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Relations between distance–based and degree–based topological indices

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ABSTRACT

Let W, Sz, PI, and WP be, respectively, the Wiener, Szeged, PI, and Wiener polarity indices of a molecular graph G. Let M_1 and M_2 be the first and second Zagreb indices of G. We obtain relations between these classical distance– and degree–based topological indices.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ ($|V(G)| = n$) and edge set $E(G)$ ($|E(G)| = m$). For a graph G, we denote by $d_G(v)$ the degree of a vertex v and by $d_G(u, v)$ denote the distance between the vertices u and v. The girth of a graph is the length of a shortest cycle contained in it. For other terminology and notation, we refer the readers to [2].

A graph invariant is a function defined on a graph that is independent of the labeling of its vertices. Till now, hundreds of graph invariants have been considered in the mathematic–chemical literature as molecular structure descriptors [33,34]. Some of these were found to be successful in chemical and physico–chemical applications, especially in QSAR/QSPR studies [6,7,24], and are referred to as *topological indices*. For details on degree–based topological indices and their comparative studies see [5,9,11,12,15,31] and the references cited therein. For analogous data on distance–based indices consult [4,5,39].

In this paper we are considering the following topological indices.

The first and the second Zagreb indices are defined as

$$M_1 = M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right] \tag{1}$$

and

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v) \tag{2}$$

respectively. These are the oldest [17,18] and best studied degree–based topological indices (see the reviews [12,16], recent papers [13,22,35], and the references cited therein).

The distance–based topological indices considered in this work are the Wiener, Szeged, PI, and the Wiener polarity indices.

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The oldest [37] and most thoroughly studied distance–based molecular structure descriptor is the Wiener index, defined as

$$W = W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v).$$

For details on its theory see the recent papers [21,26,32,39] and the references cited therein.

The Wiener polarity index $WP(G)$ of a graph G (the first time considered in [37], see also [20,27,38,39]), is the number of pairs of vertices of G at distance 3.

Let $e = uv$ be an edge of graph G, connecting the vertices u and v. Define two sets $N_u(e)$ and $N_v(e)$ as follows:

$$N_u(e) = \{w \in V(G) \mid d_G(w, u) < d_G(w, v)\} \tag{3}$$

$$N_v(e) = \{w \in V(G) \mid d_G(w, v) < d_G(w, u)\}. \tag{4}$$

The numbers of elements of $N_u(e)$ and $N_v(e)$ are denoted by $n_u(e)$ and $n_v(e)$, respectively. Thus, $n_u(e)$ counts the vertices of G lying closer to the vertex u than to the vertex v. The meaning of $n_v(e)$ is analogous. Vertices equidistant from both ends of the edge uv are not counted since these not belong either to $N_u(e)$ or to $N_v(e)$. Note that for any edge e of G, $n_u(e) \geq 1$ and $n_v(e) \geq 1$, because $u \in N_u(e)$ and $v \in N_v(e)$.

The Szeged index (see [1,14,25] and the references cited therein) is defined as

$$Sz = Sz(G) = \sum_{uv \in E(G)} n_u(e)\, n_v(e).$$

As similar, so-called “vertex PI index” is [29,30]

$$PI_v(G) = \sum_{e=uv} \left[n_u(e) + n_v(e)\right].$$

2. Difference of Zagreb indices and Wiener polarity index

Although the two Zagreb indices were introduced as early as the 1970s [17,18], and eventually extensively studied, their simplest mutual relation – namely their difference – did not attract much attention until quite recently [3,10,28].

Define the *reduced second Zagreb index* as

$$RM_2 = RM_2(G) = \sum_{uv \in E(G)} \left[d_G(u) - 1\right]\left[d_G(v) - 1\right]. \tag{5}$$

Bearing in mind Eqs. (1) and (2), one straightforwardly obtains

$$RM_2(G) = M_2(G) - M_1(G) + m$$

i.e.,

$$M_2(G) - M_1(G) = \left[\sum_{ij \in E(G)} (d_i - 1)(d_j - 1)\right] - m(G). \tag{6}$$

Relation (6), or more precisely, the reduced second Zagreb index, Eq. (5), plays an important role in the theory of Wiener polarity index WP.

Theorem 1. *[28] If the (molecular) graph G has $\#P_4$ 4-vertex path subgraphs and t triangles, then*

$$RM_2 = \#P_4 + 3t \qquad \text{i.e.,} \qquad M_2 - M_1 = \#P_4 + 3t - m. \tag{7}$$

Formula (7) seems to have been first reported in [28]. Its special case for triangle–free graphs and trees was reported or used several times [8,19,23,36].

By definition, the Wiener polarity index WP is the number of pairs of vertices whose distance is 3. Every pair of vertices at distance 3 corresponds to at least one 4-vertex path subgraph, but the opposite is not generally true. Therefore, in the general case, $WP \leq \#P_4$, implying [23]

$$WP \leq M_2 - M_1 + m. \tag{8}$$

Equality in (8) is summarized in the following:

Theorem 2. *[23] Let G be a (molecular) graph with first and second Zagreb indices M_1 and M_2, and with m edges. Then its Wiener polarity index obeys the identity*

$$WP = M_2 - M_1 + m \tag{9}$$

if and only if G is either acyclic or if its girth is greater than 6.

Special cases of Theorem 2 have been reported in [8,19].