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On Discriminativity of Vertex-Degree-Based Indices

IVAN GUTMAN•

Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia

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ABSTRACT

A recently published paper [T. Došlić, *this journal* **3** (2012) 25-34] considers the Zagreb indices of benzenoid systems, and points out their low discriminativity. We show that analogous results hold for a variety of vertex-degree-based molecular structure descriptors that are being studied in contemporary mathematical chemistry. We also show that these results are straightforwardly obtained by using some identities, well known in the theory of benzenoid hydrocarbons.

Keywords: Zagreb index, vertex-degree-based indices, benzenoid graph, catacondensed benzenoid graph.

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1. INTRODUCTION

In a recent paper [2] Došlić examined the Zagreb indices of benzenoid graphs and concluded that their discriminativity is low. In the present note we intend to offer more arguments in favor of Došlić's results, and show that such a low discriminativity is characteristic not only for Zagreb indices, but for a whole class of vertex-degree-based topological indices.

Let G be a molecular graph with vertex set $V(G)$ and edge set $E(G)$. An edge connecting the vertices u and v will be denoted by uv. The *degree* of the vertex v, denoted by $\delta(v)$, is the number of the first neighbors of v. The first and second Zagreb indices are defined as [2,8]

$$M_1(G) = \sum_{v \in V(G)} \delta(v)^2 \qquad (1)$$

and

•Corresponding author (Email: gutman@kg.ac.rs)

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

respectively. The first Zagreb index, Eq. (1), can be written also as [2,3]

$$M_1(G) = \sum_{uv \in E(G)} [\delta(u) + \delta(v)] \ . \qquad (3)$$

A large number of molecular structure descriptors (topological indices), defined in terms of vertex degrees, has been considered in the literature [7,12]. The algebraic form of many of these is analogous to Eqs. (2) and (3). The general form of such vertex-degree-based descriptors is

$$D = D(G) = \sum_{uv \in E(G)} F(\delta(u), \delta(v)) \qquad (4)$$

where the summation goes over all pairs of adjacent vertices *u*,*v* of the molecular graph *G*. In particular, the function $F = F(x, y)$ in Eq. (4) has the following form:

$F(x, y) = x + y$	for the first Zagreb index [3]
$F(x, y) = xy$	for the second Zagreb index [8]
$F(x, y) = \frac{1}{\sqrt{xy}}$	for the Randić index [11]
$F(y, y) = (xy)^{\lambda}$	for the general Randić index [9], where λ is an adjustable parameter
$F(x, y) = \sqrt{\frac{x + y - 2}{xy}}$	for the atom-bond connectivity index [4]
$F(x, y) = \frac{1}{\sqrt{x + y}}$	for the sum-connectivity index [15]
$F(x, y) = (x + y)^{\lambda}$	for the general sum-connectivity index [16], where λ is an adjustable parameter
$F(x, y) = \frac{\sqrt{xy}}{\frac{1}{2}(x + y)}$	for the geometric-arithmetic index [13]
$F(x, y) = \left(\frac{xy}{x + y - 2} \right)^3$	for the augmented Zagreb index [5]

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$F(x,y)=\dfrac{2}{x+y}$ for the harmonic index [14].

In the case of benzenoid graphs the calculation of all the above specified topological indices is much simplified by the fact that these graphs possess only vertices of degree 2 and 3, and therefore there are only three types of contributions $F(x,y)$, occurring in the summation on the right-hand side of Eq. (4), namely $F(2,2)$, $F(2,3)$, and $F(3,3)$. Indeed, if by m_{22}, m_{23}, and m_{33} we denote, respectively, the number of edges connecting two vertices of degree 2, the number of edges connecting vertices of degree 2 and 3, and the number of edges connecting two vertices of degree 3, then

$$D = m_{22}\,F(2,2) + m_{23}\,F(2,3) + m_{33}\,F(3,3). \qquad (5)$$

Moreover, in the case of benzenoid graphs, simple expressions for the structure-dependency of the coefficients m_{22}, m_{23}, m_{33} are available. These expressions are collected and systematically outlined in the book [6]. (It is worth noting that in [2] instead of the book [6], the fully irrelevant book [1] by the same authors was quoted.)

The structural features of benzenoid graphs (in mathematical literature often referred to as "hexagonal systems") are described in detail in the book [6]. In Fig. 1, self-explanatory examples of benzenoid graphs are provided.

The basic properties of benzenoid graphs are determined [6] by the number of hexagons (h) and internal vertices (i). For instance, the formula of the respective benzenoid hydrocarbon is $C_{4h+2-i}H_{2h+4-i}$.

2. MAIN RESULTS

Let b be the number of edges on the perimeter, connecting two vertices of degree 3. (This parameter is usually referred to as the *number of bays*.) Then, for a benzenoid graph B we have [6]:

$$m_{22}(B) = b + 6$$
$$m_{23}(B) = 4h - 2b - 2i - 4$$
$$m_{33}(B) = h + b + i - 1$$

which combined with Eq. (5) immediately implies

$$\begin{aligned} D(B) = {} & [6F(2,2) - 4F(2,3) - F(3,3)] + [(4F(2,3) + F(3,3)]h \\ & + [F(3,3) - 2F(2,3)]i + [F(2,2) - 2F(2,3) + F(3,3)]b \end{aligned} \qquad (6)$$

The following claims are straightforward consequences of Eq. (6):

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Proposition 1. If B_a and B_b are two benzenoid graphs with equal number of hexagons, equal number of internal vertices, and equal number of bay regions, then $D(B_a) = D(B_b)$ holds for any topological index of the form (4).

Proposition 2. If B_a and B_b are two catacondensed benzenoid graphs with equal number of hexagons and equal number of bay regions, then $D(B_a) = D(B_b)$ holds for any topological index of the form (4).

An interesting special case is encountered when the function F in Eq. (4) has the property $F(2,2) - 2F(2,3) + F(3,3) = 0$.

Proposition 3. Suppose that the condition $F(2,2) - 2F(2,3) + F(3,3) = 0$ is satisfied. Then the equality $D(B_a) = D(B_b)$ holds for two benzenoid graphs B_a and B_b if these have equal number of hexagons and equal number of internal vertices.

Proposition 4. Suppose that the condition $F(2,2) - 2F(2,3) + F(3,3) = 0$ is satisfied. Then the equality $D(B_a) = D(B_b)$ holds for any catacondensed benzenoid graphs B_a and B_b possessing equal number of hexagons.

For a benzenoid graph B, specified in Proposition 4,

$$D(B) = [6F(2,2) - 4F(2,3) - F(3,3)] + [(4F(2,3) + F(3,3)]h \quad . \qquad (7)$$

The condition $F(2,2) - 2F(2,3) + F(3,3) = 0$ is satisfied if the function F is of the form $F(x,y) = f(x) + f(y)$ for arbitrary f. Among the above listed vertex-degree-based topological indices, only the first Zagreb index (because of Eq. (3)) falls into this category. It is, of course, easy to design many other functions $F(x,y)$ with the required property. For instance,

$$F(x,y) = \frac{16}{2\sqrt{5} - \sqrt{6} - 2}\sqrt{x+y} + 2^{x+y}$$

or

$$F(x,y) = a^4(a-1)^2 b^{x+y} - b^4(b-1)^2 a^{x+y}$$

for any real-valued constants a and b. Fortunately, so far no one such topological index (in addition to the first Zagreb index) has been put forward. In view of Propositions 3 and 4, their discrimnativity would be prohibitively low.

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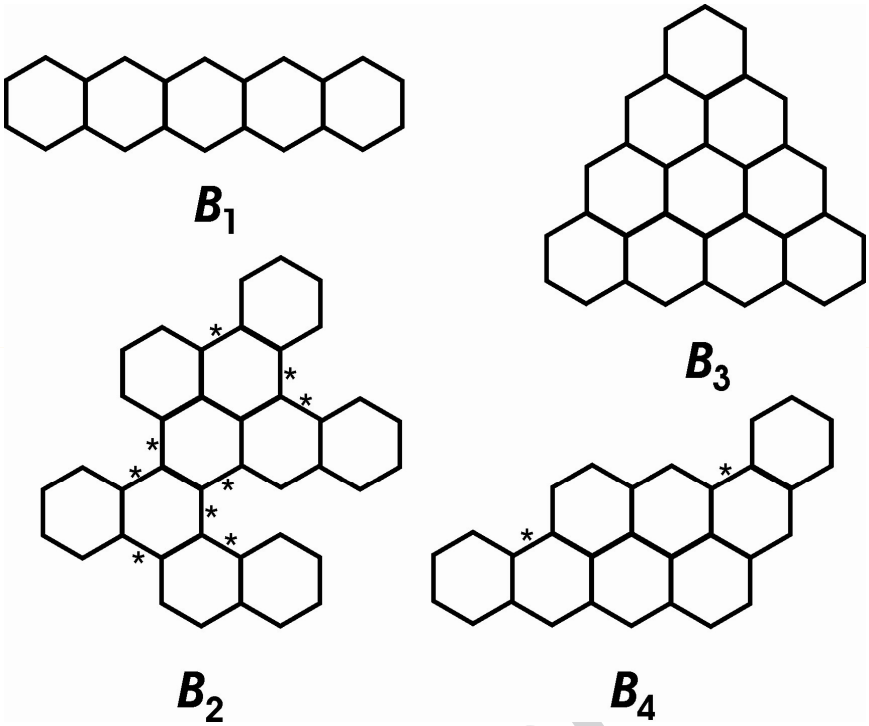

Fig. 1. Examples of benzenoid graphs: B_1 and B_2 are catacondensed ($i = 0$), whereas B_3 and B_4 are pericondensed ($i > 0$). The number h of their hexagons is 5, 10, 10, and 8, respectively; the number of their internal vertices i is 0, 0, 9, and 4, respectively. By asterisks are indicated the edges on the perimeter, connecting two vertices of degree 3; their count is b. Thus, $b(B_1) = 0$, $b(B_2) = 9$, $b(B_3) = 0$, $b(B_4) = 2$.

From Eq. (6) it is also evident that if the coefficient $F(2,2) - 2F(2,3) + F(3,3)$ is positive-valued, then the benzenoid graph with h hexagons and i internal vertices will have maximal (resp. minimal) D-index if b is maximal (resp. minimal). If this coefficient is negative-valued, then the situation is reversed.

Recall that in the case of benzenoid graphs, the minimal value of the parameter b is zero (as, for instance, for B_1 and B_3 in Fig. 1). For catacondesned benzenoids the maximal value of b was established by Rada [10] and is equal to $\lfloor (3h-6)/2 \rfloor$.

Proposition 5. For catacondensed benzenoid graphs with h hexagons, the value of the topological index D, Eq. (4), is bounded by

$$[6F(2,2) - 4F(2,3) - F(3,3)] + h[(4F(2,3) + F(3,3)] \tag{8}$$

and

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$$[6F(2,2)-4F(2,3)-F(3,3)]+h[(4F(2,3)+F(3,3)] +\left\lfloor\frac{3h-6}{2}\right\rfloor[F(2,2)-2F(2,3)+F(3,3)] \quad . \qquad (9)$$

These bounds are tight. If $F(2,2)-2F(2,3)+F(3,3)$ is positive-valued, then (8) is a lower and (9) an upper bound for *D*. If $F(2,2)-2F(2,3)+F(3,3)$ is negative-valued, then (9) is a lower and (8) an upper bound for *D*. If $F(2,2)-2F(2,3)+F(3,3)$ is equal to zero, then Proposition 4 and Eq. (7) are applicable.

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