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On the variance-type graph irregularity measures

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Abstract: Bell's degree-variance Var_B for a graph G, with the degree sequence $(d_1, d_2, \ldots, d_n)$ and size m, is defined as $Var_B(G) = \frac{1}{n}\sum_{i=1}^{n}\left[d_i - \frac{2m}{n}\right]^2$. In this paper, a new version of the irregularity measures of variance-type, denoted by Var_q, is introduced and discussed. Based on a comparative study, it is demonstrated that the newly proposed irregularity measure Var_q possess a better discrimination ability than the classical Bell's degree-variance in several cases.

Keywords: non-regular graphs, irregularity measures, degree variance

AMS Subject classification: 05C07, 05C09, 05C75

1. Introduction

In this paper, we consider only simple, connected and non-trivial graphs. For a graph G, denote by $V(G)$ and $E(G)$ the sets of vertices and edges, respectively. Let $d_{u_i}(G)$ (or simply $d_i(G)$, when there is no confusion) be the degree of vertex u_i, and denote by uv an edge of G connecting vertices u and v. The minimum degree and maximum degree of a graph G are denoted by $\delta(G)$ and $\Delta(G)$, respectively. The distance $d_G(u, v)$ between two vertices $u, v \in V(G)$ is the number of edges in a shortest $u - v$ path in a graph G. We drop the symbol "G" from the notations involving it whenever the graph under consideration is clear – for example, we will write d_i, δ and $d(u, v)$ instead of $d_i(G)$, $\delta(G)$ and $d_G(u, v)$ for simplicity.

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We use the standard terminology of graph theory, for notations not defined here, we refer the reader to [5, 19]. The eccentricity $ec(u)$ of a vertex $u \in V(G)$ is the greatest distance among all the distances from u to other vertices of G. The diameter $Diam(G)$ (respectively, radius $Rad(G)$) of a graph G is the maximum (respectively, minimum) value among the eccentricities of all the vertices of G. Let $A(G)$ (or simply A, when there is no confusion) be the adjacency matrix of a graph G. We denote by $\lambda_1(G)$ the largest eigenvalue of $A(G)$ and call it the spectral radius of G.

The set consisting of (different) degrees of all the vertices of a graph G is called the degree set of G. By a regular (respectively, bidegreed) graph, we mean a graph whose degree set consists of only one element (respectively, two elements), and by a non-regular graph we mean a graph that is not regular. By a semiregular graph, we mean a bipartite bidegreed graph in which every partite set consists of the vertices of the same degree.

The dual degree of a vertex $u \in V(G)$ is the average value of the degrees of its neighbors [16]. A graph G in which all the vertices have the same dual degree, say $p(G)$, is called a pseudo-regular graph or harmonic graph [8, 14, 32]. It is easy to check that $p(G)$ is always a positive integer and that $\lambda_1(G) = p(G)$. It is obvious that any r-regular graph G_r is also a harmonic graph with $p(G_r) = \lambda_1(G_r) = r$.

An irregularity measure (IM) of a (connected) graph G is a non-negative graph invariant satisfying the property: $IM(G) = 0$ if and only if G is regular. In literature, various irregularity measures have been proposed [12] and applied [15, 22, 33, 35, 36] till date. The majority of irregularity measures belong to the family of degree-based graph invariants [1, 2, 6, 7, 13, 18, 20, 24, 27, 29, 30, 34, 40], but there exist eigenvalue-based irregularity measures as well [11, 34]. Bell's degree-variance Var_B is one of the most popular degree-based irregularity measures. This irregularity measure for a graph G, with the degree sequence $(d_1, d_2, \ldots, d_n)$ and size m, is defined [4] as

$$Var_B(G) = \frac{1}{n}\sum_{i=1}^{n}\left[d_i - \frac{2m}{n}\right]^2.$$

We remark here that, before the appearance of the Bell's paper [4], the measure Var_B was appeared within the study of graph heterogeneity [37] (see the next section for details). The properties and applications of Var_B have been extensively studied and discussed in several papers [4, 9, 12, 23, 36, 37].

While the irregularity measure Var_B has several advantages, it also has some disadvantages. One of the drawbacks of Var_B is that its discriminatory performance is limited in certain cases. In order to overcome this drawback, several attempts have recently been made to devise some modified versions of Var_B. This research direction is focused primarily on the construction of novel graph invariants of variance type, having a higher structural selectivity and an improved discriminating sensitivity. In this paper, a new version of Var_B, denoted by Var_q and referred as the normalized degree-variance, is introduced and discussed. Based on a comparative study, it is demonstrated that the newly proposed irregularity measure Var_q possess a better discrimination ability than the classical Bell's degree-variance in several cases.

2. Preliminary Considerations

We have mentioned in the previous section that the measure Var_B was also appeared within the study of graph heterogeneity [37], before the appearance of the Bell's paper [4]. Moreover, the degree variance is mentioned by Coleman [10] as an intermediate step in the construction of a measure of hierarchization (in a sociometric context, graph heterogeneity can be interpreted as hierarchization), see [37]. Snijders [37] also proposed the following general variance for a graph G

$$Var_g(G) = \frac{1}{n}\sum_{i=1}^{n}\left[g(u_i) - \mu(G)\right]^2, \tag{1}$$

where $V(G) = \{u_1, u_2, \cdots, u_n\}$, g is a convex non-decreasing (and non-negative real) function, and

$$\mu(G) = \frac{1}{n}\sum_{i=1}^{n} g(u_i). \tag{2}$$

The function g can be taken in various ways: for example, $g(u_i) = \log(d(u_i))$ gives entropy-based measure of hierarchization [10] or $g(u_i) = d(u_i)$ gives the traditional degree-variance Var_B suggested by Bell [4] for characterizing the irregularity of a graph, or we can take $g(u_i) = ec(u_i)$, where $ec(u_i)$ is the eccentricity of a vertex $u_i \in V(G)$.

The Bell's degree-variance Var_B belongs to the family of those graph invariants that can be determined unambiguously by the degree sequence of the considered graph. In fact, in addition to Var_B, there are many irregularity measures that can be determined by the degree sequence of a graph. Some of them, which will be used in forthcoming sections, are listed below [12, 13, 20, 33, 34].

$$IRV_1(G) = nVar_B(G) = M_1(G) - \frac{4m^2}{n},$$

$$IRV_2(G) = n^2Var_B(G) = nM_1(G) - 4m^2,$$

$$IRV_3(G) = \sqrt{\frac{M_1(G)}{n}} - \frac{2m}{n} = Var_B(G)\left(\sqrt{\frac{M_1(G)}{n}} + \frac{2m}{n}\right)^{-1},$$

$$IRM_A(G) = \frac{IRV_1(G)}{2m} = \frac{M_1(G)}{2m} - \frac{2m}{n},$$

$$IRM_B(G) = F(G) - \frac{2m}{n}M_1(G),$$

$$irr_t(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}|d_i - d_j| = \sum_{i=1}^{n}\sum_{j=i+1}^{n}|d_i - d_j|,$$

where $irr_t(G)$ is the total irregularity of G introduced by Abdo *et al.* [13], $M_1(G)$ is the first Zagreb index of a graph G defined [21, 25, 28, 38, 39] as

$$M_1(G) = \sum_{i=1}^{n} d_i^2$$

and $F(G)$ is the so-called forgotten topological index [17] formulated as $F(G) = \sum_{i=1}^{n} d_i^3$. It needs to be emphasized that a common property of each of the irregularity measures listed above is that if graphs G_a and G_b have the same degree sequence, then the values of the considered irregularity measure of G_a and G_b will also be the same.

3. The Normalized Degree-Variance Irregularity Measures

In what follows, we introduce a novel variance-type irregularity measure. For a graph G with the degree sequence $(d_1, d_2, \ldots, d_n)$ and the size m, consider the graph invariants formulated as

$$D_{1,q}(G) = \sum_{i=1}^{n} p_i d_i^q = (2m)^q \sum_{i=1}^{n} p_i^{(1+q)},$$

$$D_{2,q}(G) = \sum_{i=1}^{n} p_i d_i^{2q} = (2m)^{2q} \sum_{i=1}^{n} p_i^{(1+2q)},$$

where q is a positive number and p_i is the normalized degree of a vertex u_i of the graph G, defined as

$$p_i = \frac{d_i}{\sum_{i=1}^{n} d_i} = \frac{d_i}{2m}.$$

Based on the above formulas, we define the following variant of the Bell's degree variance

$$Var_q(G) = D_{2,q}(G) - D_{1,q}^2(G) = (2m)^{2q}\left\{\sum_{i=1}^{n} p_i^{(1+2q)} - \left(\sum_{i=1}^{n} p_i^{(1+q)}\right)^2\right\}. \quad (3)$$

In what follows, we prove that Var_q is an irregularity measure. For this, we need to prove the following elementary lemma first.

Lemma 1. *Let $B_1, B_2, \cdots, B_n$ are non-negative numbers. If $w_1, w_2, \cdots, w_n$ are the non-negative numbers satisfying $w_1 + w_2 + \cdots + w_n = 1$, then it holds that*

$$\left\{\sum_{i=1}^{n} w_i B_i\right\}^2 \le \sum_{i=1}^{n} w_i B_i^2$$

with equality if and only if $B_1 = B_2 = \cdots = B_n$.

Proof. Using the Cauchy-Schwartz inequality, one gets that

$$\left\{\sum_{i=1}^{n}\sqrt{w_i}(B_i\sqrt{w_i})\right\}^2 \leq \left\{\sum_{i=1}^{n} w_i\right\}\left\{\sum_{i=1}^{n} w_i B_i^2\right\} = \sum_{i=1}^{n} w_i B_i^2.$$

□

Now, we are able to prove that the graph invariant Var_q satisfies both the properties of an irregularity measure.

Proposition 1. *If G is a connected graph with the degree sequence $(d_1, d_2, \ldots, d_n)$ and the size m, then it holds that*

$$Var_q(G) = (2m)^{2q}\left\{\sum_{i=1}^{n} p_i^{(1+2q)} - \left(\sum_{i=1}^{n} p_i^{(1+q)}\right)^2\right\} \geq 0$$

with equality if and only if G is a regular graph.

Proof. It suffices to show that

$$\left(\sum_{i=1}^{n} p_i^{(1+q)}\right)^2 \leq \sum_{i=1}^{n} p_i^{(1+2q)}.$$

Taking $w_i = p_i$ and $B_i = (p_i)^q$ for $i = 1, 2, \cdots, n$, we have

$$\left(\sum_{i=1}^{n} w_i B_i\right)^2 = \left(\sum_{i=1}^{n} p_i^{(1+q)}\right)^2$$

and

$$\sum_{i=1}^{n} w_i B_i^2 = \sum_{i=1}^{n} p_i^{(1+2q)}.$$

Thus, by using Lemma 1, we have

$$\sum_{i=1}^{n} w_i B_i^2 - \left(\sum_{i=1}^{n} w_i B_i\right)^2 = \sum_{i=1}^{n} p_i^{(1+2q)} - \left(\sum_{i=1}^{n} p_i^{(1+q)}\right)^2 \geq 0,$$

where the equality sign in the last inequality holds if and only if $(p_1)^q = (p_2)^q = \cdots = (p_n)^q$, which is true if and only if G is a regular graph. □

From Proposition 1, it follows that the graph invariant Var_q is actually an irregularity measure. We note that the irregularity measure Var_q can be rewritten as

$$Var_q(G) = D_{2,q}(G) - D_{1,q}^2(G) = \frac{1}{2m}\sum_{i=1}^{n} d_i^{(1+2q)} - \left(\frac{1}{2m}\sum_{i=1}^{n} d_i^{(1+q)}\right)^2. \quad (4)$$

The substitutions $q = 1/2$ and $q = 1$ in Equation (4) yield

$$Var_{\frac{1}{2}}(G) = \frac{1}{2m}\sum_{i=1}^{n} d_i^2 - \left(\frac{1}{2m}\sum_{i=1}^{n} d_i^{3/2}\right)^2 = \frac{1}{2m}M_1(G) - \left(\frac{1}{2m}\sum_{i=1}^{n} d_i^{3/2}\right)^2$$

and

$$Var_1(G) = D_{2,1}(G) - D_{1,1}^2(G) = \frac{F(G)}{2m} - \left(\frac{M_1(G)}{2m}\right)^2,$$

respectively. In what follows, we focus our attention to the irregularity measure Var_1. We propose to call this irregularity measure as the *normalized degree variance*.

Proposition 2. *The irregularity measures Var_B and Var_1 are incomparable.*

Proof. For the 4-vertex path P_4, one has

$$Var_B(P_4) = \frac{M_1(P_4)}{n} - \left(\frac{2m}{n}\right)^2 = \frac{10}{4} - \left(\frac{6}{4}\right)^2 = \frac{40-36}{16} = \frac{1}{4},$$

and hence

$$Var_1(P_4) = \frac{2mF(P_4) - M_1^2(P_4)}{4m^2} = \frac{6 * 18 - 10^2}{36} = \frac{2}{9} < \frac{1}{4} = Var_B(P_4).$$

On the other hand, for the 4-vertex star graph S_4 it holds that

$$Var_B(S_4) = \frac{M_1(S_4)}{n} - \left(\frac{2m}{n}\right)^2 = \frac{12}{4} - \left(\frac{6}{4}\right)^2 = \frac{48-36}{16} = \frac{3}{4}.$$

Hence

$$Var_1(S_4) = \frac{2mF(S_4) - M_1^2(S_4)}{4m^2} = \frac{6 \times 30 - 12^2}{36} = 1 > \frac{3}{4} = Var_B(S_4).$$

□

Finally, we show that for harmonic graphs there exists a strong correspondence between the sigma index $\sigma(G) = \sum_{uv \in E(G)} (d(u) - d(v))^2$, introduced in [24], and the normalized degree-variance $\mathrm{Var}_1(G)$. For this purpose, we need the following lemma.

Lemma 2. [14, 32] *If G is a harmonic graph with m edges and with the spectral radius $\lambda_1(G)$ then*

$$\lambda_1(G) = \frac{M_1(G)}{2m} = \frac{2M_2(G)}{M_1(G)},$$

where $M_2(G)$ is the second Zagreb index [25, 28] of G.

Proposition 3. *If G is a harmonic graph with m edges then*

$$Var_1(G) = \frac{1}{2m}\left(F(G) - 2M_2(G)\right) = \frac{1}{2m}\sigma(G).$$

Proof. The normalized degree-variance can be rewritten as

$$Var_1(G) = \frac{M_1(G)}{2m}\left(\frac{F(G)}{M_1(G)} - \frac{M_1(G)}{2m}\right).$$

By using Lemma 2, we get

$$Var_1(G) = \frac{M_1(G)}{2m}\left(\frac{F(G)}{M_1(G)} - \frac{2M_2(G)}{M_1(G)}\right) = \frac{1}{2m}\left(F(G) - 2M_2(G)\right).$$

□

4. Discriminatory Performance of the Normalized Degree -Variance

The discriminatory performance of the Bell's degree-variance Var_B and the normalized degree-variance Var_1 are compared and evaluated in the following examples.

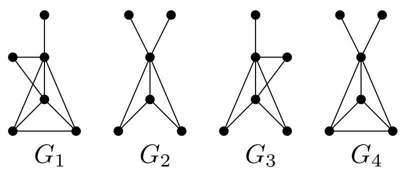

Figure 1. **Four 6-vertex non-regular graphs with the same total irregularity.**

Example 1. Consider the 6-vertex connected non-regular graphs depicted in Figure 1. It can be easily checked that all these graphs have the same value of the total irregularity, which is 26. Comparing the irregularity measures Var_B and Var_1 of the graphs shown in Figure 1, the following results are obtained.
It is easy to check that $\mathrm{Var}_B(G_1) \approx 1.667$, while the other graphs have the identical Bell's degree-variance: $Var_B(G_2) = Var_B(G_3) = Var_B(G_4) \approx 1.889$. On the other hand, for the normalized degree-variance Var_1, we get: $Var_1(G_1) \approx 1.3580$, $Var_1(G_2) \approx 2.2653$, $Var_1(G_3) \approx 1.9844$ and $Var_1(G_4) \approx 1.6094$. Thus, it can be stated that the irregularity measure Var_1 is more discriminative (more selective) than the Bell's degree variance for the considered graphs.

An n-vertex graph whose degree set consists of exactly $n-2$ elements is called an antiregular graph [3, 26, 31]. Following the references [2, 6, 7, 13], we take antiregular graphs as the graphs opposite to the regular graphs. It is interesting to note in Example 1 that the minimum values of both the measures Var_B and Var_1 are attained by the antiregular graph G_1. Thus, both of these irregularity measures may be useful in designing some irregularity measure(s) satisfying the constraints mentioned in the open problem given in [31].

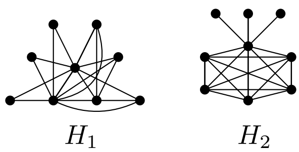

Figure 2. **Two 9-vertex non-regular graphs with 18 edges.**

Example 2. Consider the non-regular graphs H_1 and H_2 depicted in Figure 2. The degree sequences of the graphs H_1 and H_2 are $(8,8,5,3,3,3,2,2,2)$ and $(8,5,5,5,5,5,1,1,1)$, respectively. These graphs have identical first Zagreb index, $M_1(H_1) = M_1(H_2) = 192$, and different forgotten topological index, that is $F(H_1) = 1254$ and $F(H_2) = 1140$. Consequently, although the Bell's degree variance of these graphs are identical, $\mathrm{Var}_B(H_1) = Var_B(H_2) \approx 5.333$, the normalized degree variance of the graphs H_1 and H_2 are strongly different: $\mathrm{Var}_1(H_1) \approx 6.389$ and $\mathrm{Var}_1(H_2) \approx 3.222$. Comparing the discriminatory ability of the irregularity measures Var_B and Var_1, we can conclude that the normalized degree variance Var_1 possesses a better discriminatory performance for the considered graphs.

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