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TOPOLOGICAL INDICES AND IRREGULARITY MEASURES

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Abstract. It is shown that the classical vertex degree based topological indices (first and second Zagreb, Randić), as well as several their recently introduced variants, can all be viewed as measures of graph irregularity.

1. Introduction: Graph irregularity measures

Let G be a simple undirected graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. The degree of a vertex $u \in \mathbf{V}(G)$ is the number of edges incident with u, and is denoted by $d(u)$. The number of vertices and edges of the graph G will be denoted by n and m, respectively. The edge between the vertices u and v is denoted by uv. In order to avoid trivialities, it will be assumed that all graphs considered are connected.

A graph G is regular if all its vertices have the same degree. Otherwise it is irregular. Regular graphs possess countless remarkable mathematical properties and therefore play an outstanding role in graph theory. In many applications and problems it is of importance to know how much a given graph deviates from being regular, i.e., how great its irregularity is [**7**]. For this purpose, various quantitative measures of graph irregularity have been put forward. It seems that the oldest numerical measure of graph irregularity was proposed by Collatz and Sinogowitz [**8**] who defined it as

$$irr_{CS} = \lambda_1 - \frac{2m}{n}$$

where λ_1 is the largest eigenvalue of the adjacency matrix.

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A somewhat more straightforward measure of irregularity was put forward by Bell [**3**], who maintained that the variance of the vertex degrees

$$irr_B = \frac{1}{n} \sum_{u \in \mathbf{V}(G)} \left[d(u) - \frac{2m}{n} \right]^2 \tag{1.1}$$

serves for this purpose. Recall that $2m/n$ is the average vertex degree.

Albertson [**2**] defined the irregularity of G as

$$irr_A = \sum_{uv \in \mathbf{E}(G)} |d_G(u) - d_G(v)|$$

whereas two similar irregularity measures were recently introduced in [**1**] and [**14**] as

$$irr_T = irr_T(G) = \sum_{\{u,v\} \subseteq \mathbf{V}(G)} |d_G(u) - d_G(v)|$$

and

$$irr_\sigma = \sum_{uv \in E(G)} \big[d_G(u) - d_G(v) \big]^2 .$$

A few more measures of graph irregularity were proposed in [**12, 18, 20**].

Generalizing the above, we arrive at the following:

Definition 1.1. Any mapping that associates a real number $irr(G)$ to a graph G, satisfying the condition:

$$irr(G) = 0 \qquad \text{if and only if } G \text{ is regular}$$

$$irr(G) > 0 \qquad \text{otherwise}$$

is an irregularity measure. Denote by **IM** the set of all such irregularity measures.

It is worth noting that if $X \in \mathbf{IM}$ and $c > 0$, then $c\,X \in \mathbf{IM}$. If $X_1 \in \mathbf{IM}$ and $X_2 \in \mathbf{IM}$, then $X_1 + X_2 \in \mathbf{IM}$ and $X_1 \cdot X_2 \in \mathbf{IM}$.

2. Introduction: Vertex degree based topological indices

A great variety of graph invariants defined in terms of vertex degrees has been and is currently studied in the literature. One of the main reasons for this is that these invariants can be used in chemistry as structure descriptors [**9, 10, 21**]. Such chemically relevant invariants are usually referred to as *topological indices*. In this paper, we are concerned with vertex degree based (VDB) topological indices.

The oldest VDB topological indices are the *first and the second Zagreb indices*, defined as

$$M_1 = M_1(G) = \sum_{u \in \mathbf{V}(G)} d(u)^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{uv \in \mathbf{E}(G)} d(u)\, d(v) \,, \tag{2.1}$$

the Randić index, defined as

$$R = R(G) = \sum_{uv \in \mathbf{E}(G)} \frac{1}{\sqrt{d(u)\, d(v)}} \,, \tag{2.2}$$

and the zeroth–order Randić index

$$^0R = {}^0R(G) = \sum_{u\in\mathbf{V}(G)} \frac{1}{\sqrt{d(u)}}\,.$$

These all have been introduced in the 1970s, and may be considered as classical. Details of their mathematical properties and chemical applications can be found in the surveys [**5, 16, 17, 19**].

In [**4**] a topological index called *general Randić index* was introduced as

$$R_\alpha = R_\alpha(G) = \sum_{uv\in\mathbf{E}(G)} \Big[d(u)\,d(v)\Big]^\alpha\,, \tag{2.3}$$

where α is an arbitrary real number. Evidently, for $\alpha = -1/2$, R_α coindices with the ordinary Randić index.

In [**15**], the general zeroth–order Randić index was conceived as

$$^0R_\alpha = {}^0R_\alpha(G) = \sum_{u\in\mathbf{V}(G)} d(u)^\alpha\,. \tag{2.4}$$

Evidently, for $\alpha = -1/2$, $^0R_\alpha$ coindices with the ordinary zeroth–order Randić index.

For some specific values of α, the above defined general indices appear in the literature under different names. Thus, for $\alpha = 1$, R_α coincides with the second Zagreb index; for $\alpha = 1/2$, we have the reciprocal Randić index, denoted by RR. Also the index R_{-1}, is often encountered in the mathematical literature (see e.g., [**4, 6**]), and is usually referred to as the "Randić index R_{-1}".

For $\alpha = 2$, $^0R_\alpha$ reduces to the first Zagreb index, whereas for $\alpha = 3$ and $\alpha = -1$ to the forgotten topological index (denoted by F) and inverse degree (denoted by ID).

Some other recently proposed VDB topological indices are the hyper–Zagreb index

$$HM = HM(G) = \sum_{uv\in E(G)} \Big[d(u) + d(v)\Big]^2 \tag{2.5}$$

the sum–connectivity index

$$SCI = SCI(G) = \sum_{uv\in\mathbf{E}(G)} \frac{1}{\sqrt{d(u)+d(v)}}$$

the harmonic index

$$H = H(G) = \sum_{uv\in\mathbf{E}(G)} \frac{2}{d(u)+d(v)} \tag{2.6}$$

the geometric–arithmetic index

$$GA = GA(G) = \sum_{uv\in\mathbf{E}(G)} \frac{2\sqrt{d(u)\,d(v)}}{d(u)+d(v)} \tag{2.7}$$

and the atom–bond connectivity index

$$ABC = ABC(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)\, d(v)}}$$

to mention just a few; for more details see the survey [**13**].

In 2010, in a series of papers, Vukičević introduced the so-called Adriatic indices, providing a general method for constructing VDB graph invariants. Among 148 such indices, two were singled out because of the quality of their chemical applications. These were the "inverse sum indeg index" [**22**]

$$ISI = ISI(G) = \sum_{uv \in \mathbf{E}(G)} \frac{d(u)\, d(v)}{d(u) + d(v)}$$

and the "symmetric division deg index" [**23**]

$$SDD = SDD(G) = \sum_{uv \in \mathbf{E}(G)} \frac{1}{2} \left[\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)} \right] . \tag{2.8}$$

3. VDB topological indices measuring irregularity

Some VDB topological indices are in a direct and straightforward manner related to graph irregularity. First of all, it has been noticed long time ago that the Bell index and the first Zagreb index are closely related. Indeed, Eq. (1.1) can be re-written as

$$\begin{aligned} irr_B &= \frac{1}{n} \left[\sum_{u \in \mathbf{V}(G)} d(u)^2 - \frac{4m}{n} \sum_{u \in \mathbf{V}(G)} d(u) + n \left(\frac{2m}{n} \right)^2 \right] \\ &= \frac{1}{n} \left[M_1(G) - \frac{4m}{n} \cdot (2m) + \frac{4m^2}{n} \right] \end{aligned}$$

resulting in

$$M_1 = n\, irr_B + \frac{4m^2}{n}$$

implying that $M_1 - \frac{4m^2}{n} \in \mathbf{IM}$.

In view of the geometric–arithmetic inequality, the term $\frac{2\sqrt{d(u)\, d(v)}}{d(u)+d(v)}$ is equal to unity if $d(u) = d(v)$ and less than unity otherwise. Consequently, the right–hand side of Eq. (2.7) is equal to m if G is regular, and is less than m otherwise. Thus, $m - GA \in \mathbf{IM}$.

Using the simple relation

$$\big[d(u) + d(v)\big]^2 = \big[d(u) - d(v)\big]^2 + 4\, d(u)\, d(v)$$

and taking into account Eqs. (2.1) and (2.5), we immediately obtain

$$HM - 4\, M_2 = \sum_{uv \in \mathbf{E}(G)} \big[d(u) - d(v)\big]^2$$

from which we conclude that a certain linear combination of the second Zagreb and harmonic indices is a measure of graph irregularity, i.e., $HM - 4\,M_2 \in \mathbf{IM}$.

Starting with the identity

$$\frac{1}{2}\left[\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right] = 1 + \frac{1}{2}\,\frac{\big[d(u) - d(v)\big]^2}{d(u)\,d(v)}\,,$$

from Eq. (2.8) we get

$$SDD = m + \frac{1}{2}\sum_{uv\in\mathbf{E}(G)} \frac{\big[d(u) - d(v)\big]^2}{d(u)\,d(v)}\,.$$

By Definition 1.1, the right–hand summation in the above equality is an irregularity measure. Therefore $SDD - m \in \mathbf{IM}$.

Starting with the identity

$$\frac{1}{\sqrt{d(u)\,d(v)}} - \frac{2}{d(u)+d(v)} = \frac{\big[d(u) - d(v)\big]^2}{\big[d(u)+d(v)\big]\sqrt{d(u)\,d(v)}}\,,$$

from Eqs. (2.2) and (2.6) we get

$$R - H = \sum_{uv\in\mathbf{E}(G)} \frac{\big[d(u) - d(v)\big]^2}{\big[d(u)+d(v)\big]\sqrt{d(u)\,d(v)}}$$

which means that the difference of the Randić and harmonic indices is an irregularity measure, i.e., $R - H \in \mathbf{IM}$.

4. An elementary relation and its special cases

In what follows, we shall use the identity [**11**]

$$\sum_{uv\in\mathbf{E}(G)} \big[\Psi(u) + \Psi(v)\big] = \sum_{u\in\mathbf{V}(G)} d(u)\,\Psi(u) \tag{4.1}$$

valid for any function Ψ and any graph G, provided that $\Psi(u)$ is defined for all $u \in \mathbf{V}(G)$.

It is evident from Definition 1.1 that the expression

$$\Xi(\alpha) := \sum_{uv\in\mathbf{E}(G)} [d(u)^\alpha - d(v)^\alpha]^2$$

is an irregularity measure for any $\alpha \neq 0$, i.e., that $\Xi(\alpha) \in \mathbf{IM}$, $\alpha \neq 0$. Bearing in mind Eqs. (2.3), (2.4), and (4.1), we immediately obtain

$$\Xi(\alpha) = {}^0R_{2\alpha+1}(G) - 2\,R_\alpha(G)$$

implying

$${}^0R_{2\alpha+1}(G) - 2\,R_\alpha(G) \in \mathbf{IM}\,. \tag{4.2}$$

The following special cases of the relation (4.2) deserve to be separately stated:

$\alpha = 1$: A linear combination of the second Zagreb index and the forgotten topological index is an irregularity measure, namely

$$F - 2\,M_2 \in \mathbf{IM}\,.$$

$\alpha = 1/2$: A linear combination of the first Zagreb index and and the reciprocal Randić index is an irregularity measure, namely

$$M_1 - 2\,RR \in \mathbf{IM}\,.$$

$\alpha = -1/2$: The Randić index itself is directly related to an irregularity measure, via

$$R(G) = \frac{n}{2} - \frac{1}{2} \sum_{uv \in \mathbf{E}(G)} \left[\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \right]^2 \tag{4.3}$$

i.e., it satisfies

$$n - 2R \in \mathbf{IM}\,.$$

Note that (4.3) is an earlier known identity [**16**].

$\alpha = -1$: A linear combination of the Randić index R_{-1} and the inverse degree is an irregularity measure, namely

$$ID - 2\,R_{-1} \in \mathbf{IM}\,.$$

$\alpha = -3/4$: A linear combination of the zeroth–order Randić index and a particular general Randić index is an irregularity measure, namely

$${}^0R - 2\,R_{-3/4} \in \mathbf{IM}\,.$$

5. Concluding remarks

In this paper we showed that numerous and the most important VDB topological indices and/or their linear combinations are measures of graph irregularity. In spite of the extensive research in this field, this fact seems to be overlooked until now.

One may ask if there exist VDB topological indices which are not related to graph irregularity. The answer is affirmative. As far as the present author could see, among those mentioned in Section 2, such are the sum–connectivity (SCI), atom–bond–connectivity (ABC), and inverse sum indeg (ISI) indices.

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