then all numbers a, b, c and d are equal to 0.

Lemma 13. Let G_1 and G_2 be molecular graphs with the same number of vertices. If ${}^0\chi(G_1)={}^0\chi(G_2)$, then $\nu(G_1)=\nu(G_2)$.

Proof: Note that

$${}^0\chi(G_1)=\nu_1(G_1)+\frac{1}{\sqrt{2}}\nu_2(G_1)+\frac{1}{\sqrt{3}}\nu_2(G_1)+\frac{1}{2}\nu_4(G_1);$$
$${}^0\chi(G_2)=\nu_1(G_2)+\frac{1}{\sqrt{2}}\nu_2(G_2)+\frac{1}{\sqrt{3}}\nu_2(G_2)+\frac{1}{2}\nu_4(G_2),$$

hence

$$\nu_1(G_1)+\frac{1}{2}\nu_4(G_1)=\nu_1(G_2)+\frac{1}{2}\nu_4(G_2);\nu_2(G_1)=\nu_2(G_2);\nu_3(G_1)=\nu_3(G_2).$$

Since, G_1 and G_2 have the same number of vertices, we have

$$\nu_1(G_1)+\nu_2(G_1)+\nu_3(G_1)+\nu_4(G_1)=\nu_1(G_2)+\nu_2(G_2)+\nu_3(G_2)+\nu_4(G_2).$$

From the last four equations, the claim follows.

Lemma 14. Let $n \geq 3$ and let G_1 and G_2 be molecular graphs with n vertices. If ${}^{1}\chi(G_1) = {}^{1}\chi(G_2)$, then

$$\begin{aligned} 6\mu_{14}(G_1) + 6\mu_{22}(G_1) + 4\mu_{33}(G_1) + 3\mu_{44}(G_1) &= 6\mu_{14}(G_1) + 6\mu_{22}(G_1) + 4\mu_{33}(G_1) + 3\mu_{44}(G_1) \\ 2\mu_{12}(G_1) + \mu_{24}(G_1) &= 2\mu_{12}(G_2) + \mu_{24}(G_2) \\ 2\mu_{13}(G_1) + \mu_{34}(G_1) &= 2\mu_{13}(G_2) + \mu_{34}(G_2) \\ \mu_{23}(G_1) &= \mu_{23}(G_2) \end{aligned}$$

Proof: We have

$$0 = {}^{1}\chi(G_1) - {}^{1}\chi(G_2) =$$

$$= \left(\begin{array}{l} \left(6\mu_{14}(G_1) + 6\mu_{22}(G_1) + 4\mu_{33}(G_1) + 3\mu_{44}(G_1) - \mu_{14}(G_2) - 6\mu_{22}(G_2) - 4\mu_{33}(G_2) - 3\mu_{44}(G_2)\right) + \\ \frac{1}{4}\left(2\mu_{12}(G_1) + \mu_{24}(G_1) - 2\mu_{12}(G_1) - \mu_{24}(G_1)\right)\sqrt{2} + \\ \frac{1}{6}\left(2\mu_{13}(G_1) + \mu_{34}(G_1) - 2\mu_{13}(G_1) - \mu_{34}(G_1)\right)\sqrt{3} + \frac{1}{6}\left(\mu_{23}(G_1) - \mu_{23}(G_1)\right)\sqrt{6} \end{array} \right)$$

and the claim follows from Lemma 12.

Theorem 15. Let $A, B, C, D, n_1, n_2, n_3, n_4 \in \mathbb{N}$ such that $n_3 \neq 0; n_4 \neq 0$ and that $n_1 + n_2 + n_3 + n_4 \geq 3$. There are molecular graphs G_1 and G_2 such that:

$$a(G_1) = a(G_2) = A; b(G_1) = b(G_2) = B; c(G_1) = c(G_2) = C; d(G_1) = d(G_2) = D;$$

$$\nu(G_1) = \nu(G_2) = (n_1, n_2, n_3, n_4) \text{ and } \mu(G_1) \neq \mu(G_2),$$

if and only if $n_3 \geq 3$ and $n_4 \geq 4$ one of the following holds:

1) $Max - Min \geq 8$;

2) $(Max > Min)$ and $\left[(-Min - B - 2D + 4n_2 = 0) \text{ or } (D + Min > 0)\right]$;

where Min is the smallest natural number such that

$$Min \geq \max \left\{ \begin{array}{c} 0, \left\lceil \frac{b - 2d}{3} \right\rceil, \\ \left\lceil \frac{-4A + 14C - 20D}{3} \right\rceil - 5B + 6n_1 + 8n_2 + 8n_3 + 8n_4, \\ \left\lceil \frac{-4A}{3} \right\rceil - 5B - 4C - 6D + 6n_1 + 8n_2 + 6n_3 + 8n_4, \\ \left\lceil \frac{-23B - 20C + 28n_1 + 32n_4}{3} \right\rceil - 2A - 10D + 12n_2 + 12n_3, \\ \left\lceil \frac{-4A + 13C - 20D - n_3 n_4}{3} \right\rceil - 5B + 6n_1 + 8n_2 + 8n_3 + 8n_4, \end{array} \right\} \qquad (1)$$

and that $3B+2D \equiv Min \pmod 4$; and Max is the largest natural number such that

$$
Max \le \min \left\{ \begin{array}{c}
b, \\
-2A-8B-7C-10D+10n_1+12n_2+12n_3+12n_4, \\
-B+2D+4n_2, \\
\left\lfloor \frac{-4A-13C-20D}{3} \right\rfloor -5B+6n_1+8n_2+8n_3+8n_4, \\
\left\lfloor \frac{-23B-20C+37n_3}{3} \right\rfloor -2A-10D+9n_1+12n_2+12n_4, \\
\left\lfloor \frac{-4A+16n_1+28n_4}{3} \right\rfloor -5B-4C-6D+8n_2+8n_3, \\
\left\lfloor \frac{-12A-40C-58D+74n_3}{9} \right\rfloor -5B+6n_1+8n_2+8n_4, \\
-2A-7B-6C-10D+8n_1+12n_2+12n_3+14n_4, \\
\left\lfloor \frac{-1-15B-13C}{2} \right\rfloor -2A-10D+9n_1+12n_2+12n_3+12n_4, \\
\left\lfloor \frac{-1-15B-13C}{2} \right\rfloor -2A-10D+9n_1+12n_2+12n_3+12n_4, \\
\left\lfloor \frac{-1-4A-13C-19D}{3} \right\rfloor -5B+6n_1+8n_2+8n_3+8n_4, \\
\left\lfloor \frac{-4-16A-61B-52C-78D+96n_2+96n_3+96n_4}{9} \right\rfloor +8n_1 \\
\left\lfloor \frac{-4A+16n_3+2n_3^2}{3} \right\rfloor -5B-4C-6D+6n_1+8n_2+8n_4 \\
\left\lfloor \frac{-23B-20C+28n_1+31n_{44}+n_4^2}{3} -2A-10D+12n_2+12n_3 \right\rfloor
\end{array} \right\} \tag{2}
$$

and that $3B+2D \equiv Max \pmod 4$.

Proof: From Theorem 7 and Lemma 13 and 14, it follows that graphs with the required properties exist if and only if there are numbers $m_{uv,i}$, for each $1 \le u \le v \le 4$ and $1 \le i \le 2$ such that following 55 relations hold:

i,1) $m_{uv,i} \in \mathbb{Z}$, for each $1 \le u \le v \le 4$;

i,2) $m_{uv,i} \ge 0$, for each $1 \le u \le v \le 4$;

i,3) $A = 6m_{14,i} + 6m_{22,i} + 4m_{33,i} + 3m_{44,i}$;

i,4) $m_{11,i} = 0$;

i,5) $B = 2m_{12,i} + m_{24,i}$;

i,6) $C = 2m_{13,i} + m_{34,i}$;

i,7) $D = m_{23,i}$;

i,8) $n_1 = m_{11,i} + m_{12,i} + m_{13,i} + m_{14,i}$;

i,9) $2n_2 = m_{12,i} + 2m_{22,i} + m_{23,i} + m_{24,i}$;

i,10) $3n_3 = m_{13,i} + m_{23,i} + 2m_{33,i} + m_{34,i}$;

i,11) $4n_4 = m_{14,i} + m_{24,i} + m_{34,i} + 2m_{44,i}$;

i,12) $s_i = m_{23,i} + m_{24,i} - m_{12,i} \geq 0$;

i,13) s_i is an integer;

i,14) $s_i + m_{33,i} + m_{34,i} + m_{44,i} \geq n_3 + n_4 - 1$;

i,15) $n_3 \leq s_i + m_{33,i} + m_{34,i}$;

i,16) $n_4 \leq s_i + m_{34,i} + m_{44,i}$;

i,17) $n_3 \leq m_{23,i} + m_{33,i} + m_{34,i}$;

i,18) $n_4 \leq m_{24,i} + m_{34,i} + m_{44,i}$;

i,19) $m_{34,i} + m_{24,i} \geq 1$;

i,20) $m_{34,i} + m_{23,i} \geq 1$;

i,21) $m_{34,i} + s_i \geq 1$;

i,22) $(n_3 \geq 2)$ or $(\mathrm{s}_i \leq \mathrm{m}_{22,i} + m_{24,i})$;

i,23) $(n_4 \geq 2)$ or $(s \leq m_{23,i} + m_{22,i})$;

i,24) $(m_{12,i} + m_{23,i} + m_{24,i} > 0)$ or $(m_{22,i} = 0)$;

i,25) $m_{33,i} \leq \frac{n_3 \cdot (n_3 - 1)}{2}$;

i,26) $m_{34,i} \leq n_3 \cdot n_4$;

i,27) $m_{44,i} \leq \frac{n_4 \cdot (n_4 - 1)}{2}$.

28) $\begin{pmatrix} m_{11,1}, m_{12,1}, m_{13,1}, m_{14,1}, m_{22,1}, \\ m_{23,1}, m_{23,1}, m_{33,1}, m_{34,1}, m_{44,1} \end{pmatrix} \neq \begin{pmatrix} m_{11,2}, m_{12,2}, m_{13,2}, m_{14,2}, m_{22,2}, \\ m_{23,2}, m_{23,2}, m_{33,2}, m_{34,2}, m_{44,2} \end{pmatrix}$,

where $1 \leq i \leq 2$. Note that, for $i = 1,2$, relations i,3) - i,11) can be rewritten as i,1*) $m_{11,i}=0$

i,2*) $m_{12,i}=\frac{B}{2}-\frac{m_{24,i}}{2}$

i,3*) $m_{13,i}=\frac{m_{24,i}}{2}+\frac{1}{2}(4A+15B+14C+20D-18n_1-24n_2-24n_3)$

i,4*) $m_{14,i}=-2A-8B-7C-10D+10n_1+12n_2+12n_3+12n_4$;

i,5*) $m_{22,i}=-\frac{m_{24,i}}{4}+\frac{1}{4}(-B-2D+4n_2)$;

i,6*) $m_{23,i}=D$;

i,7*) $m_{33,i}=\frac{3m_{24,i}}{4}+\frac{1}{4}(4a+15b+12c+18d-18n_1-24n_2-18n_3-24n_4)$;

i,8*) $m_{34,i}=-3m_{24,i}-4a-15b-13c-20d+18n_1+24n_2+24n_3+24n_4$;

i,9*) $m_{44,i}=\frac{3m_{24,i}}{2}+\frac{1}{2}(6a+23b+20c+30d-28n_1-36n_2-36n_3-32n_4)$.

Hence, $(m_{11,i},m_{12,i},m_{13,i},m_{14,i},m_{22,i},m_{23,i},m_{24,i},m_{33,i},m_{34,i},m_{44,i})$ is uniquely determined by the value of $m_{24,i}$, therefore

1*) $m_{24,i}\neq m_{24,j}$

Denote right-handside of (1) as *Minv* and denote right-handside of (2) as *Maxv*. Note that i,1) and i,13) can be rewritten as

i,11*) $m_{24,i}\equiv 3B+2D \pmod 4$.

Relations i,2), i,12), i,15) – i,21) and i,25) – i,27) are equivalent to $Minv\leq m_{24,i}\leq Maxv$. Taking into account the relation i,11*), these can be rewritten as:

i,12*) $Min\leq m_{24,i}\leq Max$.

Relations i,24) can be rewritten as

i,13*) $(-m_{24,i}-B-2D+4n_2=0)$ or $(D+m_{24,i}>0)$

From 10*) and i,11*) it follows that $Maxv-Minv\geq 4$. Specially, it follows that

$$\left(\left\lfloor\frac{-23B-20C+28n_1+31n_4+n_4^2}{3}-\right\rfloor\right)-\left(\left\lceil\frac{-23B-20C+28n_1+32n_4}{3}\right\rceil-\right)\geq 4$$
$$\left(\left\lfloor -2A-10D+12n_2+12n_3\right\rfloor\right)\quad\left(-2A-10D+12n_2+12n_3\right)$$

$$\left(\left\lfloor \frac{-4A+16n_3+2n_3^2}{3} \right\rfloor - \atop -5B-4C-6D+6n_1+8n_2+8n_4\right) - \left(\left\lceil \frac{-4A}{3} \right\rceil - 5B-4C-6D+ \atop 6n_1+8n_2+6n_3+8n_4\right) \geq 4.$$

From these relations easily follows that

14*) $n_3 \geq 3$ and $n_4 \geq 4$. Hence, the relations i,14), i,22) and i,23) are fulfilled.

So far, we have proved that graphs G_1 and G_2 with the required properties exist if and only if 14*) holds and there are nonnegative integers $m_{24,1}$ and $m_{24,2}$ that satisfy 10*) and i,11*) – i,13*).

Distinguish three cases:

CASE 1: $Max - Min < 4$.

There is a single number that satisfies relations i,11*) and i,12*), therefore the relation 10*) can not be satisfied, so there are no graphs with the required properties.

CASE 2: $4 \leq Max - Min \leq 7$.

The only two different numbers that satisfy the relations 10), i,11*) and i,12*) are Min and $Min+4$. Note that $D+Min+4>0$, therefore graphs G_1 and G_2 with the required properties exist if and only if $\left[\left(-Min-B-2D+4n_2=0\right) \text{ or } \left(D+Min>0\right)\right]$.

CASE 3: $Max - Min \geq 8$.

Note that $D+Min+4>0$ and $D+Min+8>0$, so it is sufficient to take $m_{24,1}=Min+4$ and $m_{24,1}=Min+8$.

This concludes the proof of our theorem.

Now, we shall utilize this theorem to create the following algorithm:

1) $n=7$

2) For each (n_1,n_2,n_3,n_4) generated by $GenNumVer(n)$ do

2.1) if $n_3 \geq 3$ and $n_4 \geq 4$ then

2.1.1) for each d such that $0 \leq d \leq \min\{2n_2, 3n_3\}$

2.1.1.1) for each c such that $0 \leq c \leq 2(3n_3 - d)$

2.1.1.1.1) for each b such that $0 \leq b \leq 2(2n_2 - d)$

2.1.1.1.1.1) for each a such that $0 \le a \le 6\left(n_1 + 2n_2 + 3n_3 + 4n_4 - \frac{b}{2} - \frac{c}{2} - d\right)$

2.1.1.1.1.1.1) If$(Max - Min \ge 8)$

2.1.1.1.1.1.1.1) Put $m_{23,1} = Min + 4$ and $m_{23,2} = Min + 8$

2.1.1.1.1.1.1.2) Calculate numbers $m_{uv,i}, 1 \le u \le v \le 4, 1 \le i \le 2$ using formulas I,1*) - I,9*)

from the last Theorem

2.1.1.1.1.1.1.3) Output numbers $n_i, 1 \le i \le 4; m_{uv,i}, 1 \le u \le v \le 4, 1 \le i \le 2; A, B, C, D$

2.1.1.1.1.1.1.4) Exit program

2.1.1.1.1.1.2) If $(Max > Min)$ and $[(-Min - B - 2D + 4n_2 = 0)$ or $(D + Min > 0)]$ then

2.1.1.1.1.1.2.1) Put $m_{23,1} = Min$ and $m_{23,2} = Min + 4$

2.1.1.1.1.1.1.2) Calculate numbers $m_{uv,i}, 1 \le u \le v \le 4, 1 \le i \le 2$ using formulas i,1*) - i,9*)

from the last Theorem

2.1.1.1.1.1.2.3) Output numbers $n_i, 1 \le i \le 4; m_{uv,i}, 1 \le u \le v \le 4, 1 \le i \le 2; A, B, C, D$

2.1.1.1.1.1.2.4) Exit program

3) Increment n and go to 2)

The output of this algorithm is:

$n_1 = 7;\ n_2 = 3;\ n_3 = 5;\ n_4 = 4;\ a = 30;\ b = 4;\ c = 14;\ d = 2;$

$m_{12,1} = 2;\ m_{13,1} = 1;\ m_{14,1} = 4;\ m_{22,1} = 1;\ m_{23,1} = 2;\ m_{24,1} = 0;\ m_{33,1} = 0;\ m_{34,1} = 12;\ m_{44,1} = 0;$

$m_{12,2} = 0;\ m_{13,2} = 7;\ m_{14,2} = 0;\ m_{22,2} = 0;\ m_{23,2} = 2;\ m_{24,2} = 4;\ m_{33,2} = 3;\ m_{34,2} = 0;\ m_{44,2} = 6.$

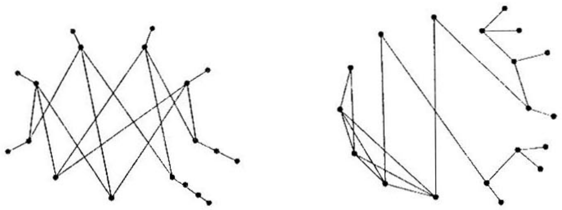
Therefore, for graphs G_1 and G_2 with at most 18 vertices holds

$$\left[{}^0\chi(G_1) = {}^0\chi(G_2) \text{ and } {}^1\chi(G_1) = {}^1\chi(G_2)\right] \Rightarrow \mu(G_1) = \mu(G_2),$$

and there are graphs G_1 and G_2 with 19 vertices such that

$${}^0\chi(G_1) = {}^0\chi(G_2) \text{ and } {}^1\chi(G_1) = {}^1\chi(G_2) \text{ and } \mu(G_1) \ne \mu(G_2).$$

Namely, for graphs G_1 and G_2 given on the following diagrams



we have:

$n(G_1) = n(G_2) = 19$

${}^0\chi(G_1) = {}^0\chi(G_2) = 9 + \frac{3}{2}\sqrt{2} + \frac{5}{3}\sqrt{3}$

${}^1\chi(G_1) = {}^1\chi(G_2) = \frac{15}{6} + \sqrt{2} + \frac{7}{3}\sqrt{3} + \frac{1}{3}\sqrt{6}$

$\mu(G_1) = (0,2,1,4,1,2,0,0,12,0)$

$\mu(G_2) = (0,0,7,0,0,2,4,3,0,6)$

6. Concluding remarks

We presented an efficacious algorithm for studying the discriminatory power of molecular descriptors, that was tested on the Zagreb M_2 index and the modified Zagreb $^*M_2$ index for all kinds of (molecular) graphs. The result of our analysis is surprising — Zagreb M_2 index is more discriminative than the modified Zagreb $^*M_2$ index. One would expect the reverse result because the Zagreb M_2 indices belong to the set of *natural* numbers and the modified Zagreb $^*M_2$ indices to the set of *rational* numbers.

We also investigated the discriminatory power of the first two Randić connectivity indices: ${}^0\chi$ and ${}^1\chi$. We did this because the Randić indices are grounded in the Zagreb indices though they were obtained in quite a different way. In this case we obtained that ${}^0\chi$ and ${}^1\chi$ indices discriminate all graphs with up to 18 vertices. We also found a pair of graphs with 19 vertices for which the above is not valid.

Acknowledgment – We thank the Ministry of Science and Technology of Croatia for support.

References

1. F. Harary, *Graph Theory*, 2nd printing, Addison-Wesley, Reading, MA, 1971.
2. I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972). 535-538.
3. I. Gutman, B. Ruščić, N. Trinajstić and C.F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399-3405.
4. A.T. Balaban, Highly discriminating distance-based topological index, *Chem. Phys. Lett.* **89** (1982) 399-404.
5. D.H. Rouvray, The search for useful topological indices in chemistry, Sci. *Am.* **61** (1973) 729-735.
6. N. Trinajstić, *Chemical Graph Theory*, 2nd revised edition, CRC Press, Boca Raton, FL, 1992.
7. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
8. S.C. Basak, D.K. Harriss and V.R. Magnuson, POLLY 2.3, Copyright of the University of Minnesota, 1988.
9. R. Todeschini, DRAGON, WebSite - http://www.disat.unimib.it/chm/
10. S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113-124; see also K.C. Das and I Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103-112.
11. D. Vukičević and N. Trinajstić, Modified Zagreb M2 index — comparison with the Randić connectivity index for benzenoid systems, *Croat. Chem. Acta* **76** (2003) 183-187.
12. M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609-6615.