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Computational and Analytical Studies of the Harmonic Index on Erdös–Rényi Models

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Abstract

A main topic in the study of topological indices is to find bounds of the indices involving several parameters and/or other indices. In this paper we perform statistical (numerical) and analytical studies of the harmonic index $H(G)$, and other topological indices of interest, on Erdős-Rényi (ER) graphs $G(n,p)$ characterized by n vertices connected independently with probability $p \in (0,1)$. Particularly, in addition to $H(G)$, we study here the (-2) sum-connectivity index $\chi_{-2}(G)$, the modified Zagreb index $MZ(G)$, the inverse degree index $ID(G)$ and the Randić index $R(G)$. First, to perform the statistical study of these indices, we define the averages of the normalized indices to their maximum value: $\langle \overline{H}(G) \rangle$, $\langle \overline{\chi}_{-2}(G) \rangle$, $\langle \overline{MZ}(G) \rangle$, $\langle \overline{ID}(G) \rangle$ and $\langle \overline{R}(G) \rangle$. Then, from a detailed scaling analysis, we show that the averages of the normalized indices scale with the product $\xi \approx np$. Moreover, we find two different behaviors. On the one hand, $\langle H(G) \rangle$ and $\langle R(G) \rangle$, as a function

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of the probability p, show a smooth transition from zero to $n/2$ as p increases from zero to one. Indeed, after scaling, it is possible to define three regimes: a regime of mostly isolated vertices when $\xi < 0.01$ ($H(G), R(G) \approx 0$), a transition regime for $0.01 < \xi < 10$ (where $0 < H(G), R(G) < n/2$), and a regime of almost complete graphs for $\xi > 10$ ($H(G), R(G) \approx n/2$). On the other hand, $\langle \chi_{-2}(G) \rangle$, $\langle MZ(G) \rangle$ and $\langle ID(G) \rangle$ increase with p until approaching their maximum value, then they decrease by further increasing p. Thus, after scaling the curves corresponding to these indices display bell-like shapes in log scale, which are symmetric around $\xi \approx 1$; i.e. the percolation transition point of ER graphs. Therefore, motivated by the scaling analysis, we analytically (i) obtain new relations connecting the topological indices H, χ_{-2}, MZ, ID and R that characterize graphs which are extremal with respect to the obtained relations and (ii) apply these results in order to obtain inequalities on H, χ_{-2}, MZ, ID and R for graphs in ER models.

1 Introduction

A single number which represents a chemical structure in graph-theoretical terms via the molecular graph is called a *topological descriptor*; besides, if it correlates with a molecular property, it is called *topological index* and it is used to understand physicochemical properties of chemical compounds. The interest in topological indices lies in the fact that they synthesize some of the properties of a molecule into a single number. With this in mind, hundreds of topological indices have been introduced and studied so far; it is worth noting the seminal work by Wiener [27] in which he used the sum of all shortest-path distances of a (molecular) graph in order to model physical properties of alkanes.

Topological indices based on end-vertex degrees of edges have been used for more than 40 years and some of them are recognized tools in chemical research. Probably, the best known among such descriptors are the Randić connectivity index and the Zagreb indices.

The *Randić connectivity index* was defined in [2] as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} ,$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u. There are more than a thousand papers and a couple of books dealing with this index (see, e.g., [3–5] and the references therein).

Also, there is a vast amount of research into the Zagreb indices. For details of their chemical applications and mathematical theory see [6–8] and the references therein. In [9–11], the *variable first and second Zagreb indices* are defined as

$$M_1^\alpha(G) = \sum_{u \in V(G)} d_u^\alpha, \qquad M_2^\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,$$

with $\alpha \in \mathbb{R}$.

Note that M_1^2 is the first Zagreb index M_1, M_1^{-1} is the *inverse degree index*

$$ID(G) = \sum_{u \in V(G)} \frac{1}{d_u} = \sum_{uv \in E(G)} \left(\frac{1}{d_u^2} + \frac{1}{d_v^2}\right),$$

M_1^3 is the forgotten index, etc. Also, $M_2^{-1/2}$ is the usual Randić index R and M_2^1 is the second Zagreb index M_2.

The concept of *variable molecular descriptors* was proposed as a new way of characterizing heteroatoms in molecules (see [12, 13]), but also to assess structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes [14]). The idea behind the variable molecular descriptors is that the variables are determined during the regression; this allows to make the standard error of the estimate for a particular property (targeted in the study) as small as possible (see, e.g., [11]).

Gutman and Tošović [15] tested the correlation abilities of 20 vertex-degree-based topological indices used in the chemical literature for the case of standard heats of formation and normal boiling points of octane isomers. It is noteworthy that the variable second Zagreb index M_2^α with exponent $\alpha = -1$ (and to a lesser extent with exponent $\alpha = -2$) performs significantly better than the Randić index ($R = M_2^{-1/2}$). M_2^{-1} is also known as the *modified Zagreb* index:

$$MZ(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v} .$$

The modified Zagreb index has been used in the structure-boiling point modeling of benzenoid hydrocarbons [16]. Also, variable Zagreb indices exhibit a potential applicability for deriving multi-linear regression models [17]. Various properties and relations of these indices are discussed in several papers (see, e.g., [10, 18, 19]).

Other related indices have attracted great interest in the last years. Among them we can mention the *harmonic index*, defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

in [20] (see examples of recent studies in [21–25]), and the *general sum-connectivity index*, defined by Zhou and Trinajstić in [26] as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha .$$

Note that χ_1 is the first Zagreb index M_1, $2\chi_{-1}$ is the harmonic index H, $\chi_{-1/2}$ is the sum-connectivity index χ, etc. Some relations of these indices are reported in [22].

A topic of current interest in the study of topological indices is to find bounds of the indices involving relevant parameters and/or other indices. In this paper we perform statistical and analytical studies of the harmonic index $H(G)$, the (-2) sum-connectivity index $\chi_{-2}(G)$, the modified Zagreb index $MZ(G)$, the inverse degree index $ID(G)$ and the Randić index $R(G)$ on Erdős-Rényi graphs.

We want to stress that the statistical study of topological indices we perform here is justified by the random nature of the Erdős-Rényi graphs $G(n,p)$ we are interested in; i.e. random graphs characterized by n vertices connected independently with probability $p \in (0,1)$. Since a given parameter pair (n,p) represents an infinite-size ensemble of random graphs, the computation of a topological index on a single graph is irrelevant. In contrast, the computation of a given topological index on a large ensemble of random graphs, all characterized by the same parameter pair (n,p), may provide useful *average* information about the full ensemble. This *statistical* approach, well known in random matrix theory studies, is not widespread in studies of topological indices, mainly because topological indices are not commonly applied to random graphs; for an exception see [28]. However, we believe that topological indices may well serve as complimentary tools, in addition to the well known random matrix theory spectral indicators, in the study and characterization of random matrix models.

This paper is organized as follows. In Sec. 2 we perform a detailed scaling analysis of the average of the indices $H(G)$, $\chi_{-2}(G)$, $MZ(G)$, $ID(G)$ and $R(G)$ on Erdős-Rényi graphs. The scaling analysis allows us to define a *universal* parameter able to predict the average values of indices under study. However, since other relevant quantities (like the variance and minimal and maximal values of the indices) are not fixed by the universal scaling parameter, in Sec. 3 we analytically (i) obtain new relations connecting the topological indices and characterize graphs which are extremal with respect to the relations obtained and (ii) apply our results in order to obtain inequalities of the topological indices on graphs in Erdős-Rényi models.

2 Scaling analysis of vertex-degree-based topological indices on Erdős-Rényi graphs

In this Section we perform a statistical study of the harmonic index $H(G)$, the (-2) sum-connectivity index $\chi_{-2}(G)$, the modified Zagreb index $MZ(G)$ and the inverse degree index $ID(G)$. For completeness we include results for the Randić index $R(G)$, some of them already reported in [28]. We recall that we consider random graphs G from the standard Erdős-Rényi model $G(n,p)$.

In Fig. 1(a) we show the average harmonic index $\langle H(G)\rangle$ as a function of the probability p on Erdős-Rényi graphs $G(n,p)$ of several sizes n. Here and in all the following calculations, the averages $\langle\cdot\rangle$ are computed over 10^6 random graphs $G(n,p)$. We observe that the curves of $\langle H(G)\rangle$, for all the values of n considered here, have a very similar functional form as a function of p: $\langle H(G)\rangle$ shows a smooth transition (in log scale) from zero to $n/2$ when p increases from zero (isolated vertices) to one (complete graphs). Note that $n/2$ is the maximal value that $H(G)$ can take.

Similarly, in Fig. 1(b) we present the average (-2) sum-connectivity index $\langle\chi_{-2}(G)\rangle$. Note that (in contrast to the curves of $\langle H(G)\rangle$ vs. p which are monotonically increasing), for small p, $\langle\chi_{-2}(G)\rangle$ increases with p until approaching its maximum value, then $\langle\chi_{-2}(G)\rangle$ decreases from that maximum by further increasing p, giving to the curves $\langle\chi_{-2}(G)\rangle$ vs. p a bell-like shape in log scale. A similar behavior can be observed for $\langle MZ(G)\rangle$ and $\langle ID(G)\rangle$; see Figs. 1(c) and 1(d), respectively. In the case of the harmonic index, the maximum value is well known and corresponds to $n/2$. While for the average (-2) sum-connectivity, modified Zagreb and inverse degree indices we have obtained the maximum average values numerically ($\max[\langle\chi_{-2}(G)\rangle]$, $\max[\langle MZ(G)\rangle]$ and $\max[\langle ID(G)\rangle]$, respectively); they are plotted in the insets of Figs. 1(b-d) as a function of n. The linear trend of the data $\max[\langle\cdot\rangle]$ vs. n allows us to propose the equation

$$\max[\langle\cdot\rangle] = \alpha n + \beta, \tag{1}$$

which, indeed, describes very well the numerical data; see the black lines in the insets of Figs. 1(b-d). The values of the parameters obtained from the fittings of Eq. (1) to the data in Figs. 1(b-d) are reported in Table 1.

For completeness, in Fig. 1(e) we report $\langle R(G)\rangle$ vs. p; see also [28]. In fact, we observe that the behavior of $\langle R(G)\rangle$ is very similar to that of $\langle H(G)\rangle$; compare Figs. 1(a) and 1(e).

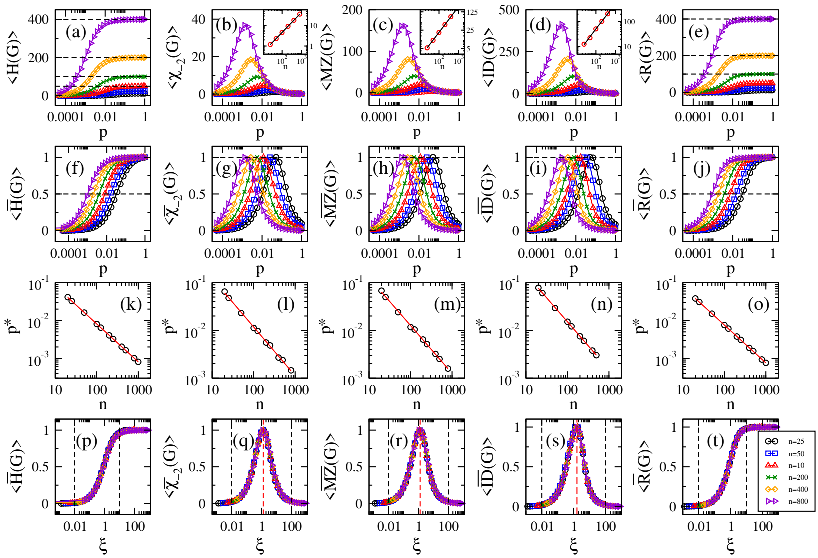

Figure 1. Average (a) harmonic index $\langle H(G)\rangle$, (b) (-2) sum-connectivity index $\langle \chi_{-2}(G)\rangle$, (c) modified Zagreb index $\langle MZ(G)\rangle$, (d) inverse degree index $\langle ID(G)\rangle$ and (e) Randić index $\langle R(G)\rangle$ as a function of the probability p of Erdős-Rényi graphs $G(n,p)$ of different sizes $n \in [25, 800]$. Dashed lines in (a) and (e) indicate $n/2$ for $n \in [200, 800]$. Insets in (b-d) are $\max[\langle \cdot \rangle]$ vs. n; black lines are fittings of Eq. (1) to the data with fitting parameters given in Table 1. (f-j) Average indices normalized to their maximum values $\langle \overline{\cdot} \rangle = \langle \cdot \rangle / \max[\langle \cdot \rangle]$ as a function of p. The dashed lines in (f,j) [(g-i)] indicate $\langle \overline{\cdot} \rangle = 0.5$ [$\langle \overline{\cdot} \rangle = 1$]; i.e. the values of $\langle \overline{\cdot} \rangle$ used to define p^*. (k-o) p^* as a function of the graph size n. The black lines are fittings of Eq. (2) to the data with fitting parameters given in Table 2. (p-t) $\langle \overline{\cdot} \rangle$ as a function of $\xi = np$, seeEq. (3). Each symbol was computed by averaging over 10^6 random graphs $G(n,p)$.

Also, $\max[\langle R(G)\rangle] = n/2$.

Now, to ease our statistical analysis, in Figs. 1(f-j) we present again $\langle H(G)\rangle$, $\langle \chi_{-2}(G)\rangle$, $\langle MZ(G)\rangle$, $\langle ID(G)\rangle$ and $\langle R(G)\rangle$, respectively, but now normalized to their maximum values: $\langle \overline{\cdot} \rangle = \langle \cdot \rangle / \max[\langle \cdot \rangle]$, From these figures we can clearly see that the main effect of increasing n is the displacement of the curves $\langle \overline{\cdot} \rangle$ vs. p to the left on the p-axis. Moreover, the fact that these curves, plotted in semi-log scale, are shifted the same amount on the p-axis when doubling n makes us anticipate the existence of a scaling parameter that depends on n. In order to look for that scaling parameter we first define a quantity to characterize the position of the curves on the p-axis: For the harmonic and Randić indices,

Table 1. Values of α and β obtained from the fittings of Eq. (1) to the data $\max[\langle \cdot \rangle]$ vs. n of the insets of Figs. 1(b-d).

Index	α	β
(-2) sum-connectivity $\chi_{-2}(G)$	0.0459	0.0337
modified Zagreb $MZ(G)$	0.2001	0.2595
inverse degree $ID(G)$	0.5197	-1.1175

we choose the value of p, that we label as p^*, for which $\langle \overline{\cdot} \rangle \approx 0.5$; see the dashed lines in Figs. 1(f,j). Notice that p^* characterizes the transition from isolated vertices to complete Erdős-Rényi graphs of size n. For the other indices (χ_{-2}, MZ, and ID), we define p^* as the value of p for which $\langle \overline{\cdot} \rangle \approx 1$.

Then, in Figs. 1(k-o) we present p^* as a function of n for all indices. The linear trend of the data (in log-log scale) implies a power-law relation of the form

$$p^* = \mathcal{C} n^{\delta}. \tag{2}$$

In fact, Eq. (2) provides excellent fittings to the data, as shown in Figs. 1(k-o); the values of the fitting parameters are reported in Table 2. Note that in all cases $\delta \approx -1$. Then we define the scaling parameter ξ as:

$$\xi \equiv \frac{p}{p^*} \propto \frac{p}{n^{\delta}} \approx \frac{p}{n^{-1}} = np \, . \tag{3}$$

Table 2. Values of $\mathcal{C}$ and δ obtained from the fittings of the curves p^* vs. n of Fig. 1 (i-l) with Eq. (2)

Index	$\mathcal{C}$	δ
harmonic	0.8215	-1.0023
(-2) sum-connectivity	1.1836	-1.0051
modified Zagreb	1.1542	-0.9846
inverse degree	1.4791	-0.9965
Randić	0.7678	-1.0021

Therefore, by plotting again the curves of the normalized average indices $\langle \overline{\cdot} \rangle \approx 1$ now as a function of ξ, we observe that curves for different graph sizes n fall on top of single *universal* curves, see Figs. 1(p-t). This means that once the product np is fixed, the average harmonic, (-2) sum-connectivity, modified Zagreb, inverse degree and Randić indices (on Erdős-Rényi graphs) are also fixed. This statement is in accordance with the results reported in [29–31], where the spectral and transport properties of Erdős-Rényi graphs where shown to be universal for the scaling parameter np, see also [32, 33].

Moreover, once we have found the scaling parameter of the indices studied here, it is expected that other quantities related to the same indices could also be scaled by the same scaling parameter. Indeed, we validate the universality of the scaling parameter ξ by applying it to the energies $E(n,p)$ of the matrices corresponding to each of the indices above on Erdös-Rényi graphs. $E(n,p)$ is defined as [34, 35]

$$E(n,p) = \sum_{i=1}^{n} |e_i| \;, \tag{4}$$

where e_i are the eigenvalues of the following matrices:

(i) Randić matrix,

$$(R)_{ij} = \begin{cases} (d_i d_j)^{-1/2} & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise,} \end{cases}$$

(ii) harmonic matrix,

$$(H)_{ij} = \begin{cases} 2(d_i + d_j)^{-1} & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise,} \end{cases}$$

(iii) (-2) sum-connectivity matrix,

$$(\chi_{-2})_{ij} = \begin{cases} (d_i + d_j)^{-2} & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise,} \end{cases}$$

(iv) modified Zagreb matrix,

$$(MZ)_{ij} = \begin{cases} (d_i d_j)^{-1} & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise,} \end{cases}$$

(v) inverse degree matrix,

$$(ID)_{ij} = \begin{cases} d_i^{-2} + d_j^{-2} & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise.} \end{cases}$$

Thus in Figs. 2(a-e) we present the energy E as a function of the probability p of the harmonic, (-2) sum-connectivity, modified Zagreb, inverse degree and Randić indices on Erdös-Rényi graphs of several sizes n. The curves E vs. p show a similar behavior for different values of n: For small p, E increases with p until reaching a maximum value, then E decreases from that maximum by further increasing p. Now, for convenience, we normalize E to the maximum value, $\overline{E} = E/\max(E)$, and plot it in Figs. 2(f-j). Here, it

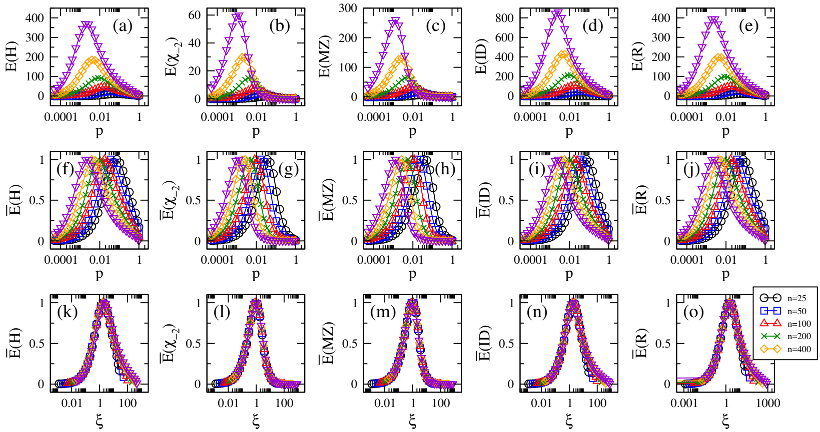

Figure 2. Energy of the (a) harmonic, (b) (-2) sum-connectivity, (c) modified Zagreb, (d) inverse degree, and (e) Randić matrices as a function of the probability p for Erdös-Rényi graphs of size n. (f-j) $\overline{E} = E/\max(E)$ as a function p. (k-o) $\overline{E}$ as a function ξ.

is clear that the curves $\overline{E}$ vs. p are very similar but shifted to the left on the p-axis for increasing n. Finally, in Figs. 2(k-o) we plot $\overline{E}$ as a function of the scaling parameter ξ, see Eq. (3), and show that all curves fall one on top of the other (except for finite size effects at large ξ). Therefore we confirm that the energies, given by Eq. (4), of the indices we study here are scaled with the parameter ξ; that is, once ξ is fixed the normalized energy $\overline{E}$ of a given index is (statistically) the same for different parameter combinations (n, p). Additionally, from Figs. 2(k-o) we can conclude that the maximum value of E occurs in the interval $1 < \xi < 2$, in close agreement with the delocalization transition value for the eigenvectors of Erdös-Rényi graphs reported in [29, 36–39] to be $\xi \approx 1.4$. Therefore, the index energy E appears to be a good delocalization transition indicator for random graphs. That is, for $E < 1$ [$E > 1$] the eigenvectors of the adjacency matrices of the corresponding random graphs are expected to be in a localized [delocalized] regime.

Even though we have shown that ξ scales the normalized average indices studied here reasonably well, it is fair to say that there are additional quantities related to these indices which are still size dependent for fixed ξ. See for example Fig. 3(a-e), where we show probability distribution functions of $\overline{H}(G)$, $\overline{\chi}_{-2}(G)$, $\overline{MZ}(G)$, $\overline{ID}(G)$ and $\overline{R}(G)$, respectively, for $\xi = 1$. In these figures we observe that, even for fixed ξ (or equivalently, for fixed $\langle\overline{H}(G)\rangle$, $\langle\overline{\chi}_{-2}(G)\rangle$, $\langle\overline{MZ}(G)\rangle$, $\langle\overline{ID}(G)\rangle$ and $\langle\overline{R}(G)\rangle$), the

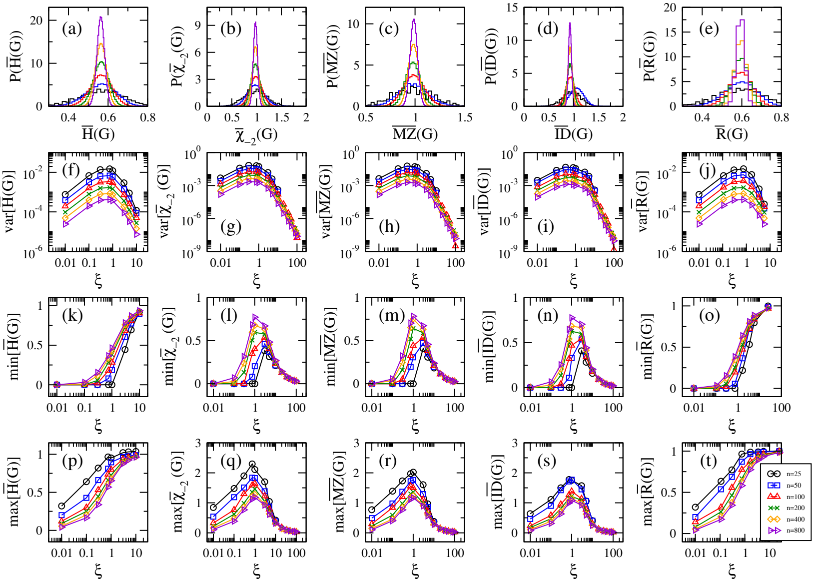

Figure 3. Probability distribution functions of (a) $\overline{H}(G)$, (b) $\overline{\chi}_{-2}(G)$, (c) $\overline{MZ}(G)$, (d) $\overline{ID}(G)$, and (e) $\overline{R}(G)$ for several graph sizes n at the fixed value of $\xi = 1$. (f-j) Variance of the normalized indices var$[\overline{\cdot}]$ as a function of ξ. (k-o) Minimum value of the normalized indices min$[\overline{\cdot}]$ as a function of ξ. (p-t) Maximum value of the normalized indices max$[\overline{\cdot}]$ as a function of ξ.

corresponding distributions become narrower when increasing n. This means that the variance and the minimal and maximal values of these distributions change with n, as can be clearly seen in Figs. 3(f-t). This motivate us to look for bounds and inequalities on these indices on Erdős-Rényi graphs, which is the main topic of the following Section.

3 Inequalities for vertex-degree-based topological indices on Erdős-Rényi models

We start by recalling that in this work we consider random graphs G from the standard Erdős-Rényi model $G(n, p)$; i.e., G has n vertices and each edge appears independently with probability $p \in (0, 1)$. Throughout this Section, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) graph such that each connected component of G has, at least, one edge (there are no isolated vertices).

We say that a statement holds for *almost every* (a.e.) *graph* if the probability of the set of graphs for which the statement fails tends to 0 as $n \to \infty$.

The following facts about the Erdős-Rényi model are well-known [40] (see also [41]):

(1) Almost every graph G has $m = p\,n(n-1)/2 + o\,(n^2)$ edges.

(2) Almost every graph G has maximum degree $\Delta = p(n-1) + (2pqn \log n)^{1/2} + o\,((n \log n)^{1/2})$, with $p \in [1/2, 1)$ and $q = 1 - p$.

(3) Almost every graph G has minimum degree $\delta = q(n-1) - (2pqn \log n)^{1/2} + o\,((n \log n)^{1/2})$, with $p \in [1/2, 1)$ and $q = 1 - p$.

Recall that $f(n) = g(n) + o(a(n))$ means that

$$\lim_{n\to\infty} \frac{f(n) - g(n)}{a(n)} = 0,$$

and $f(n) = g(n) + O(a(n))$ means that

$$\frac{f(n) - g(n)}{a(n)}$$

is a bounded sequence.

The following technical result appears in [42, Corollary 2.3].

Lemma 1 *Let g be the function $g(x,y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \le x, y \le b$. Then*

$$\frac{2\sqrt{ab}}{a+b} \le g(x,y) \le 1.$$

The equality in the lower bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$. Besides, $g(x,y) = g(x',y')$ if and only if x/y is equal to either x'/y' or y'/x'.

Recall that a (Δ, δ)-*biregular graph* (or simply a *biregular graph*) is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ.

Given a graph G, let us define

$$\delta_G = \min_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}, \qquad \Delta_G = \min_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

A similar result to the following proposition is proved in [41].

Proposition 2 *If G is a graph with n vertices, then*

$$\delta_G R(G) \le H(G) \le \Delta_G R(G)\,,$$

and the equality is attained in both bounds if G is a regular or biregular graph. Furthermore, if G is connected, then the equality is attained in both bounds if and only if G is regular or biregular.

Proof. Denote by δ and Δ the minimum degree and the maximum degree of G, respectively. We have, for every $uv \in E(G)$,

$$\delta_G \le \frac{2\sqrt{d_u d_v}}{d_u + d_v} \le \Delta_G, \qquad \frac{\delta_G}{\sqrt{d_u d_v}} \le \frac{2}{d_u + d_v} \le \frac{\Delta_G}{\sqrt{d_u d_v}}\,,$$

and the inequalities hold.

If G is a regular or biregular graph, then

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} = \frac{2\sqrt{\delta\Delta}}{\delta + \Delta} = \delta_G = \Delta_G$$

for every $uv \in E(G)$, and so, the lower and upper bounds are the same.

Assume now that G is connected and that the equality is attained in both bounds. Thus,

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} = \frac{2\sqrt{\delta\Delta}}{\delta + \Delta} = \delta_G = \Delta_G$$

for every $uv \in E(G)$. Lemma 1 gives $d_u/d_v \in \{\delta/\Delta,\, \Delta/\delta\}$ for every $uv \in E(G)$. Choose $v_0 \in V(G)$ with $d_{v_0} = \Delta$. If $u_0 v_0 \in E(G)$, then $d_{u_0}/d_{v_0} = \delta/\Delta$, and so, $d_{u_0} = \delta$; if $u_0 v \in E(G)$, then $d_v = \Delta$. Since G is connected, by iterating this argument we conclude that G is a regular or biregular graph. ■

As a consequence of Proposition 2 and Lemma 1, we obtain the known inequalities

$$\frac{\sqrt{\delta\Delta}}{\delta + \Delta}\, R(G) \le H(G) \le R(G)\,.$$

The following result relates the harmonic and the modified Zagreb indices.

Theorem 3 *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$\delta\, MZ(G) \le H(G) \le \Delta\, MZ(G).$$

Each equality is attained if and only if G is regular.

Proof. Let us consider the function $f : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}$ given by

$$f(x, y) = \frac{x + y}{xy} = \frac{1}{x} + \frac{1}{y} .$$

Hence, $2/\Delta \le f(x, y) \le 2/\delta$; the lower bound is attained if and only if $x = y = \Delta$, and the upper bound is attained if and only if $x = y = \delta$. Thus, we have for every $uv \in E(G)$

$$\frac{1}{\Delta}\frac{2}{d_u + d_v} \le \frac{1}{d_u d_v} \le \frac{1}{\delta}\frac{2}{d_u + d_v} ,$$
$$\frac{1}{\Delta} H(G) \le MZ(G) \le \frac{1}{\delta} H(G).$$

If the equality in the last lower (respectively, upper) bound is attained, then $d_u = d_v = \Delta$ (respectively, $d_u = d_v = \delta$) for every $uv \in E(G)$; thus, G is regular.

If G is regular, then both bounds are the same, and so, both equalities are attained.

■

Theorem 3 has the following consequence on random graphs.

Corollary 4 *In the Erdős-Rényi model $G(n, p)$, with $p \in [1/2, 1)$ and $q = 1 - p$, almost every graph G satisfies*

$$qn - (2pqn \log n)^{1/2} + o\left((n \log n)^{1/2}\right) \le \frac{H(G)}{MZ(G)}$$
$$\le pn + (2pqn \log n)^{1/2} + o\left((n \log n)^{1/2}\right) .$$

The following result relates the harmonic and the (-2) sum-connectivity indices.

Theorem 5 *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

$$4\,\delta\,\chi_{-2}(G) \le H(G) \le \min\{4\Delta, 2(m + 1)\}\chi_{-2}(G) .$$

The equality in the lower bound is attained if and only if G is regular.

Proof. We are going to compute the minimum value of the function $f : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}$ given by

$$f(x, y) = \frac{\frac{2}{x+y}}{\frac{1}{(x+y)^2}} = 2(x + y).$$

Hence, $4\delta \le f(x, y) \le 4\Delta$.

Thus, we have for every $uv \in E(G)$

$$\frac{4\delta}{(d_u + d_v)^2} \le \frac{2}{d_u + d_v} \le \frac{4\Delta}{(d_u + d_v)^2} ,$$
$$4\delta\chi_{-2}(G) \le H(G) \le 4\Delta\chi_{-2}(G) .$$

If the equality in the lower bound is attained, then $4\delta\chi_{-2}(G) = H(G)$ and so, $d_u = d_v = \delta$ for every $uv \in E(G)$; thus, G is regular.

If G is regular, then $4\delta\chi_{-2}(G) = 4\delta m(2\delta)^{-2} = m/\delta = H(G)$.

Since $d_u + d_v \le m + 1$, we have that $f(d_u, d_v) \le 2(m + 1)$ for every $uv \in E(G)$, and so,

$$H(G) \le 2(m+1)\chi_{-2}(G)\,.$$

■

Theorem 5 has the following consequence on random graphs.

Corollary 6 *In the Erdős-Rényi model $G(n,p)$, with $p \in [1/2, 1)$ and $q = 1-p$, almost every graph G satisfies*

$$4qn - 4(2pqn\log n)^{1/2} + o\left((n\log n)^{1/2}\right) \le \frac{H(G)}{\chi_{-2}(G)} \le 4pn + 4(2pqn\log n)^{1/2} + o\left((n\log n)^{1/2}\right).$$

In the same paper, where Zagreb indices were introduced, the *forgotten topological index* (or F-index) is defined as

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

Both the forgotten topological index and the first Zagreb index were employed in the formulas for total π-electron energy in [43], as a measure of branching extent of the carbon-atom skeleton of the underlying molecule. However, this index never got attention except recently, when Furtula and Gutman in [44] established some basic properties of the F-index and showed that its predictive ability is almost similar to that of first Zagreb index and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. Besides, in [44] the importance of the F-index was pointed out: it can be used to obtain a high accuracy of the prediction logarithm of the octanol-water partition coefficient.

The *Albertson index* is defined in [45] as

$$Alb(G) = \sum_{uv\in E(G)} |d_u - d_v|\,.$$

This index is much used as a measure of non-regularity of a graph. The Albertson index is also known as *misbalance deg index* (see [46] and [47]). This is a significant predictor of standard enthalpy of vaporization for octane isomers (see [46]).

Theorem 7 *If G is a graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$, then*

$$H(G) \le \frac{F(G)}{2\delta^3} - \frac{(2\Delta)^{\alpha-1} Alb(G)^2}{\delta^2 \chi_\alpha(G)}, \quad \text{if } \alpha \le 1,$$

$$H(G) \le \frac{F(G)}{2\delta^3} - \frac{(2\delta)^{\alpha-1} Alb(G)^2}{\delta^2 \chi_\alpha(G)}, \quad \text{if } \alpha \ge 1,$$

and each equality is attained if and only if G is regular.

Proof. Since

$$\frac{d_u^2 + d_v^2}{2\delta} \ge \frac{d_u^2 + d_v^2}{d_u + d_v} = \frac{2d_u d_v}{d_u + d_v} + \frac{(d_u - d_v)^2}{d_u + d_v} \ge \frac{2\delta^2}{d_u + d_v} + \frac{(d_u - d_v)^2}{d_u + d_v},$$

for every $uv \in E(G)$, and

$$F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} \left(d_u^2 + d_v^2\right),$$

we have

$$\frac{F(G)}{2\delta} \ge \delta^2 H(G) + \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v}.$$

If $\alpha \le 1$, then $(1-\alpha)/2 \ge 0$ and Cauchy-Schwarz inequality gives

$$\begin{aligned} (2\Delta)^{\alpha-1} Alb(G)^2 &= \left(\frac{Alb(G)}{(2\Delta)^{(1-\alpha)/2}} \right)^2 \le \left(\sum_{uv \in E(G)} \frac{|d_u - d_v|}{(d_u + d_v)^{(1-\alpha)/2}} \right)^2 \\ &\le \left(\sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v} \right) \left(\sum_{uv \in E(G)} (d_u + d_v)^\alpha \right) \\ &= \chi_\alpha(G) \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v}, \end{aligned}$$

and we conclude

$$\frac{F(G)}{2\delta} \ge \delta^2 H(G) + \frac{(2\Delta)^{\alpha-1} Alb(G)^2}{\chi_\alpha(G)}.$$

If $\alpha \ge 1$, then $(1-\alpha)/2 \le 0$ and

$$(2\delta)^{\alpha-1} Alb(G)^2 \le \chi_\alpha(G) \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v},$$

and the previous argument provides the desired inequality.

The previous argument gives that if some bound is attained, then $d_u d_v = \delta^2$ for every $uv \in E(G)$. Thus, $d_u = \delta$ for every $u \in V(G)$ and G is regular.

If the graph G is regular, then

$$\begin{aligned}\frac{F(G)}{2\delta^3} - \frac{(2\Delta)^{\alpha-1}Alb(G)^2}{\delta^2\chi_\alpha(G)} &= \frac{F(G)}{2\delta^3} - \frac{(2\delta)^{\alpha-1}Alb(G)^2}{\delta^2\chi_\alpha(G)} \\ &= \frac{F(G)}{2\delta^3} = \frac{2\delta^2 m}{2\delta^3} = \frac{m}{\delta} = H(G)\,.\end{aligned}$$

■

Theorem 8 *If G is a graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$, then*

$$(\Delta-\delta)^2 H(G) \ge \frac{2^\alpha \Delta^{\alpha-1} Alb(G)^2}{\chi_\alpha(G)}\,, \quad \text{if } \alpha \le 1,$$
$$(\Delta-\delta)^2 H(G) \ge \frac{2^\alpha \delta^{\alpha-1} Alb(G)^2}{\chi_\alpha(G)}\,, \quad \text{if } \alpha \ge 1,$$

and for each $\alpha \ne 1$ the equality is attained if and only if G is regular.

Proof. We have

$$\frac{1}{2}(\Delta-\delta)^2 H(G) = \sum_{uv\in E(G)} \frac{(\Delta-\delta)^2}{d_u+d_v} \ge \sum_{uv\in E(G)} \frac{(d_u-d_v)^2}{d_u+d_v}\,.$$

The argument in the proof of Theorem 7 gives

$$\sum_{uv\in E(G)} \frac{(d_u-d_v)^2}{d_u+d_v} \ge \frac{(2\Delta)^{\alpha-1}Alb(G)^2}{\chi_\alpha(G)}\,, \quad \text{if } \alpha \le 1,$$
$$\sum_{uv\in E(G)} \frac{(d_u-d_v)^2}{d_u+d_v} \ge \frac{(2\delta)^{\alpha-1}Alb(G)^2}{\chi_\alpha(G)}\,, \quad \text{if } \alpha \ge 1,$$

and we obtain the desired inequalities.

If the graph is regular, then $Alb(G) = 0$, $\Delta = \delta$ and

$$(\Delta-\delta)^2 H(G) = \frac{2^\alpha \Delta^{\alpha-1} Alb(G)^2}{\chi_\alpha(G)} = \frac{2^\alpha \delta^{\alpha-1} Alb(G)^2}{\chi_\alpha(G)} = 0.$$

The previous argument gives that if some bound is attained, then we have either $d_u + d_v = 2\delta$ for every $uv \in E(G)$ or $d_u + d_v = 2\Delta$ for every $uv \in E(G)$. Thus, $d_u = \delta$ for every $u \in V(G)$ or $d_u = \Delta$ for every $u \in V(G)$, and so, G is regular. ■

Theorem 8 has the following consequence on random graphs.

Corollary 9 *For each $\alpha \in \mathbb{R}$, in the Erdős-Rényi model $G(n,p)$, with $p \in [1/2, 1)$ and $q = 1-p$, almost every graph G satisfies*

$$\frac{Alb(G)^2}{H(G)\chi_\alpha(G)} \le 2^{-\alpha}(p-q)^2 p^{1-\alpha} n^{3-\alpha} + O\left(n^{5/2-\alpha}(\log n)^{1/2}\right), \quad \text{if } \alpha \le 1,$$
$$\frac{Alb(G)^2}{H(G)\chi_\alpha(G)} \le 2^{-\alpha}(p-q)^2 q^{1-\alpha} n^{3-\alpha} + O\left(n^{5/2-\alpha}(\log n)^{1/2}\right), \quad \text{if } \alpha \ge 1.$$

Proof. If $\alpha \le 1$, then Theorem 8 gives

$$\begin{aligned}\frac{Alb(G)^2}{H(G)\chi_\alpha(G)} &\le 2^{-\alpha}(\Delta-\delta)^2\Delta^{1-\alpha}\\ &= 2^{-\alpha}\left((p-q)n+O\left((n\log n)^{1/2}\right)\right)^2\left(pn+O\left((n\log n)^{1/2}\right)\right)^{1-\alpha}\\ &= 2^{-\alpha}\left((p-q)^2n^2+O\left(n^{3/2}(\log n)^{1/2}\right)\right)\left(p^{1-\alpha}n^{1-\alpha}+O\left(n^{1/2-\alpha}(\log n)^{1/2}\right)\right)\\ &= 2^{-\alpha}(p-q)^2p^{1-\alpha}n^{3-\alpha}+O\left(n^{5/2-\alpha}(\log n)^{1/2}\right),\end{aligned}$$

for almost every graph. The same argument gives the inequality when $\alpha \ge 1$. ■

The following Szőkefalvi-Nagy inequality appears in [48] (see also [49]).

Lemma 10 *If $a_j \ge 0$ for $1 \le j \le k$, $R = \max_j a_j$ and $r = \min_j a_j$, then*

$$k\sum_{j=1}^{k} a_j^2 - \left(\sum_{j=1}^{k} a_j\right)^2 \ge \frac{k}{2}(R-r)^2.$$

In many papers the hypothesis $a_j \ge 0$ for $1 \le j \le k$, $R = \max_j a_j$ and $r = \min_j a_j$, is replaced by $0 < r \le a_j \le R$ for $1 \le j \le k$. However, the conclusion of Lemma 10 does not hold in general with the hypothesis $0 < r \le a_j \le R$ for $1 \le j \le k$, as the following example shows:

If $a_j = a$ for $1 \le j \le k$ and $r \le a < R$, then

$$k\sum_{j=1}^{k} a_j^2 - \left(\sum_{j=1}^{k} a_j\right)^2 = k^2a^2 - k^2a^2 = 0 < \frac{k}{2}(R-r)^2,$$

a contradiction.

The following Popoviciu's inequality on variances [48] shows a converse of Lemma 10.

Lemma 11 *If $a_j \ge 0$ for $1 \le j \le k$, $R = \max_j a_j$ and $r = \min_j a_j$, then*

$$k\sum_{j=1}^{k} a_j^2 - \left(\sum_{j=1}^{k} a_j\right)^2 \le \frac{k^2}{4}(R-r)^2.$$

Theorem 12 *If G is a graph with m edges,*

$$Q = \max_{uv\in E(G)} \frac{1}{d_u+d_v}, \qquad q = \min_{uv\in E(G)} \frac{1}{d_u+d_v},$$

then

$$\sqrt{4m\chi_{-2}(G) - m^2(Q-q)^2} \le H(G) \le \sqrt{4m\chi_{-2}(G) - 2m(Q-q)^2}\,.$$

The equality in the each bound is attained if G is a regular or biregular graph.

Proof. If we choose $a_j = \frac{1}{d_u+d_v}$, Lemma 10 gives

$$
\begin{aligned}
m\chi_{-2}(G) - \frac{H(G)^2}{4} &= m \sum_{uv\in E(G)} \frac{1}{(d_u+d_v)^2} - \left(\sum_{uv\in E(G)} \frac{1}{d_u+d_v} \right)^2 \\
&\geq \frac{m}{2}(Q-q)^2,
\end{aligned}
$$

and this gives the second inequality.

By using Lemma 11 instead of Lemma 10, we obtain

$$
m\chi_{-2}(G) - \frac{H(G)^2}{4} \leq \frac{m^2}{4}(Q-q)^2,
$$

and this gives the first inequality.

If G is a regular or biregular graph, then

$$
\frac{1}{d_u+d_v} = \frac{1}{\Delta+\delta} = Q = q
$$

for every $uv \in E(G)$. Thus,

$$
\begin{aligned}
\sqrt{4m\chi_{-2}(G) - m^2(Q-q)^2} &= \sqrt{4m\chi_{-2}(G) - 2m(Q-q)^2} \\
&= \sqrt{4m\frac{m}{(\Delta+\delta)^2}} = \frac{2m}{\Delta+\delta} = H(G).
\end{aligned}
$$

■

The following result provides some inequalities relating harmonic and inverse degree indices (see [50] for other inequalities relating these indices).

Theorem 13 *Let G be a graph with minimum degree δ and maximum degree Δ. Then*

$$
\begin{aligned}
&ID(G) \geq \frac{2}{\Delta} H(G), \\
&ID(G) \leq \frac{2}{\delta} H(G), \qquad \text{if } \delta \geq (\sqrt{2}-1)\Delta, \\
&ID(G) \leq \frac{(\Delta^2+\delta^2)(\Delta+\delta)}{2\Delta^2\delta^2} H(G), \qquad \text{if } \delta < (\sqrt{2}-1)\Delta.
\end{aligned}
$$

Furthermore, the first inequality is attained if and only if G is regular; if $\delta \geq (\sqrt{2}-1)\Delta$, then the second inequality is attained if and only if G is regular; if $\delta < (\sqrt{2}-1)\Delta$, then the third inequality is attained if and only if G is (Δ,δ)-biregular.

Proof. We are going to compute the maximum and minimum values of the function $f : [\delta,\Delta] \times [\delta,\Delta] \to \mathbb{R}$ given by

$$
f(x,y) = \left(\frac{1}{x^2} + \frac{1}{y^2} \right) \frac{x+y}{2}.
$$

By symmetry, we can assume that $x \le y$. We have

$$\frac{\partial f}{\partial x}(x,y) = \frac{1}{2y^2} - \frac{1}{2x^2} - \frac{y}{x^3} = \frac{y}{2x^3}\left(\frac{x^3}{y^3} - \frac{x}{y} - 2\right).$$

If we define $g(t) := t^3 - t - 2$, then

$$\frac{\partial f}{\partial x}(x,y) = \frac{y}{2x^3}\, g\Big(\frac{x}{y}\Big).$$

Since g increases on $(-\infty, -3^{-1/2}) \cup (3^{-1/2}, \infty)$, decreases on $(-3^{-1/2}, 3^{-1/2})$ and $g(-3^{-1/2}) < 0$, the function g has just a real zero t_0. Since $g(1) < 0$ and $g(2) > 0$, we have $t_0 \in (1,2)$.

Hence,

$$\frac{\partial f}{\partial x}(x,y) < 0 \qquad \text{if } \delta \le x \le y \le \Delta,$$

and so, the maximum value of f is attained on the set $\{x = \delta, \delta \le y \le \Delta\}$, and the minimum value of f is attained on the set $\{\delta \le x = y \le \Delta\}$. Thus,

$$f(x,y) \ge \min_{\delta \le x \le \Delta} f(x,x) = \min_{\delta \le x \le \Delta} \frac{2}{x^2}x = \frac{2}{\Delta},$$

$$\frac{1}{d_u^2} + \frac{1}{d_v^2} \ge \frac{2}{\Delta}\frac{2}{d_u + d_v},$$

$$ID(G) \ge \frac{2}{\Delta}\, H(G).$$

Since

$$\frac{\partial f}{\partial y}(x,y) = \frac{1}{2x^2} - \frac{1}{2y^2} - \frac{x}{y^3}, \qquad \frac{\partial^2 f}{\partial y^2}(x,y) = \frac{1}{y^3} + \frac{3x}{y^4} > 0,$$

f is a convex function (for each fixed x), and we have

$$f(x,y) \le \max_{\delta \le y \le \Delta} f(\delta, y) = \max\{f(\delta,\delta), f(\delta,\Delta)\} = \max\left\{\frac{2}{\delta}, \left(\frac{1}{\delta^2} + \frac{1}{\Delta^2}\right)\frac{\delta+\Delta}{2}\right\}.$$

Note that the function

$$h(t) := t^3 + t^2 - 3t + 1 = (t-1)(t+1-\sqrt{2}\,)(t+1+\sqrt{2}\,)$$

satisfies $h(t) > 0$ if $t \in (0, \sqrt{2}-1)$, and $h(t) \le 0$ if $t \in [\sqrt{2}-1, 1]$. Thus, we have for $\delta < (\sqrt{2}-1)\Delta$,

$$\frac{\delta^3}{\Delta^3} + \frac{\delta^2}{\Delta^2} + \frac{\delta}{\Delta} + 1 > 4\,\frac{\delta}{\Delta}, \qquad \frac{\delta^2}{\Delta^2} + \frac{\delta}{\Delta} + 1 + \frac{\Delta}{\delta} > 4,$$

$$\left(1 + \frac{\delta^2}{\Delta^2}\right)\left(\frac{\Delta}{\delta} + 1\right) > 4, \qquad \left(\frac{1}{\delta^2} + \frac{1}{\Delta^2}\right)\frac{\delta+\Delta}{2} > \frac{2}{\delta},$$

and we conclude

$$f(x,y) \le \max\left\{\frac{2}{\delta}, \left(\frac{1}{\delta^2}+\frac{1}{\Delta^2}\right)\frac{\delta+\Delta}{2}\right\} = \frac{(\Delta^2+\delta^2)\,(\Delta+\delta)}{2\Delta^2\delta^2},$$

$$\frac{1}{d_u^2}+\frac{1}{d_v^2} \le \frac{(\Delta^2+\delta^2)(\Delta+\delta)}{2\Delta^2\delta^2}\,\frac{2}{d_u+d_v},$$

$$ID(G) \le \frac{(\Delta^2+\delta^2)(\Delta+\delta)}{2\Delta^2\delta^2}\,H(G).$$

If $\delta \ge (\sqrt{2}-1)\Delta$, then $f(x,y) \le 2/\delta$ and

$$ID(G) \le \frac{2}{\delta}\,H(G).$$

The previous argument gives that the first inequality is attained if and only if $d_u = d_v = \Delta$ for every $uv \in E(G)$, and this happens if and only if G is regular.

Assume that $\delta \ge (\sqrt{2}-1)\Delta$. Thus, the second inequality is attained if and only if $d_u = d_v = \delta$ for every $uv \in E(G)$, i.e., if and only if G is regular. Assume that $\delta < (\sqrt{2}-1)\Delta$. Thus, the third inequality is attained if and only if $\{d_u, d_v\} = \{\Delta, \delta\}$ for every $uv \in E(G)$, i.e., if and only if G is (Δ,δ)-biregular (note that G can not be a regular graph since $\delta < (\sqrt{2}-1)\Delta < \Delta$. ■

Theorem 13 has the following consequence on random graphs.

Corollary 14 *In the Erdős-Rényi model $G(n,p)$, with $p \in [1/2,1)$ and $q = 1-p$, almost every graph G satisfies*

$$\frac{1}{2}\,qn + O\left((n\log n)^{1/2}\right) \le \frac{H(G)}{ID(G)} \le \frac{1}{2}\,pn + O\left((n\log n)^{1/2}\right), \quad \text{if } p < \sqrt{2}/2,$$

$$\frac{2p^2q^2}{p^2+q^2}\,n + O\left((n\log n)^{1/2}\right) \le \frac{H(G)}{ID(G)} \le \frac{1}{2}\,pn + O\left((n\log n)^{1/2}\right), \quad \text{if } p > \sqrt{2}/2.$$

Proof. Assume first that $p < \sqrt{2}/2$. Thus,

$$q = 1-p > (\sqrt{2}-1)p \quad \Rightarrow \quad \delta > (\sqrt{2}-1)\Delta,$$

for almost every graph, and Theorem 13 gives

$$\frac{1}{2}\,\delta \le \frac{H(G)}{ID(G)} \le \frac{1}{2}\,\Delta.$$

Assume now that $p > \sqrt{2}/2$. Therefore, $\delta < (\sqrt{2}-1)\Delta$ for almost every graph, and Theorem 13 gives

$$\frac{2\Delta^2\delta^2}{(\Delta^2+\delta^2)\,(\Delta+\delta)} \le \frac{H(G)}{ID(G)} \le \frac{1}{2}\,\Delta.$$

We have the desired inequalities since

$$\begin{aligned}\frac{2\Delta^2\delta^2}{(\Delta^2+\delta^2)(\Delta+\delta)} &= \frac{2\left(p^2n^2+O\left(n^{3/2}(\log n)^{1/2}\right)\right)\left(q^2n^2+O\left(n^{3/2}(\log n)^{1/2}\right)\right)}{\left((p^2+q^2)n^2+O\left(n^{3/2}(\log n)^{1/2}\right)\right)\left(n+O\left((n\log n)^{1/2}\right)\right)}\\ &= \frac{2p^2q^2n^4+O\left(n^{7/2}(\log n)^{1/2}\right)}{(p^2+q^2)n^3+O\left(n^{5/2}(\log n)^{1/2}\right)}\\ &= \frac{2p^2q^2n+O\left((n\log n)^{1/2}\right)}{p^2+q^2+O\left(n^{-1/2}(\log n)^{1/2}\right)}\\ &= \left(2p^2q^2n+O\left((n\log n)^{1/2}\right)\right)\left(\frac{1}{p^2+q^2}+O\left(n^{-1/2}(\log n)^{1/2}\right)\right)\\ &= \frac{2p^2q^2}{p^2+q^2}n+O\left((n\log n)^{1/2}\right),\end{aligned}$$

for almost every graph. ■

We prove now several inequalities for H involving the variable second Zagreb index.

Remark 15 *Recall that α in $M_2^\alpha(G)$ is a parameter rather than an exponent.*

Theorem 16 *If G is a graph with maximum degree Δ and minimum degree δ, and $\alpha\in\mathbb{R}$, then*

$$H(G)\ge\frac{2M_2^\alpha(G)^2}{\Delta^{4\alpha}M_1(G)},\qquad \text{if } \alpha\ge 0,$$

$$H(G)\ge\frac{2M_2^\alpha(G)^2}{\delta^{4\alpha}M_1(G)},\qquad \text{if } \alpha\le 0,$$

and the equality is attained for some $\alpha\neq 0$ if and only if G is regular.

Proof. If $\alpha\ge 0$, then Cauchy-Schwarz inequality gives

$$\begin{aligned}M_2^\alpha(G)^2 &= \left(\sum_{uv\in E(G)}\frac{(d_ud_v)^\alpha}{(d_u+d_v)^{1/2}}(d_u+d_v)^{1/2}\right)^2\\ &\le \sum_{uv\in E(G)}\frac{(d_ud_v)^{2\alpha}}{d_u+d_v}\sum_{uv\in E(G)}(d_u+d_v)\le\frac{\Delta^{4\alpha}}{2}H(G)M_1(G).\end{aligned}$$

If the equality is attained for some $\alpha>0$, then the previous argument gives $d_ud_v=\Delta^2$ for every $uv\in E(G)$; thus, $d_u=\Delta$ for every $u\in V(G)$ and G is regular.

If G is a regular graph, then

$$\frac{2M_2^\alpha(G)^2}{\Delta^{4\alpha}M_1(G)}=\frac{2(\Delta^{2\alpha}m)^2}{\Delta^{4\alpha}2\Delta m}=\frac{m}{\Delta}=H(G).$$

If $\alpha\le 0$, then a similar argument gives the result. ■

Corollary 17 *If G is a graph with minimum degree δ, then*

$$H(G) \geq 2\,\delta^4\,\frac{MZ(G)^2}{M_1(G)}\,,$$

and the equality is attained if and only if G is regular.

Theorem 16 has the following consequence on random graphs.

Corollary 18 *For each $\alpha \in \mathbb{R}$, in the Erdős-Rényi model $G(n,p)$, with $p \in [1/2, 1)$ and $q = 1 - p$, almost every graph G satisfies*

$$\frac{H(G)M_1(G)}{M_2^{\alpha}(G)^2} \geq 2p^{-4\alpha}n^{-4\alpha} + O\left(n^{-4\alpha-1/2}(\log n)^{1/2}\right), \quad \text{if } \alpha \geq 0,$$
$$\frac{H(G)M_1(G)}{M_2^{\alpha}(G)^2} \geq 2q^{-4\alpha}n^{-4\alpha} + O\left(n^{-4\alpha-1/2}(\log n)^{1/2}\right), \quad \text{if } \alpha \leq 0.$$

Proof. Assume first that $\alpha \geq 0$. Thus, Theorem 16 gives

$$\begin{aligned}\frac{H(G)M_1(G)}{M_2^{\alpha}(G)^2} &\geq \frac{2}{\Delta^{4\alpha}} = \frac{2}{\left(pn + O\left((n\log n)^{1/2}\right)\right)^{4\alpha}} \\ &= \frac{2}{p^{4\alpha}n^{4\alpha}\left(1 + O\left(n^{-1/2}(\log n)^{1/2}\right)\right)^{4\alpha}} \\ &= 2p^{-4\alpha}n^{-4\alpha}\left(1 + O\left(n^{-1/2}(\log n)^{1/2}\right)\right) \\ &= 2p^{-4\alpha}n^{-4\alpha} + O\left(n^{-4\alpha-1/2}(\log n)^{1/2}\right),\end{aligned}$$

for almost every graph. If $\alpha \leq 0$, then the same argument gives the desired result. ■

We need the following well-known result, that provides a converse of Cauchy-Schwarz inequality (see, e.g., [51, Lemma 3.4]).

Lemma 19 *If $a_j, b_j \geq 0$ and $\omega b_j \leq a_j \leq \Omega b_j$ for $1 \leq j \leq k$, then*

$$\left(\sum_{j=1}^{k} a_j^2\right)^{1/2}\left(\sum_{j=1}^{k} b_j^2\right)^{1/2} \leq \frac{1}{2}\left(\sqrt{\frac{\Omega}{\omega}} + \sqrt{\frac{\omega}{\Omega}}\right)\sum_{j=1}^{k} a_j b_j.$$

If $a_j > 0$ for some $1 \leq j \leq k$, then the equality holds if and only if $\omega = \Omega$ and $a_j = \omega b_j$ for every $1 \leq j \leq k$.

A family of Adriatic indices was introduced in [46] and [47]. An especially interesting subclass of these descriptors consists of 148 discrete Adriatic indices. Most of the indices showed good predictive properties on the testing sets provided by the International Academy of Mathematical Chemistry. Twenty of them were selected as significant predictors. One of them, the *inverse sum indeg index*, ISI, was selected in [47] as a significant predictor of total surface area of octane isomers. This index is defined as

$$ISI(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v} = \sum_{uv\in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}}.$$

In the last years there has been an increasing interest in this index (see, e.g., [52–54]).

We report that in the proof of [53, Theorem 2.7] there is a small mistake produced by a change in a lower and an upper bounds in the argument of its proof. The following result provides a similar inequality without mistakes.

Theorem 20 *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

$$ISI(G) \geq \frac{\Delta^{3/2}\delta^{3/2}}{(\Delta^3 + \delta^3)\, m}\, M_2(G)H(G),$$

and the equality is attained if and only if G is regular.

Proof. Cauchy-Schwarz inequality gives

$$M_2(G) = \sum_{uv\in E(G)} d_u d_v \leq \left(\sum_{uv\in E(G)} (d_u d_v)^2 \right)^{1/2} \left(\sum_{uv\in E(G)} 1 \right)^{1/2},$$

$$\left(\sum_{uv\in E(G)} (d_u d_v)^2 \right)^{1/2} \geq m^{-1/2} M_2(G)\,,$$

and

$$\frac{1}{2}\, H(G) = \sum_{uv\in E(G)} \frac{1}{d_u + d_v} \leq \left(\sum_{uv\in E(G)} \left(\frac{1}{d_u + d_v} \right)^2 \right)^{1/2} \left(\sum_{uv\in E(G)} 1 \right)^{1/2},$$

$$\left(\sum_{uv\in E(G)} \left(\frac{1}{d_u + d_v} \right)^2 \right)^{1/2} \geq \frac{1}{2}\, m^{-1/2} H(G)\,.$$

We have for every $uv \in E(G)$

$$2\delta^3 \leq d_u d_v \,(d_u + d_v) = \frac{d_u d_v}{\frac{1}{d_u + d_v}} \leq 2\Delta^3.$$

Thus, Lemma 19 gives

$$\sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v} \geq \frac{\left(\sum_{uv\in E(G)} (d_u d_v)^2 \right)^{1/2} \left(\sum_{uv\in E(G)} \frac{1}{(d_u + d_v)^2} \right)^{1/2}}{\frac{1}{2}\left(\sqrt{\frac{\Delta^3}{\delta^3}} + \sqrt{\frac{\delta^3}{\Delta^3}} \right)}.$$

Therefore,

$$ISI(G) \geq \frac{2\Delta^{3/2}\delta^{3/2}}{\Delta^3+\delta^3}\, m^{-1/2} M_2(G)\, \frac{1}{2}\, m^{-1/2} H(G)$$
$$= \frac{\Delta^{3/2}\delta^{3/2}}{(\Delta^3+\delta^3)\, m}\, M_2(G)H(G).$$

If G is regular, then

$$\frac{\Delta^{3/2}\delta^{3/2}}{(\Delta^3+\delta^3)\, m}\, M_2(G)H(G) = \frac{\Delta^3}{2\Delta^3 m}\, \Delta^2 m\, \frac{m}{\Delta} = \frac{\Delta}{2}\, m = ISI(G).$$

If the equality is attained, then Lemma 19 gives $2\delta^3 = 2\Delta^3$ and G is regular. ■

The *Platt number* of a graph G is the topological index defined (see, e.g., [55]) as

$$P(G) = \sum_{uv\in E(G)} (d_u + d_v - 2).$$

Proposition 21 *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

$$m - \frac{1}{2\delta}\, P(G) \leq H(G) \leq m - \frac{1}{2\Delta}\, P(G),$$

and each equality is attained if and only if G is a regular graph.

Proof. We have

$$\frac{d_u+d_v-2}{2\Delta} \leq \frac{d_u+d_v-2}{d_u+d_v} = 1 - \frac{2}{d_u+d_v} \leq \frac{d_u+d_v-2}{2\delta},$$
$$\frac{1}{2\Delta}\, P(G) \leq m - H(G) \leq \frac{1}{2\delta}\, P(G).$$

Each equality is attained if and only if $d_u+d_v = 2\Delta$ for every $uv \in E(G)$ or $d_u+d_v = 2\delta$ for every $uv \in E(G)$; this is equivalent to $d_u = \Delta$ for every $u \in V(G)$ or $d_u = \delta$ for every $u \in V(G)$, and this holds if and only if G is a regular graph. ■

Multiplicative versions of the first and the second Zagreb indices, Π_1 and Π_2, were first considered in [56], defined as

$$\Pi_1(G) = \prod_{u\in V(G)} d_u^2, \qquad \Pi_2(G) = \prod_{uv\in E(G)} d_u d_v.$$

Also, the multiplicative sum-Zagreb index Π_1^* was introduced in [57] as

$$\Pi_1^*(G) = \prod_{uv\in E(G)} (d_u + d_v)\,.$$

Theorem 22 *If G is a graph with m edges, then*

$$H(G) \geq \frac{2m}{\Pi_1^*(G)^{1/m}},$$

and the equality is attained if G is a regular or biregular graph. If G is a connected graph, then the equality is attained if and only if G is regular or biregular.

Proof. Using the fact that the geometric mean is at most the arithmetic mean, we obtain

$$\frac{1}{2m} H(G) = \frac{1}{m} \sum_{uv \in E(G)} \frac{1}{d_u + d_v} \geq \left(\prod_{uv \in E(G)} \frac{1}{d_u + d_v} \right)^{1/m} = \frac{1}{\Pi_1^*(G)^{1/m}}.$$

If G is a regular or biregular graph, then $d_u + d_v = \Delta + \delta$ is constant for every $uv \in E(G)$, and so the geometric mean is equal to the arithmetic mean; hence, the equality is attained.

Assume now that G is a connected graph and that the equality is attained. Thus, the equality of arithmetic and geometric means holds and, consequently, there exists a constant c such that $d_u + d_v = c$ for every $uv \in E(G)$. Therefore, if $uv, vw \in E(G)$, we have $d_v = c - d_u = c - d_w$ and so, $d_u = d_w$. Since G is connected, the set $\{d_a : a \in V(G)\}$ has at most two values, and G is regular or biregular. ■

Lemma 23 *Let h be the function $h(x, y) = \frac{2xy}{x+y}$ with $\delta \leq x, y \leq \Delta$. Then*

$$\delta \leq h(x, y) \leq \Delta.$$

Furthermore, the lower (respectively, upper) bound is attained if and only if $x = y = \delta$ (respectively, $x = y = \Delta$).

Theorem 24 *We have for any graph G with m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}\backslash\{0\}$,*

$$\frac{2^\alpha m^2}{\delta^\alpha M_2^{-\alpha}(G)} \leq \chi_\alpha(G) \leq \frac{(\Delta^{3\alpha/2} + \delta^{3\alpha/2})^2}{\Delta^{5\alpha/2}\delta^{3\alpha/2}} \frac{2^{\alpha-2} m^2}{M_2^{-\alpha}(G)}, \qquad \text{if } \alpha < 0,$$

$$\frac{2^\alpha m^2}{\Delta^\alpha M_2^{-\alpha}(G)} \leq \chi_\alpha(G) \leq \frac{(\Delta^{3\alpha/2} + \delta^{3\alpha/2})^2}{\Delta^{3\alpha/2}\delta^{5\alpha/2}} \frac{2^{\alpha-2} m^2}{M_2^{-\alpha}(G)}, \qquad \text{if } \alpha > 0,$$

and each inequality is attained for some value of α if and only if G is regular.

Proof. By Lemma 23, we have

$$\left(\frac{2}{\Delta}\right)^{\alpha/2} \le \frac{(d_u+d_v)^{\alpha/2}}{(d_ud_v)^{\alpha/2}} \le \left(\frac{2}{\delta}\right)^{\alpha/2}, \qquad \text{if } \alpha > 0,$$

$$\left(\frac{2}{\delta}\right)^{\alpha/2} \le \frac{(d_u+d_v)^{\alpha/2}}{(d_ud_v)^{\alpha/2}} \le \left(\frac{2}{\Delta}\right)^{\alpha/2}, \qquad \text{if } \alpha < 0.$$

Cauchy-Schwarz inequality gives

$$\left(\sum_{uv\in E(G)} \frac{(d_u+d_v)^{\alpha/2}}{(d_ud_v)^{\alpha/2}}\right)^2 \le \left(\sum_{uv\in E(G)} (d_u+d_v)^{\alpha}\right)\left(\sum_{uv\in E(G)} (d_ud_v)^{-\alpha}\right) = \chi_\alpha(G)M_2^{-\alpha}(G).$$

These inequalities provide the lower bounds.

If $\alpha > 0$, then the following inequalities hold

$$2^{\alpha/2}\delta^{3\alpha/2} \le (d_ud_v)^{\alpha/2}(d_u+d_v)^{\alpha/2} = \frac{(d_u+d_v)^{\alpha/2}}{\frac{1}{(d_ud_v)^{\alpha/2}}} \le 2^{\alpha/2}\Delta^{3\alpha/2}.$$

If $\alpha < 0$, then the converse inequalities hold. Hence, for every $\alpha \neq 0$, Lemma 19 gives

$$\left(\sum_{uv\in E(G)} \frac{(d_u+d_v)^{\alpha/2}}{(d_ud_v)^{\alpha/2}}\right)^2 \ge \frac{\left(\sum_{uv\in E(G)} (d_u+d_v)^{\alpha}\right)\left(\sum_{uv\in E(G)} (d_ud_v)^{-\alpha}\right)}{\frac{1}{4}\left(\left(\frac{\Delta}{\delta}\right)^{3\alpha/4} + \left(\frac{\delta}{\Delta}\right)^{3\alpha/4}\right)^2} = \frac{4(\Delta\delta)^{3\alpha/2}}{(\Delta^{3\alpha/2}+\delta^{3\alpha/2})^2}\,\chi_\alpha(G)M_2^{-\alpha}(G),$$

and this gives the upper bounds.

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $\chi_\alpha(G)$. If some bound is attained for some value of α, then Lemma 23 gives $d_u = d_v = \delta$ for every $uv \in E(G)$ or $d_u = d_v = \Delta$ for every $uv \in E(G)$; hence, G is regular. ■

Corollary 25 *We have for any graph G with m edges, maximum degree Δ and minimum degree δ,*

$$\frac{m^2\delta}{2M_2(G)} \le H(G) \le \frac{(\Delta^{3/2}+\delta^{3/2})^2}{\Delta^{1/2}\delta^{3/2}}\frac{m^2}{8M_2(G)},$$

and each inequality is attained if and only if G is regular.

4 Summary

Motivated by the importance of the theoretical-practical applications of several topological indices, in this paper we have studied statistically and analytically the properties of the harmonic index $H(G)$, the (-2) sum-connectivity index $\chi_{-2}(G)$, the modified Zagreb index $MZ(G)$, the inverse degree index $ID(G)$ and the Randić index $R(G)$ on Erdős-Rényi graphs characterized by n vertices connected independently with probability $p \in (0,1)$.

First, by the proper scaling analysis of the average (and normalized) indices ($\langle \overline{H}(G) \rangle$, $\langle \overline{\chi}_{-2}(G) \rangle$, $\langle \overline{MZ}(G) \rangle$, $\langle \overline{ID}(G) \rangle$ and $\langle \overline{R}(G) \rangle$) we found that $\xi \approx np$ works as the scaling parameter of all the indices under study. That is, for fixed ξ, $\langle \overline{\cdot} \rangle$ is also fixed for all the above indices, see Figs. 1(p-t).

Moreover, we report two different behaviors. On the one hand, $\langle H(G) \rangle$ and $\langle R(G) \rangle$, as a function of the probability p, show a smooth transition from zero to $n/2$ as p increases from zero to one. Indeed, after scaling, our analysis provides a way to predict the values of H and R on Erdős-Rényi graphs once the value of ξ is known: $H(G), R(G) \approx 0$ for $\xi < 0.01$ (when the vertices in the graph are mostly isolated), the transition from isolated vertices to complete graphs occurs in the interval $0.01 < \xi < 10$ where $0 < H(G), R(G) < n/2$, while when $\xi > 10$ the graphs are almost complete and $H(G), R(G) \approx n/2$; see Figs. 1(p,t).[1] On the other hand, $\langle \chi_{-2}(G) \rangle$, $\langle MZ(G) \rangle$ and $\langle ID(G) \rangle$ increase with p until approaching their maximum value, then they decrease by further increasing p. Thus, after scaling the curves corresponding to these indices display bell-like shapes in log scale, which are symmetric around $\xi \approx 1$; i.e. the percolation transition point of ER graphs, see Figs. 1(q-s).

We validated our scaling hypothesis by applying the scaling parameter to the energy $E(n,p)$ corresponding to the indices under study. Indeed, we showed that ξ also scales the energy $E(n,p)$, see Figs. 1(k-o). Moreover, we also found that that the maximum value of E occurs in the interval $1 < \xi < 2$, in close agreement with the delocalization transition value for the eigenvectors of Erdös-Rényi graphs. Therefore, we propose the index energy E as a delocalization transition indicator for random graphs. That is, for $E < 1$ [$E > 1$] the eigenvectors of the adjacency matrices of the corresponding random graphs are expected to be in a localized [delocalized] regime.

Therefore, motivated by the scaling analysis, we analytically (i) obtain new relations connecting the topological indices H, χ_{-2}, MZ, ID and R that characterize graphs which are extremal with respect to the obtained relations and (ii) apply these results in order to obtain inequalities on H, χ_{-2}, MZ, ID and R for graphs in Erdős-Rényi models.

We would like to add that our analytical results, even though focused on H, χ_{-2},

[1]It is important to mention that the statistical results for $R(G)$ were already reported in [28]. However, we decided to include them here to provide a complete overview.

MZ, ID and R, are not restricted to them. In fact, we are also reporting results relating these indices with other topological indices of interest: the forgotten index $F(G)$ (see Theorem 7), the Albertson index $Alb(G)$ (see Theorems 7 and 8), the general sum-connectivity index $\chi_\alpha(G)$ (see Theorems 7 and 8), the variable second Zagreb index $M_2^\alpha(G)$ (see Theorems 16 and 24), the inverse sum indeg index $ISI(G)$ (see Theorem 20), the Platt number $P(G)$ (see Proposition 21) and the multiplicative sum-Zagreb index Π_1^* (see Theorem 22).

We hope that our study may motivate the use of topological indices in studies of random graphs but also in studies of generic *sparse* random matrix models.

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