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Research Article

Weighted Graph Irregularity Indices Defined on the Vertex Set of a Graph

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Performing comparative tests, some possibilities of constructing novel degree- and distance-based graph irregularity indices are investigated. Evaluating the discrimination ability of different irregularity indices, it is demonstrated (using examples) that in certain cases two newly constructed irregularity indices, namely $IRDE_A$ and $IRDE_B$, are more selective.

1. Introduction

Only connected graphs without loops and parallel edges are considered in this study. For a graph G with n vertices and m edges, $V(G)$ and $E(G)$ denote the sets of vertices and edges, respectively. Let $d(u)$ be the degree of vertex u of G. Let uv be an edge of G connecting the vertices u and v. Let $\Delta = \Delta(G)$ and $\delta = \delta(G)$ be the maximum and the minimum degrees, respectively, of G. In what follows, we use the standard terminology in graph theory; for notations not defined here, we refer the readers to the books [1, 2].

For a connected graph G, the set of numbers n_j of vertices with degree j is denoted by $\{n_j = n_j(G)\colon n_j > 0, 1 \leq j \leq \Delta\}$. For simplicity, the numbers $n_j(G)$ are called the vertex-parameters of graph G. For two vertices $u, v \in V(G)$, the distance $d(u,v)$ between u and v is the number of edges in a shortest path connecting them.

Two connected graphs G_1 and G_2 are said to be vertex-degree equivalent if they have an identical vertex-degree sequence. Certainly, if G_1 and G_2 are vertex-degree equivalent, then their vertex-parameters sets satisfy the equation $n_j(G_1) = n_j(G_2)$ for every j. A graph is called k-regular if all its vertices have the same degree k. A graph which is not regular is called a nonregular graph. A connected graph G is said to be *bidegreed* if its degree set consists of only two elements, where a degree set of G is the set of all distinct elements of its degree sequence.

2. Preliminary Considerations

A topological index TI of a graph G is any number associated with G (in some way) provided that the equation $TI(G) = TI(G')$ holds for every graph G' isomorphic to G. A lot of existing topological indices are degree- and distance-based ones [3–5]. Graph irregularity indices form a notable subclass of the class of traditional topological indices; where a topological index TI of a (connected) graph G is called a graph irregularity index if $TI(G) \geq 0$, and $TI(G) = 0$ if and only if graph G is a regular graph. Details about the existing graph irregularity indices can be found in [6, 7]. The readers interested in the general concept of irregularity in graphs may consult the book [8].

In several situations, it is crucial to know how much irregular a given graph is; for example, see [9, 10] where irregularity measures are used to predict physicochemical properties of chemical compounds, and see [11–14] for some applications of irregularity measures in network theory.

Most of the existing irregularity indices used in mathematical chemistry are degree-based irregularity indices. There exist irregularity indices which form a particular subset Φ of the set of degree-based irregularity indices; we say that an irregularity index ϕ belongs to the set Φ if for every pair of vertex-degree equivalent graphs G_1 and G_2, the equation $\phi(G_1) = \phi(G_2)$ holds.

The most popular topological indices that are used in defining degree-based irregularity indices, are the first and second Zagreb indices (see for example [15]), denoted by M_1 and M_2, respectively, and the so-called forgotten topological index [15], denoted by F. The first and second Zagreb indices of a graph G are defined as

$$\begin{aligned} M_1(G) &= \sum_{u\in V(G)} d_u^2, \\ M_2(G) &= \sum_{uv\in E(G)} d_u d_v, \end{aligned} \tag{1}$$

and the forgotten topological index is defined as

$$F(G) = \sum_{u\in V(G)} d_u^3. \tag{2}$$

There exist numerous degree-based graph irregularity indices in literature, some of them are listed below.

The variance Var is a degree-based graph irregularity index introduced by Bell [16]. The variance Var of a graph G of order n and size m is defined as

$$Var(G) = \frac{1}{n}\sum_{u\in V(G)}\left(d_u - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \frac{4m^2}{n^2}. \tag{3}$$

We also consider the following four irregularity indices:

$$IRV(G) = n^2\mathrm{Var}(G) = nM_1(G) - 4m^2, \tag{4}$$

$$IR_1(G) = \sqrt{\frac{M_1(G)}{n}} - \frac{2m}{n}, \tag{5}$$

$$IR_2(G) = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n}, \tag{6}$$

$$IR_3(G) = F(G) - \frac{2m}{n}M_1(G). \tag{7}$$

It is remarked here that, except IR_2, all the irregularity indices formulated above belong to the set Φ.

3. Weighted Irregularity Indices Defined on the Vertex Set of a Graph

In this section, we consider irregularity indices defined on the set of vertices of a graph G. The majority of these indices are weighted degree- and distance-based topological indices. Most of them may be considered as extended versions of the Wiener index; for example, see [17]. Let us consider the weighted vertex-based topological index of a graph G formulated as

$$ZW(G) = \frac{1}{2}\sum_{u,v\in V(G)} Z(u,v)W(u,v), \tag{8}$$

where $Z(u,v)$ and $W(u,v)$ are appropriately selected non-negative 2-variable symmetric functions; both of them are defined on the vertex set $V(G)$ of G. For simplicity, we call the function $W(u,v)$ as the weight function of G. By taking

$$Z(u,v) = |d_u - d_v|^p. \tag{9}$$

in Equation (8), we get the following graph irregularity index

$$IRR_p(G) = \frac{1}{2}\sum_{u,v\in V(G)} |d_u - d_v|^p W(u,v), \tag{10}$$

where p is a positive real number. Depending on the choice of the parameter p and the weight function $W(u,v)$, various types of irregularity indices can be deduced. For instance, the choices $p = 1$ and $W(u,v) = 1$ lead to the so-called total irregularity of a graph G defined by

$$Irrt_1(G) = \frac{1}{2}\sum_{u,v\in V(G)} |d_u - d_v|. \tag{11}$$

It was introduced by Abdo et al. in [18]. Also, assuming that $p = 2$ and $W(u,v) = 1$, we have the irregularity index $Irrt_2(G)$, introduced in Ref. [19]:

$$Irrt_2(G) = \frac{1}{2}\sum_{u,v\in V(G)} (d_u - d_v)^2. \tag{12}$$

At this point, the following known proposition [19] concerning $Irrt_2$ needs to be stated.

Proposition 1. *For every graph G with n vertices and m edges, it holds that*

$$\begin{aligned} Irrt_2(G) &= \frac{1}{2}\sum_{u,v\in V(G)} (d_u - d_v)^2 = nM_1(G) - 4m^2 \\ &= n^2\mathrm{Var}(G) = IRV(G). \end{aligned} \tag{13}$$

In Equation (9), by taking $Z(u,v) = (d_u - d_v)^2$ and $W(u,v) = d(u,v)$, we obtain the following irregularity index:

$$IRD(G) = \frac{1}{2}\sum_{u,v\in V(G)} (d_u - d_v)^2 d(u,v). \tag{14}$$

Note that IRD is a weighted degree- and distance-based irregularity index. Although IRD is a new irregularity index which is not known in the literature, but we prove in the next proposition that this irregularity index can be written in the linear combination of the following two topological indices

$$DG(G) = \sum_{u\in V(G)} d_u^2 D_G(u), \tag{15}$$

and

$$\mathrm{Gut}(G) = \frac{1}{2}\sum_{u,v\in V(G)} (d_u d_v) d(u,v), \tag{16}$$

where $D_G(u)$ is identical to the transmission $\mathrm{Tr}(u)$ of the vertex $u \in V(G)$ and $\mathrm{Gut}(G)$ is the so-called Gutman index; for example, see [20].

Proposition 2. *For a (connected) graph G, it holds that*

$$IRD(G) = \frac{1}{2}\sum_{u,v\in V(G)} (d_u - d_v)^2 d(u,v) = DG(G) - 2\mathrm{Gut}(G). \tag{17}$$

Proof. Note that

$$\frac{1}{2}\sum_{u,v\in V(G)} (d_u - d_v)^2 d(u,v) = \frac{1}{2}\sum_{u,v\in V(G)} \left(d_u^2 + d_v^2\right) d(u,v) - 2Gut(G). \tag{18}$$

For the graph G, it holds [21] that

$$\frac{1}{2}\sum_{u,v\in V(G)} (\omega(u) + \omega(v)) d(u,v) = \sum_{u\in V(G)} \omega(u) D_G(u), \tag{19}$$

where $\omega(u)$ is any quantity associated with the vertex u of G. By taking $\omega(u) = d_u^2$ in (19) and using the obtained identity in (18), we get

$$\begin{aligned}\frac{1}{2}\sum_{u,v\in V(G)} (d_u - d_v)^2 d(u,v) &= \sum_{u\in V(G)} d_u^2 D_G(u) - 2\mathrm{Gut}(G) \\ &= DG(G) - 2\mathrm{Gut}(G).\end{aligned} \tag{20}$$

□

Remark 1. From Proposition 2, it follows that the inequality

$$DG(G) \geq 2\mathrm{Gut}(G) \tag{21}$$

holds for every (connected) graph G, with equality if and only if G is regular.

Remark 2. Because IRD is a weighted version of the irregularity index $Irrt_2$, it is expected that its discrimination power is better than that of $Irrt_2$.

Remark 3. Based on identity Equation (20), one can establish another irregularity index IRQ defined by

$$IRQ(G) = \frac{DG(G) - 2\mathrm{Gut}(G)}{2\mathrm{Gut}(G)} = \frac{DG(G)}{2\mathrm{Gut}(G)} - 1. \tag{22}$$

As $\mathrm{Gut}(G) > 1/2$ for every (connected) graph of order at least 3, one has

$$IRQ(G) = \frac{DG(G)}{2\mathrm{Gut}(G)} - 1 < DG(G) - 2\mathrm{Gut}(G) = IRD(G). \tag{23}$$

4. Discriminating Ability of Novel Weighted Irregularity Indices

For comparing the discrimination ability of the irregularity indices IRD and IRQ with the traditional degree-based irregularity indices Var, IR_1, IR_2, and IR_3, we use the 6-vertex graphs G_i $(i = 1, 2, 3, 4)$ depicted in Figure 1. It is remarked here that the graphs shown in Figure 1 belong to the family of connected threshold graphs, and graph G_1 is isomorphic to the connected 6-vertex antiregular graph (for example, see [22, 23]).

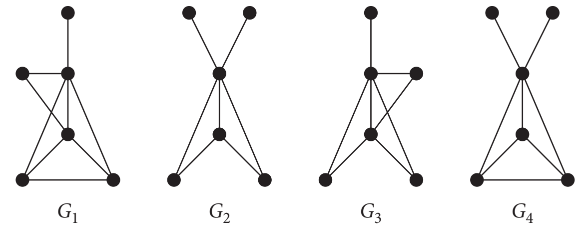

Figure 1: Four 6-vertex nonregular graphs selected for tests.

For the four graphs depicted in Figure 1, computed values of preselected topological indices M_1, M_2, F, and corresponding irregularity indices are summarized in Tables 1 and 2.

Comparing irregularity indices listed in Tables 1 and 2, the following conclusions can be drawn. Among the four tested graphs, the index G_1 achieves the maximum value (that is, 249) of IR_3. The irregularity indices IR_1 and IR_2 are maximum for the graph G_2 (namely, $IR_1(G_2) \approx 0.375$ and $IR_2(G_2) \approx 0.5202$). As it can be seen that $\mathrm{Var}(G_1) \approx 1.667$, while $\mathrm{Var}(G_2) = \mathrm{Var}(G_3) = \mathrm{Var}(G_3) \approx 1.889$ and that all the four graphs have the same value of $Irrt_1$, which is 26. Also, the relation $Irrt_2(G) = n^2\mathrm{Var}(G)$ is confirmed for the considered graphs: $Irrt_2(G_1) = 60$ and $Irrt_2(G_2) = Irrt_2(G_3) = Irrt_2(G_4) = 68$. Moreover, we have $IRD(G_1) = IRD(G_2) = IRD(G_3) = 80$ and $IRD(G_4) = 92$, while the computed values of the irregularity index IRQ are different for all four graphs. From these observations, one can conclude that the degree variance Var, the total irregularity index Irr_1, together with the irregularity indices Irr_2, and IRD have a limited discrimination ability for the considered four graphs.

5. Novel Irregularity Indices Constructed by Using the External Weight Concept

The weight function $W(u,v)$ included in (9) can be considered as an "internal" weight function. Introducing the external weight concept, one can construct novel irregularity indices. By using them, the original sequence of previously determined irregularity values can be appropriately modified for a given set of graphs considered.

By definition, an external weight $EW(G)$ for a graph G is a positive-valued topological index computed as a function of one or more traditional topological indices. By means of an external weight $EW(G)$ a novel irregularity index $IRE(G)$ can be created as defined below:

$$IRE(G) = EW(G) \times IR(G), \tag{24}$$

where $IR(G)$ is an arbitrary irregularity index. By appropriately selected external weights $EW(G)$, one can establish several different versions of irregularity indices $IRE(G)$ satisfying some restrictions or desired expectations. As an

Table 1: Computed topological indices of the four graphs shown in Figure 1.

Graph	m	M_1	M_2	F	Var	IR_1	IR_2	IR_3
G_1	9	64	106	252	5/3	0.266	0.4319	249.0
G_2	7	44	57	170	17/9	0.375	0.5202	167.7
G_3	8	54	79	214	17/9	0.333	0.4758	211.3
G_4	8	54	82	208	17/9	0.333	0.5349	205.3

Table 2: Computed topological indices of the four graphs shown in Figure 1.

Graph	m	$Irrt_1$	$Irrt_2$	DG	Gut	IRD	IRQ
G_1	9	26	60	388	154	80	0.2597
G_2	7	26	68	270	95	80	0.4211
G_3	8	26	68	326	123	80	0.3252
G_4	8	26	68	332	120	92	0.3833

example, consider the three external weights defined for a graph G of order n and size m as follows:

$$EW_A(G) = \frac{m^2}{100n}, \tag{25}$$

$$EW_B(G) = \frac{M_2(G) + F(G)}{n^2}, \tag{26}$$

$$EW_C(G) = \frac{1}{2 \times \mathrm{Gut}(G)}. \tag{27}$$

Using the three external weights listed above, the following irregularity indices of new type are obtained:

$$IRDE_A(G) = EW_A(G) \times IRD(G), \tag{28}$$

$$IRDE_B(G) = EW_B(G) \times IRD(G), \tag{29}$$

$$IRDE_C(G) = EW_C(G) \times IRD(G). \tag{30}$$

For graphs shown in Figure 1, the computed external weights and the corresponding irregularity indices are summarized in Table 3.

Comparing the computed irregularity indices mentioned in Table 3, one can conclude that the graph G_1 has the maximum irregularity indices $IRDE_A(G_1) = 10.8$ and $IRDE_B(G_1) = 795.6$, while the maximum value of the irregularity index $IRDE_C$ is attained by the graph G_2 where $IRDE_C(G_2) = 0.4211$ (it should be emphasized here that the graph G_1 is identical to the 6-vertex connected antiregular graph, and it is usually desired that the connected antiregular graph attains the maximum value of an irregularity index among all connected graphs of a fixed order.)

It is remarked here that the irregularity indices IRQ and $IRDE_C$ are identical to each other because

$$\begin{aligned} IRQ(G) &= \frac{DG(G)}{2\mathrm{Gut}(G)} - 1 = \frac{DG(G) - 2\mathrm{Gut}(G)}{2\mathrm{Gut}(G)} \\ &= EW_C(G) \times IRD(G) = IRDE_C(G). \end{aligned} \tag{31}$$

Table 3: Computed topological indices of the four graphs shown in Figure 1.

Graph	m	EW_A	$IRDE_A$	EW_B	$IRDE_B$	EW_C	$IRDE_C$
G_1	9	0.1350	10.800	9.944	795.6	0.0032	0.2597
G_2	7	0.0817	6.533	6.306	504.4	0.0053	0.4211
G_3	8	0.1067	8.533	8.139	651.1	0.0041	0.3252
G_4	8	0.1067	9.813	8.056	741.1	0.0042	0.3833

6. Additional Considerations

An interesting open problem can be formulated as follows: find a deterministic relationship between the following weighted bond-additive indices (see [24]).

$$BA_p(G) = \sum_{uv\in E(G)} \left|d_u - d_v\right|^p W(u,v) \tag{32}$$

and weighted atoms-pair-additive indices

$$IRR_p(G) = \frac{1}{2}\sum_{u,v\in V(G)} \left|d_u - d_v\right|^p W(u,v). \tag{33}$$

Depending on the definitions of the above irregularity indices, we observe that there exist graphs for which the mentioned relationship is perfect. As an example, when $p = 1$ and $W(u,v) = d(u,v)$ then for the wheel graph W_n of order n with $n \geq 5$, one has

$$\frac{1}{2}\sum_{u,v\in V(W_n)} \left|d_u - d_v\right| d(u,v) = \sum_{uv\in E(W_n)} \left|d_u - d_v\right| = AL(W_n), \tag{34}$$

where AL is the Albertson irregularity index [25].

The sigma index $\sigma(G)$ of a graph G is defined (for example, see [26]) as

$$\sum_{uv\in E(G)} (d_u - d_v)^2. \tag{35}$$

This irregularity index is a natural generalization of the Albertson irregularity index. For the wheel graph W_n of order n with $n \geq 5$, the following identity holds:

$$\begin{aligned} IRD(W_n) &= \frac{1}{2}\sum_{u,v\in V(W_n)} (d_u - d_v)^2 d(u,v) \\ &= \sum_{uv\in E(W_n)} (d_u - d_v)^2 = \sigma(W_n). \end{aligned} \tag{36}$$

It is possible to construct a particular graph family for which the concept outlined above can be extended. For two graphs J_1 and J_2 with disjoint vertex sets, $J_1 \cup J_2$ denotes the disjoint union of J_1 and J_2. The join $J_1 + J_2$ of J_1 and J_2 is the graph obtained from $J_1 \cup J_2$ by adding edges between every vertex of J_1 and every vertex of J_2.

Proposition 3. *Define the bidegreed graph H_n of order n as follows:*

$$H = H_0 + \left(\cup_{j\geq 1} H_j\right), \tag{37}$$

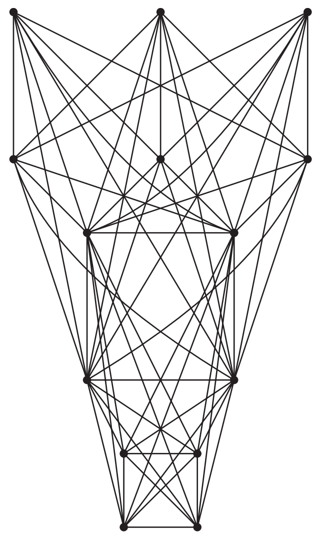

Figure 2: The bidegreed graph H_{14}.

where H_0 is an r-regular graph and each H_j is an r'-regular graph. It holds that

$$\begin{aligned} \mathrm{BAD}_p(H_n) &= \frac{1}{2} \sum_{u,v \in V(H_n)} \left|d_u - d_v\right|^p d(u,v) \\ &= \sum_{uv \in E(H_n)} \left|d_u - d_v\right|^p = AL_p(H_n), \end{aligned} \tag{38}$$

where AL_pG is a modified version of the generalized Albertson irregularity index (see [27]).

Proof. We note that

$$BAD_p(H_n) = \sum_{uv \in E(H_n)} \left|d_u - d_v\right|^p + \sum_{uv \notin E(H_n)} \left|d_u - d_v\right|^p d(u,v). \tag{39}$$

Observe that $d_x = d_y$ for every pair of nonadjacent vertices $x, y \in V(H_n)$, which implies that

$$\sum_{uv \notin E(H_n)} \left|d_u - d_v\right|^p d(u,v) = 0. \tag{40}$$

and hence Equation (39) yields the desired result.

As an example concerning Proposition 3, consider the bidegreed graph H_{14} of order 14 and size 59 constructed as follows:

$$H_{14} = C_4 + \left(K_{3,3} \cup K_4\right), \tag{41}$$

where C_4 is the (2-regular) cycle graph with 4 vertices, $K_{3,3}$ is the (3-regular) complete bipartite graph of order 6, and K_4 is the (3-regular) complete graph on 4 vertices (see Figure 2. The graph H_{14} contains ten vertices of degree 7 and four vertices of degree 12. Note that if $uv \notin E(H_{14})$, then $u \in V(J)$ and $v \in V(K)$, where $J, K \in \left\{K_{3,3}, K_4\right\}$, and both the vertices u, v have the degree 7 in H_{14}. Thus,

$$\sum_{uv \notin E(H_{14})} \left|d_u - d_v\right|^p d(u,v) = 0 \tag{42}$$

and the desired conclusion holds. □

Data Availability

The data about this study may be requested from the authors.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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