Novel Degree-based Molecular Descriptors with Increased Discriminating Power

Tomislav Došlić

Faculty of Civil Engineering, University of Zagreb
Kačićeva 26, Zagreb, Croatia
doslic@grad.hr

Tamás Réti

Óbuda University
Bécsi út 96/B, H-1034 Budapest, Hungary
reti.tamas@bgk.uni-obuda.hu

Abstract: In the present study we investigate some general problems concerning the degeneracy of widely used topological indices (graph invariants), and we propose a novel family of molecular descriptors characterized by a decreased degeneracy level. A special feature of topological indices of novel type is that they take into account the degrees of vertices on increasing distances from a single vertex. According to the comparative tests performed on samples of isospectral graphs and of graphs of small diameter, the new descriptors are judged to be more efficient for discriminating between topological structures of molecular graphs than several traditional molecular indices.

Keywords: Zagreb indices; pseudo-regular graphs; QSAR/QSPR studies

1 Introduction

A promising trend in theoretical and structural chemistry is the employment of graph invariants (topological indices) for the characterization of the combinatorial structure of carbon-based chemical compounds and the prediction of their physico-chemical properties. Topological invariant is a real number derived from the structure of a graph in such a way that it does not depend on the labeling of vertices. Hundreds topological invariants (indices) have been invented so far, and numerous reviews have been published on their applications in the QSAR/QSPR studies [1-10].

One of the main difficulties when using topological indices for discriminating and prediction purposes is their degeneracy, i.e., the fact that two (or more) non-isomorphic graphs have the same value of a topological index. The degeneracies are unavoidable; however, it makes sense to search for indices whose degeneracy is as low as reasonably possible [11, 12].

In the present study we investigate the discriminating potential (application limits) of traditional degree-based descriptors, especially, how to decrease the degeneracy by an appropriate modification or generalization of their structure, and finally we propose a set of novel topological invariants having improved discriminating potential.

2 Definitions, Basic Notions

All graphs considered in this study are finite, simple and connected graphs (without loops and multiple edges). We use the standard terminology; for the concepts not defined here, we refer the reader to any of standard graph theory monographs such as, e.g., [13] or [14]. For a connected graph G, V(G) and E(G) denote the set of vertices and edges, and $|V(G)|$ and $|E(G)|$ the numbers of vertices and edges, respectively.

An edge of G connecting vertices u and v is denoted by (u,v). The diameter of a graph G (written by diam(G)) is defined as the greatest distance between any pairs of vertices in G. The degree of vertex u, denoted by d(u), is the number of edges incident to u. We denote by $\Delta=\Delta(G)$ and $\delta=\delta(G)$ the maximum and the minimum degrees, respectively, of vertices of G. A graph is called regular (R-regular), if all its vertices have the same degree R. To avoid trivialities we always assume that $|V(G)| \geq 3$, and $d(u)\geq 1$. A connected graph with maximum vertex degree at most 4 is said to be a "chemical graph".

Consider the topological descriptor X(G) defined in the general form

$$X(G) = F(Z_1(G), Z_2(G), ..., Z_J(G))$$

where F is a J-variable, non-negative real function, $Z_1(G)$, $Z_2(G)$,...,$Z_j(G)$,... $Z_J(G)$ are appropriately selected topological invariants given as

$$Z_j(G) = \sum_r \sum_{s\leq r} E(r,s) f_j(r,s),$$

where $f_j(x,y)$ are real symmetric functions for $1\leq j\leq J$, and quantities E(r,s) denote the number of edges in G with end-vertices of degree r and s. (The number E(r,s) are sometimes denoted by $m_{r,s}$).

The descriptors represented by X(G) are called *the generalized edge-additive topological indices*.

It follows that if for graphs Hu and Hv the equalities $E_{Hu}(r,s)=E_{Hv}(r,s)$ are fulfilled, then $Z_j(Hu)=Z_j(Hv)$ and $X(Hu)=X(Hv)$ hold, independently of the type of functions $f_j(x,y)$ and the J-variable function F. This means that the topological descriptors of the type X(G) are not suitable for discriminating between graphs Hu and Hv.

By specializing functions F and $f_j(x,y)$ one can obtain several indices (molecular descriptors) from recent literature [3-10]. In a particular case, by selecting topological parameters $Z_1(G)$ and $Z_2(G)$ as

$$Z_1(G)=\sum_r\sum_{s\le r}E(r,s)\left(\frac{r}{s}+\frac{s}{r}\right) \quad \text{and} \quad Z_2(G)=|V(G)|=\sum_r\sum_{s\le r}E(r,s)\left(\frac{1}{r}+\frac{1}{s}\right),$$

we can construct the topological index $X_E(G)=Z_1(G)/Z_2(G)$ introduced in a recent paper [10]. It has been verified that for index $X_E(G)$ the following identity is fulfilled:

$$X_E(G)=\frac{Z_1(G)}{Z_2(G)}=\frac{1}{|V(G)|}\sum_r\sum_{s\le r}E(r,s)\left(\frac{r}{s}+\frac{s}{r}\right)=\frac{1}{|V(G)|}\sum_{u\in V(G)}m(u)$$

In the above formula m(u) stands for the average degree of the vertices adjacent to vertex u in G.

In certain cases the discriminating ability of topological descriptors of the type X(G) (for example $X_E(G)$) is strongly limited. This is demonstrated in the following example. In Fig. 1 a pair of isospectral graphs, G_1 and G_2, are shown [15]. For them the equality $X_E(G_1)= X_E(G_2)$ holds; consequently, they cannot be distinguished by the topological index $X_E(G)$.

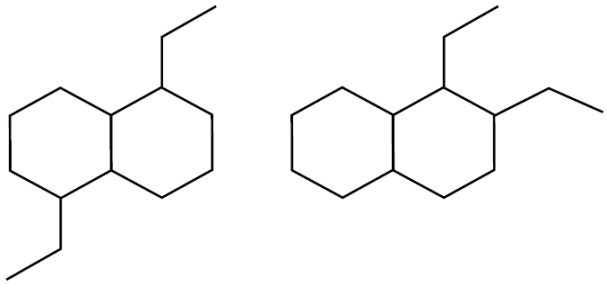

Figure 1
A pair of isospectral chemical graphs that cannot be distinguished by indices of the type X(G)

A possible solution to improve the discriminativity of a topological index is to modify it so as to include more information encoded in the graph adjacency matrix. For this purpose, it seems logical to take into account the degrees of vertices on increasing distances from a single vertex [16-18]. Hence, for i ≥1 we define the quantitites

$$Q_i(u) = \sum_{v \in N_i(u)} d(v)$$

where $N_i(u)$ denotes the set of all vertices at distance i from vertex u. If $N_i(u)$ is empty, we set $Q_i(u) = 0$ by definition. Obviously, $Q_i(u)$ is equal to zero for all i that exceed the diameter of G. Now we define

$$m_i(u) = \frac{Q_i(u)}{n_i(u)}$$

where $n_i(u)$ is the cardinality of $N_i(u)$. It is assumed that $m_i(u) = 0$ if $N_i(u)$ is empty. It is easy to see that relations $\delta \le m_i(u) \le \Delta$ and $\sum n_i(u) = |V(G)| - 1$ hold for any vertex u. By averaging $m_i(u)$ over all vertices of G we obtain global topological indices

$$\langle m_i(G) \rangle = \frac{1}{|V(G)|} \sum_{u \in V(G)} m_i(u),$$

and topological parameters defined as

$$Q_i(G) = \sum_{u \in V(G)} Q_i(u) = \sum_{u \in V(G)} m_i(u) n_i(u) = \sum_{u \in V(G)} \sum_{v \in N_i(u)} d(v)$$

for $1 \le i \le \mathrm{diam}(G)$. From the previous considerations if follows that the topological index $X_E(G)$ now appears as a special case $X_E(G) = \langle m_1(G) \rangle$.

3 Some Theoretical Considerations

The Zagreb indices belong to the family of the widely used molecular descriptors. In what follows we analyse some correspondances between the quantities $Q_i(u)$, $m_i(u)$, $n_i(u)$ and the Zagreb indices.

Recall that the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined as

$$M_1 = M_1(G) = \sum_{u \in V(G)} d^2(u) = \sum_r \sum_{s \le r} E(r,s)(r+s)$$

$$M_2 = M_2(G) = \sum_{(u,v)\in E(G)} d(u)d(v) = \sum_r \sum_{s\le r} E(r,s)rs$$

We refer the reader to surveys [4, 5, 19-21] for more information on Zagreb indices.

Proposition 1 ([10]): Let [d(G)] denote the average degree of a connected graph G. Then $\langle m_1(G)\rangle \ge [d(G)]$ holds with equality if and only, if G is regular. ■

Proposition 2 ([22]): Let G be a connected graph. Then

$$M_1(G) = \sum_{u\in V(G)} m_1(u)d(u) \quad \text{and} \quad 2M_2(G) = \sum_{u\in V(G)} m_1(u)d^2(u)$$ ■

Corollary 2.1 Because $\delta \le m_1(u) \le \Delta$ this imples that

$$2|E(G)|\delta \le Q_1(G) = M_1(G) \le 2|E(G)|\Delta$$

$$\delta M_1(G) \le 2M_2(G) \le \Delta M_1(G)$$

Lemma 1 ([19]): Let G be a connected graph. Then

$$Q_1(u) = d(u)m_1(u) \le 2|E(G)| - d(u) - (|V(G)| - 1 - d(u))\delta$$ ■

Lemma 2 Let G be a connected graph. Then

$$Q_1(u) = d(u)m_1(u) \le 2|E(G)| - |V(G)| + 1$$

Proof. Because $\delta \ge 1$ and $d(u) \le |V(G)| - 1$, from Lemma 1 it follows the claim. ■

From Lemma 2 the following proposition yields:

Proposition 3 Let G be a connected graph. Then for k=1,2,...positive integers

$$\sum_{u\in V(G)} Q_1^k(u) = \sum_{u\in V(G)} (d(u)m_1(u))^k \le |V(G)|(2|E(G)| - |V(G)| + 1)^k$$

with equality if G is a complete graph K_n or a star graph S_n on $n\ge 3$ vertices. ■

Corollary 3.1 ([31]): As a particular case, for k=1 we have

$$M_1(G) = \sum_{u\in V(G)} d(u)m_1(u) \le |V(G)|(2|E(G)| - |V(G)| + 1)$$

with equality if G is a complete graph K_n or a star graph S_n on $n\ge 3$ vertices.

Proposition 4 ([23]): Let G be a connected graph. Then

$$Q_1(u) = d(u)m_1(u) = \sum_{v\in N_1(u)} d(v) \ge d(u) + n_2(u)$$

and

$$d(u)Q_1(u) = d^2(u)m_1(u) \geq d^2(u) + d(u)n_2(u)$$

with equality if and only if G is a triangle- and quadrangle-free graph. ■

Corollary 4.1 Consider the Gordon-Scantlebury index S(G) of a graph G [1, 24]. This is a widely-used molecular descriptor of the type X(G) which can be calculated as

$$S(G) = \frac{1}{2}\sum_{u\in V(G)} d(u)\big(d(u)-1\big) = \frac{1}{2}\big\{M_1(G) - 2|E(G)|\big\}$$

From the prevous considerations it follows that

$$\sum_{u\in V(G)} n_2(u) \leq \sum_{u\in V(G)} Q_1(u) - 2|E(G)| = M_1(G) - 2|E(G)| = 2S(G)$$

and

$$2M_2(G) = \sum_{u\in V(G)} d^2(u)m_1(u) \geq M_1(G) + \sum_{u\in V(G)} d(u)n_2(u)$$

with equality if and only if G is a triangle- and quadrangle-free graph.

Proposition 5 Let G be a connected graph. Then

$$Q_2(G) = \sum_{u\in V(G)} Q_2(u) = \sum_{u\in V(G)} m_2(u)n_2(u) = \sum_{u\in V(G)} d(u)n_2(u)$$

Proof. It is based on the following identity:

$$\sum_{u\in V(G)} Q_2(u) = \sum_{u\in V(G)}\sum_{v\in N_2(u)} d(v) = \sum_{u\in V(G)} d(u)n_2(u) \qquad ■$$

Proposition 6 Let G be a connected graph. Then

$$\sum_{i\geq 2} Q_i(G) = 2|E(G)|\big(|V(G)|-1\big) - M_1(G)$$

Proof. For any vertex u we have

$$2|E(G)| - d(u) = \sum_{v\in N_1(u)} d(v) + \sum_{i\geq 2}\sum_{v\in N_i(u)} d(v) = \sum_{v\in N_1(u)} d(v) + \sum_{i\geq 2} Q_i(u)$$

The claim now follows by summing over all vertices. ■

Corollary 6.1 Let $G \neq K_n$ where K_n denotes the complete graph on n-vertices. Then

$$M_1(G) + Q_2(G) \leq 2|E(G)|\big(|V(G)|-1\big)$$

with equality if and only if, diam(G) =2.

Proposition 7 Let G be a connected graph. Then

$$\sum_{u\in V(G)} m_1^2(u) \geq M_1(G)$$

with equality if and only if G is regular.

Proof. From the Cauchy-Schwarz inequality one obtains

$$Q_1(G) = \sum_{u\in V(G)} m_1(u)d(u) \leq \sqrt{\sum_{u\in V(G)} m_1^2(u)} \sqrt{\sum_{u\in V(G)} d^2(u)}$$

Since $M_1(G)= Q_1(G)$, we have

$$M_1(G) \leq \sqrt{\sum_{u\in V(G)} m_1^2(u)} \sqrt{M_1(G)}$$

and the claim follows. ■

A connected graph is called pseudo-regular [25, 26] if there exists a positive constant p=p(G) such that each vertex of G has the average neighbor degree number equal to p, i.e., $m_1(u)=p(G)$ for any vertex u in G. Of course, every regular graph is also pseudo-regular. Moreover, it is obvious that $\langle m_1(G)\rangle = p(G)$ for any pseudo-regular graph.

In Fig. 2 two infinite sequences of pseudo-regular graphs denoted by $G_A(k)$ and $G_B(k)$ are shown [27]. It is interesting to note that $m_1(u)=3$ holds for any vertex u of graphs $G_A(k)$ and $G_B(k)$, where $k\geq 3$.

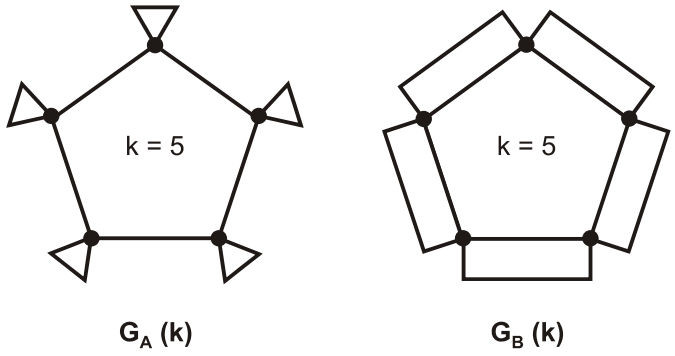

Figure 2
Pseudo-regular chemical graphs $G_A(5)$ and $G_B(5)$ that are not regular

Moreover, for graphs $G_A(k)$ and $G_B(k)$ the identities E(2,2,)=k, E(4,2)=2k, E(4,4)=k, $|E(G)| = 4k$ are fulfilled. This implies that graphs $G_A(k)$ and $G_B(k)$ cannot be distinguished by topological indices of the type X(G).

Proposition 8 Let G be a pseudo-regular graph. Then

$$p(G) = \langle m_1(G) \rangle = \frac{2M_2(G)}{M_1(G)}$$

Proof. From Proposition 2 it follows directly that if G is pseudo-regular then $M_1(G) = 2|E(G)|p$ and $M_2(G) = |E(G)|p^2$. ■

Proposition 9 Let G be a connected graph. Then

$$\sqrt{\frac{\sum_{u \in V(G)} Q_1^2(u)}{M_1(G)}} = \sqrt{\frac{\sum_{u \in V(G)} d^2(u) m_1^2(u)}{\sum_{u \in V(G)} d^2(u)}} \geq \frac{2M_2(G)}{M_1(G)}$$

with equality if and only if G is pseudo-regular.

Proof: We start from the Chebyshev inequality ([28], p 43). By specializing $b_j = a_j$ and $\sum_{j=1}^{J} w_j = 1$ we obtain the inequality

$$\sum_{j=1}^{J} w_j a_j^2 \geq \left(\sum_{j=1}^{J} w_j a_j \right)^2$$

with equality if and only if $a_1 = a_2, \ldots = a_J$. Now we denote by u_j the j-th vertex of G and define $a_j = m_1(u_j)$ and $w_j = d^2(u_j)/M_1(G)$ for $1 \leq j \leq J = |V(G)|$. We have

$$\frac{\sum_{u \in V(G)} d^2(u) m_1^2(u)}{\sum_{u \in V(G)} d^2(u)} \geq \left(\frac{1}{M_1(G)} \sum_{u \in V(G)} d^2(u) m_1(u) \right)^2 = \left(\frac{2M_2(G)}{M_1(G)} \right)^2$$

Now the claim follows with equality if and only if G is pseudoregular. ■

It is interesting to note that the left-hand side of the inequality of Proposition 9 is a sharp lower bound of the spectral radius of G ([25]).

Proposition 10 Let G be a connected graph. Then

$$\sqrt{\frac{\sum_{u \in V(G)} (d^2(u) + Q_1(u))^2}{\sum_{u \in V(G)} d^2(u)}} = \sqrt{\frac{\sum_{u \in V(G)} (d^2(u) + d(u) m_1(u))^2}{M_1(G)}} \geq 2\sqrt{\frac{M_1 G)}{|V(G)|}}$$

with equality if and only if G is regular.

Proof. We compute the variance of quantities defined as $b_j = d^2(u_j) + d(u_j)m_1(u_j)$ for $1 \leq j \leq J = |V(G)|$. We have

$$\mathrm{Var}(b) = \frac{1}{J} \sum_{j=1}^{J} b_j^2 - \left(\frac{1}{J} \sum_{j=1}^{J} b_j \right)^2 \geq 0$$

Consequently,

$$\frac{1}{|V(G)|}\sum_{u\in V(G)}(d^2(u)+d(u)m_1(u))^2 \geq \left(\frac{1}{|V(G)|}\sum_{u\in V(G)}(d^2(u)+d(u)m_1(u))\right)^2 = \frac{4M_1^2G)}{|V(G)|^2}$$

and this further implies

$$\frac{1}{M_1(G)}\sum_{u\in V(G)}(d^2(u)+d(u)m_1(u))^2 \geq \frac{4M_1G)}{|V(G)|}.$$

From there the claim follows, with equality if and only if G is regular. ■

The left-hand side of the inequality of Proposition 10 represents a sharp lower bound on the Laplacian spectral radius of G [29].

4 Possibilities of Increasing the Discriminativity

Comparing the topological indices $\langle m_1(G)\rangle$ and $\langle m_2(G)\rangle$ it is clear that $\langle m_2(G)\rangle$ should be more discriminative than $\langle m_1(G)\rangle$. Considering the pseudo-regular graphs $G_A(k)$ and $G_B(k)$ in Fig. 2, from the previous considerations it follows that $\langle m_1(G_A(k))\rangle = \langle m_1(G_B(k))\rangle = 3$ for $k \geq 3$, and $\langle m_2(G_A(k))\rangle = 28/9$ and $\langle m_2(G_A(k))\rangle = 32/9$ hold for $k \geq 5$.

For isospectral graphs G_1 and G_2 depicted in Fig. 1 it can be verified that $\langle m_1(G_1)\rangle = \langle m_1(G_2)\rangle = 16/7$, moreover $\langle m_2(G_1)\rangle = 177/70 \approx 2.52857$ and $\langle m_2(G_2)\rangle = 2117/840 \approx 2.52024$. As we can observe the numerical values of $\langle m_2(G_1)\rangle$ and $\langle m_2(G_2)\rangle$ are very close.

In the following, we will analyse the situations where employing the topological descriptor $\langle m_2(G)\rangle$ does not result in an improvement of disriminating performance. One such situation is, obviously, when G is regular; another one is when the graph is, in a sense, "small".

Proposition 11 Let G be a connected graph of diameter 2. Then the descriptors $\langle m_1(G)\rangle$ and $\langle m_2(G)\rangle$ are algebraically dependent quantities.

Proof. If the diameter of G is equal to 2, we have $n_1(u) = d(u)$ and $n_2(u) = |V(G)| - 1 - d(u)$ for any vertex u. By Proposition 6, one obtains

$$2|E(G)| - d(u) = \sum_{v\in N_1(u)} d(v) + \sum_{v\in N_2(u)} d(v) = Q_1(u) + Q_2(u)$$

This implies that

$$Q_2(u) = 2|E(G)| - d(u) - Q_1(u) = 2|E(G)| - d(u)\big(1 + m_1(u)\big)$$

From there it follows that

$$\langle m_2(G)\rangle = \frac{1}{|V(G)|}\sum_{u\in V(G)}\frac{Q_2(u)}{n_2(u)} = \frac{1}{|V(G)|}\sum_{u\in V(G)}\frac{2|E(G)| - d(u)\big(1+m_1(u)\big)}{|V(G)|-1-d(u)}$$

Hence, if two graphs of diameter 2 have identical d(u) and $m_1(u)$ for all vertices, we cannot discriminate between them based solely on the values of $\langle m_1(G)\rangle$ and $\langle m_2(G)\rangle$. ■

For an illustration, look at the polyhedral graphs of diameter 2 shown in Fig. 3.

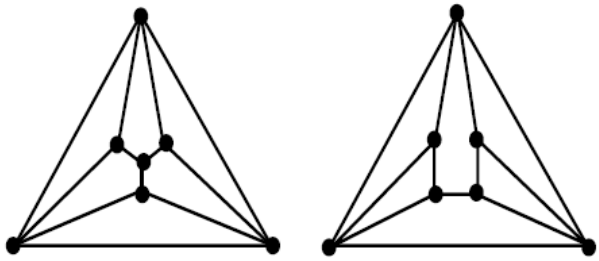

Figure 3
Graphs of diameter 2 that cannot be distinguished by $\langle m_1(G)\rangle$ and $\langle m_2(G)\rangle$

It can be easily verified that graphs G_b and G_c are characterized by the following identical topological parameters: E(3,3)=3, E(4,3)=6, E(4,4)=3, moreover, $\langle m_1(G_b)\rangle = \langle m_1(G_c)\rangle = 7/2$, $\langle m_2(G_b)\rangle = \langle m_2(G_c)\rangle = 23/7 = 3.285714$. It should be noted that for G_b and G_c the corresponding Wiener indices (W) are also identical, namely $W(G_b)=W(G_c)=30$ [1, 11].

The above examples demonstrate that there exist several molecular graphs having the same $\langle m_1(G)\rangle$ index. Moreover, in certain cases, indices $\langle m_i(G)\rangle$ for small values of i (i=1,2) still suffer from degeneracy and narrow numerical range.

As we have already mentioned the occurrence of degeneracy can be decreased by taking into account the degrees of neighboring vertices in $N_i(u)$, that is, the degrees of all vertices at distance i≥1 from u. Based on this concept, Randić and Plavšić proposed a descriptor of the following type [17]:

$$AVS(G) = \sum_{u\in V(G)} d(u) + \sum_{u\in V(G)}\sum_{i\geq 1} Q_i(u)P_i(u)$$

In the above formula, constants $P_i(u)$ are appropriately selected positive weights. In general, the weight is a strictly decreasing positive function of i. In the chemical literature, when $P_i = 1/2^i$ for i=1,2, ..., the AVS(G) index is called "the augmented valence sum" [17]. This is a useful measure of complexity of chemical graphs. It is interesting to note, that if $P_i(u)=1$ for any $i\geq 1$ and for any vertex u, then it follows from the Proposition 6

$$AVS(G) = \sum_{u\in V(G)} d(u) + \sum_{u\in V(G)} \sum_{i\geq 1} Q_i(u) = 2|E(G)| + \sum_{i\geq 1} Q_i(G) = 2|E(G)||V(G)|$$

Moreover, if $P_i(u)=1/m_i(u)$ for $i\geq 1$, then we get the equality

$$AVS(G) = 2|E(G)| + \sum_{u\in V(G)} \sum_{i\geq 1} n_i(u) = 2|E(G)| + |V(G)|\left(|V(G)| - 1\right)$$

Finally, if $P_i(u)=1/n_i(u)$ for $i\geq 1$, then one obtains

$$AVS(G) = 2|E(G)| + \sum_{u\in V(G)} \sum_{i\geq 1} m_i(u) = 2|E(G)| + |V(G)| \sum_{i\geq 1} \langle m_i(G) \rangle$$

as a particular case. The descriptor AVS(G) has a better discriminating ability than most other traditional topological indices [17]. The only drawback to the computation of AVS(G) descriptors is that in every cases, it is necessary to determine the corresponding graph distance matrix.

5 A Novel Set of Molecular Descriptors Based on Dissimilarity Functions

An alternative approach to improve the discriminating ability is to try to combine the information captured by $\langle m_1(G) \rangle$ and $\langle m_2(G) \rangle$. That would amount to quantifying the change in the average degree when one passes from distance 1 to distance 2 from a given vertex. Starting with this concept, we selected a topological quantity of the type

$$\frac{1}{|V(G)|} \sum_{u\in V(G)} D\left(m_1(u), m_2(u)\right).$$

In the expression above the non-negative function D(x,y) is a measure of dissimilarity of its arguments. There are several ways to meaningfully choose D(x, y). As a particular case, we consider here the dissimilarity function defined as D(x,y)= min(x,y)/max(x,y). In that way we obtain a new topological index

$$T(G) = \frac{1}{|V(G)|} \sum_{u\in V(G)} \frac{\min(m_1(u), m_2(u))}{\max(m_1(u), m_2(u))} \leq 1$$

It can be verified that T(G) discriminates between chemical graphs G_1 and G_2 in Fig. 1. Indeed, $T(G_1)=9553/11760=0.81233$ and $T(G_2)=19391/23520= 0.82447$. The result is even more interesting when we take into account the fact that G_1 and G_2 are isospectral [15]. A imilareffect appears on a pair of isospectral graphs depicted in Fig. 4. [30].

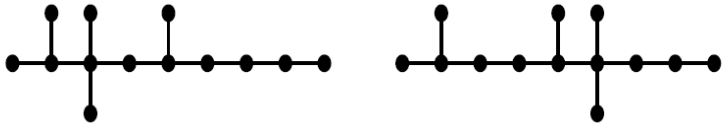

Figure 4
A pair of isospectral trees that cannot be distinguished by indices of the type X(G), but are discriminated by index T(G)

Moreover, for graphs of diameter 2 in Fig. 3 we have $T(G_b) = 0.8641002$ and $T(G_c)= 0.8868275$. Hence we have reasons to consider T(G) as a valuable addition to the repertoire of topological indices discriminating among isospectral and/or graphs of small diameter.

Concluding Remarks

We conclude the paper with some remarks on the properties of the topological descriptor T(G). According to our comparative studies performed on isospectral graphs and graphs of small diameter, it was found that the topological index T(G) has a quite low degeneracy. This is a favorable property when considering the efficiency of discrimination among real chemical graphs. Additionally, a practical advantage is that descriptors T(G) are simply computed. For this purpose, it is enough to determine the degree-distribution of the first and second order neighboring vertices (i.e. degrees of vertices at distances i= 1 and 2 from a given vertex u).

It is obvious from the definition that T(G) is equal to one for regular graphs. That suggests that T(G) could be used as a kind of measure of non-regularity of a graph. For a path P_n on n vertices we easily obtain $T(P_n) = 1 – 1/n$, in accordance with our perception of a path as a quite regular tree. Computing the value of T(G) for a star graph S_n on n vertices, however, we face a serious problem since $m_2(u)$ is equal to zero for the central vertex u. It follows that $T(S_n) = 1/n$, a result difficult to reconcile with the fact that the star is also a fairly regular tree. On the other hand, the drastic changes in the average degree of neighbors on distances 1 and 2 in the star graph are well captured by the index.

Generally, T(G) is likely to have problems whenever G has a well-connected vertices, i.e., vertices adjacent to all other vertices. However, that is not a serious problem in practical applications, since well-connected vertices are necessarily of a high degree, while chemically interesting and relevant graphs contain vertices of degree at most four.

Acknowledgment

Partial support of the Ministry of Science, Education and Sport of the Republic of Croatia (Grants No. 037-0000000-2779 and 177-0000000-0884 and a bilateral cooperation project) is gratefully acknowledged. This work was partially supported by the Hungarian National Office for Research and Technology (NKTH) as a part of a Bilateral Cooperation Program (under contract no. HR-38/2008).

References

[1] N. Trinajstić, Chemical Graph Theory, 2nd revised ed. CRC Press, Boca Raton, USA, 1992

[2] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, 2nd ed., Wiley–VCH, Weinheim, 2009

[3] M. Randić, The Connectivity Index 25 Years after, Journal of Molecular Graphics and Modelling, 20 (2001) 19-35

[4] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb Indices 30 Years After, Croat. Chem. Acta, 76 (2003) 113-124

[5] I. Gutman, K. Ch. Das, The First Zagreb Index 30 Years after, MATCH Commun. Math. Comput. Chem. 50 (2004) 83-92

[6] B. Zhou, N. Trinajstić, On a Novel Connectivity Index, J Math Chem 46, (2009) 1252-1270

[7] B. Furtula, A. Graovac, D. Vukičević, Atom-bond Connectivity Index of Trees, Discrete Applied Mathematics, 157 (2009) 2828-2835

[8] D. Vukičević, B. Furtula, Topological Index Based on the Ratios of Geometrical and Arithmetical Means of End-vertex Degrees of Edges, J Math Chem 46 (2009) 1369-1376

[9] D. Vukičević, M. Gašperov, Bond Additive Modeling 1. Adriatic Indices, Croat. Chem. Acta, 83 (2010) 243-260

[10] T. Došlić, T. Réti, D. Vukičević, On the Vertex Degree Indices of Connected Graphs, Chem. Phys. Lett. 512 (2011) 283-286

[11] I. Gutman, Y-N. Yeh, S-L. Lee, Y-L. Luo, Some Recent Results in the Theory of the Wiener Number, Indian Journal of Chemistry, 32A (1993) 651-661

[12] I. Gutman, Y-L. Luo, Y-N. Yeh, S-L. Lee, The Mean Isomer Degeneracy of the Wiener Index, Journal of the Chinese Chemical Society, 40 (1993) 195-198

[13] F. Buckley, F. Harary, Distance in Graphs, Addison–Wesley, Redwood, 1990

[14] D. B. West, Introduction to Graph Theory, Prentice-Hall, Upper Saddle River, NJ, 1996

[15] K. Balasubramanian, C. S. Basak, Characterization of Isospectral Graphs Using Graph Invariants and Derived Orthogonal Parameters, J. Chem. Inf. Comput. Sci. 38 (1998) 367-373

[16] M. Randić, On Complexity of Transitive Graphs Representing Degenerate Rearrangements, Croat. Chem. Acta, 74 (2001) 683-705

[17] M. Randić, D. Plavšić, On the Concept of Molecular Complexity, Croat. Chem. Acta, 75 (2002) 107-116

[18] I. Lukovits, S. Nikolić, N. Trinajstić, On Relationships between Vertex-degrees, Path-numbers and Graph Valence-shells in Trees, Chem. Phys. Lett. 354 (2002) 417-422

[19] K. Ch. Das, I. Gutman, Some Properties of the Second Zagreb Index, MATCH Commun. Math. Comput. Chem. 52, (2004) 103-112

[20] A. Ilić, D. Stefanović, On Comparing Zagreb indices, MATCH Commun. Math. Comput. Chem. 62 (2009) 681-687

[21] D. Vukičević, I. Gutman, B. Furtula, V. Andova, D. Dimitrov, Some Observations on Comparing Zagreb Indices, MATCH Commun. Math. Comput. Chem. 66 (2011) 627-645

[22] K. Ch. Das, Maximizing the Sum of Squares of Degrees, Discrete Math. 285 (2004) 57-66

[23] S. Yamaguchi, Estimating the Zagreb Indices and the Spectral Radius of Triangle- and Quadrangle-free Connected Graphs, Chem. Phys. Lett. 458 (2008) 396-398

[24] M. Gordon, G. R. Scantlebury, Non-Random Polycondensation: Statistical Theory of the Substitution Effect, Trans. Faraday Soc. 60 (1964) 604-621

[25] A. Yu, M. Lu, F. Tian, On the Spectral Radius of Graphs, Linear Algebra and its Applications 387 (2004) 41-49

[26] T. Réti, I. Gutman, D. Vukičević, On Zagreb Indices of Pseudo-Regular Graphs, Journal of Mathematical Nanoscience, 1 (2012) 1-12

[27] H. Hargitai, personal communication

[28] G. H. Hardy, J. E. Littlewood, G. Pólya, Inequalities, Cambridge University Press, Cambridge, 1952

[29] G.-X. Tian, T.-Z. Huang, B. Zhou, A Note on Sum of Powers of the Laplacian Eigenvalues of Bipartite Graphs, Linear Algebra and its Applications, 430 (2009) 2503-2510

[30] E. R. van Dam, W. H. Haemens, Which Graphs Are Determined by Their Spectrum? Linear Algebra and its Applications, 373 (2003) 241-272

[31] B. Zhou, Zagreb Indices, MATCH Commun. Math. Comput. Chem. 52 (2004) 113-118