AIMS Mathematics

http://www.aimspress.com/journal/Math

AIMS Mathematics, 9(2): 3646–3670.
DOI: 10.3934/math.2024179
Received: 20 September 2023
Revised: 21 December 2023
Accepted: 25 December 2023
Published: 09 January 2024

Research article

Multiplicative topological indices: Analytical properties and application to random networks

R. Aguilar-Sánchez[1], **J. A. Mendez-Bermudez**[2], **José M. Rodríguez**[3,*] **and José M. Sigarreta**[4]

[1] Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla, Puebla 72570, Mexico

[2] Instituto de Física, Benemérita Universidad Autónoma de Puebla, Puebla 72570, Mexico

[3] Departamento de Matemáticas, Universidad Carlos III de Madrid, Avenida de la Universidad 30, Leganés, Madrid 28911, Spain

[4] Facultad de Matemáticas, Universidad Autónoma de Guerrero, Carlos E. Adame No. 54 Col. Garita, Acapulco, Guerrero 610101, Mexico

* **Correspondence:** Email: jomaro@math.uc3m.es.

Abstract: We consider two general classes of multiplicative degree-based topological indices (MTIs), denoted by $X_{\Pi,F_V}(G) = \prod_{u\in V(G)} F_V(d_u)$ and $X_{\Pi,F_E}(G) = \prod_{uv\in E(G)} F_E(d_u, d_v)$, where uv indicates the edge of G connecting the vertices u and v, d_u is the degree of the vertex u, and $F_V(x)$ and $F_E(x, y)$ are functions of the vertex degrees. This work has three objectives: First, we follow an analytical approach to deal with a classical topic in the study of topological indices: to find inequalities that relate two MTIs between them, but also to their additive versions $X_\Sigma(G)$. Second, we propose some statistical analysis of MTIs as a generic tool for studying average properties of random networks, extending these techniques for the first time to the context of MTIs. Finally, we perform an innovative scaling analysis of MTIs which allows us to state a scaling law that relates different random graph models.

Keywords: multiplicative topological index; degree-based topological index; random graphs
Mathematics Subject Classification: 05C50, 05C80, 05C92, 60B20

1. Introduction

We can identify two types of graph invariants which are currently being studied in chemical graph theory. Namely,

$$X_\Sigma(G) = X_{\Sigma,F_V}(G) = \sum_{u\in V(G)} F_V(d_u) \qquad \text{or}$$
$$X_\Sigma(G) = X_{\Sigma,F_E}(G) = \sum_{uv\in E(G)} F_E(d_u, d_v) \tag{1.1}$$

and

$$X_\Pi(G) = X_{\Pi,F_V}(G) = \prod_{u\in V(G)} F_V(d_u) \qquad \text{or}$$
$$X_\Pi(G) = X_{\Pi,F_E}(G) = \prod_{uv\in E(G)} F_E(d_u, d_v)\,. \tag{1.2}$$

Here, uv denotes the edge of the graph $G = (V(G), E(G))$ connecting the vertices u and v, d_u is the degree of the vertex u, and $F_V(x)$ and $F_E(x, y)$ are appropriately defined functions (see e.g., [1]). Since $X_\Sigma(G)$ and $X_\Pi(G)$ are usually known as topological indices in the literature, here we will refer to $X_\Pi(G)$ as multiplicative topological indices (MTIs) to make a clear difference between both types of indices.

Among the vast amount of topological indices of the form $X_\Sigma(G)$, the first and second Zagreb indices [2] stand out, and they are defined as

$$M_1(G) = \sum_{u\in V(G)} d_u^2 = \sum_{uv\in E(G)} (d_u + d_v) \tag{1.3}$$

and

$$M_2(G) = \sum_{uv\in E(G)} d_u d_v, \tag{1.4}$$

respectively. Also, the Randić connectivity index [3]

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}\,, \tag{1.5}$$

the harmonic index [4]

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v}\,, \tag{1.6}$$

the sum-connectivity index [5]

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}\,, \tag{1.7}$$

and the inverse degree index [4]

$$ID(G) = \sum_{u\in V(G)} \frac{1}{d_u} = \sum_{uv\in E(G)} \left(\frac{1}{d_u^2} + \frac{1}{d_v^2}\right). \tag{1.8}$$

The topological indices mentioned above and many others of the form $X_\Sigma(G)$ have been widely studied during recent decades.

More recently, MTIs have attracted a lot of attention, see e.g., [6–12]. Indeed, several MTIs have already been deeply analyzed in the literature (see e.g., the work of V. R. Kulli). Among the most relevant ones, the Narumi-Katayama index [13] should be mentioned:

$$NK(G) = \prod_{u\in V(G)} d_u. \tag{1.9}$$

Additionally, multiplicative versions of the Zagreb indices [14]

$$\Pi_1(G) = \prod_{u\in V(G)} d_u^2, \tag{1.10}$$

$$\Pi_2(G) = \prod_{uv\in E(G)} d_u d_v \tag{1.11}$$

and

$$\Pi_1^*(G) = \prod_{uv\in E(G)} (d_u + d_v). \tag{1.12}$$

In addition to the MTIs of Eqs (1.9)–(1.12), in this work we also consider multiplicative versions of the indices in Eqs (1.5)–(1.8): the multiplicative Randić connectivity index

$$R_\Pi(G) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}, \tag{1.13}$$

the multiplicative harmonic index

$$H_\Pi(G) = \prod_{uv\in E(G)} \frac{2}{d_u + d_v}, \tag{1.14}$$

the multiplicative sum-connectivity index

$$\chi_\Pi(G) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}, \tag{1.15}$$

and the multiplicative inverse degree index

$$ID_\Pi(G) = \prod_{uv\in E(G)} \left(\frac{1}{d_u^2} + \frac{1}{d_v^2}\right). \tag{1.16}$$

Therefore, motivated by their potential applications, in this work we perform an analytical as well as computational study of MTIs. Specifically, the purpose of this work is threefold:

First, we follow an analytical viewpoint to find several new inequalities that relate two MTIs indices between them as well as to their additive versions in Section 2. Note that the search for inequalities between different indices is a classical topic in the study of topological indices. See e.g., [6–12] for previous results relating MTIs.

Second, we want to establish the statistical analysis of MTIs as a generic tool for the study of average properties of random networks in Section 3. For some previous works dealing with the statistical analysis of (non-multiplicative) topological indices, see, e.g., [15–19].

Finally, in this paper we perform for the first time (to our knowledge) a scaling study of MTIs on random networks which let us state a scaling law that relates different random graph models in Section 4.

2. Inequalities involving multiplicative topological indices

There are many works studying particular MTIs; see, e.g., [20, 21] and the references therein. However, in this section we obtain several analytical inequalities involving the general MTIs $X_{\Pi,F_V}(G)$ and $X_{\Pi,F_E}(G)$.

The following equalities are direct:

$$X_{\Pi,F_V}(G) = \prod_{u\in V(G)} F_V(d_u) = e^{\sum_{u\in V(G)} \log F_V(d_u)} = e^{X_{\Sigma,\log F_V}(G)},$$
$$X_{\Pi,F_E}(G) = \prod_{uv\in E(G)} F_E(d_u, d_v) = e^{\sum_{uv\in E(G)} \log F_E(d_u,d_v)} = e^{X_{\Sigma,\log F_E}(G)}.$$

Since the geometric mean is at most the arithmetic mean (by Jensen's inequality), we have the following inequalities.

Proposition 2.1. *Let G be a graph with n vertices and m edges. Then,*

$$X_{\Pi,F_V}(G)^{1/n} \le \frac{1}{n} X_{\Sigma,F_V}(G), \qquad X_{\Pi,F_E}(G)^{1/m} \le \frac{1}{m} X_{\Sigma,F_E}(G).$$

This general result has as a particular consequence the following known inequality, see [9, Theorem 2.1].

Corollary 2.1. *Let G be a graph with n vertices and m edges. Then,*

$$\Pi_1(G) \le \Big(\frac{2m}{n}\Big)^{2n}.$$

Proof. If we take $F_V(d_u) = d_u$, then

$$X_{\Pi,F_V}(G) = \Pi_1(G)^{1/2}, \qquad X_{\Sigma,F_V}(G) = 2m,$$

and Proposition 2.1 gives

$$\Pi_1(G)^{1/(2n)} \le \frac{2m}{n},$$

which implies the desired inequality. □

Proposition 2.1 has several consequences:

Proposition 2.2. *Let G be a graph with n vertices and m edges.*

(1) *If $F_E(d_u, d_v) = h(d_u) + h(d_v)$ and $F_V(d_u) = d_u h(d_u)$ for some function h, then*

$$X_{\Pi,F_V}(G)^{1/n} \le \frac{1}{n} X_{\Sigma,F_E}(G), \qquad X_{\Pi,F_E}(G)^{1/m} \le \frac{1}{m} X_{\Sigma,F_V}(G).$$

(2) *If $F_E(d_u, d_v) = h(d_u)h(d_v)$ and $F_V(d_u) = h(d_u)^{d_u}$ for some function h, then*

$$X_{\Pi,F_E}(G)^{1/n} \le \frac{1}{n} X_{\Sigma,F_V}(G), \qquad X_{\Pi,F_V}(G)^{1/m} \le \frac{1}{m} X_{\Sigma,F_E}(G).$$

Proof. Let G be a graph with n vertices and m edges.

If $F_E(d_u, d_v) = h(d_u) + h(d_v)$ and $F_V(d_u) = d_u h(d_u)$ for some function h, then

$$\begin{aligned} X_{\Sigma,F_E}(G) &= \sum_{uv\in E(G)} F_E(d_u, d_v) = \sum_{uv\in E(G)} (h(d_u) + h(d_v)) \\ &= \sum_{u\in V(G)} d_u h(d_u) = X_{\Sigma,F_V}(G). \end{aligned}$$

Consequently, Proposition 2.1 implies

$$\begin{aligned} X_{\Pi,F_V}(G)^{1/n} &\le \frac{1}{n} X_{\Sigma,F_V}(G) = \frac{1}{n} X_{\Sigma,F_E}(G), \\ X_{\Pi,F_E}(G)^{1/m} &\le \frac{1}{m} X_{\Sigma,F_E}(G) = \frac{1}{m} X_{\Sigma,F_V}(G). \end{aligned}$$

If $F_E(d_u, d_v) = h(d_u)h(d_v)$ and $F_V(d_u) = h(d_u)^{d_u}$ for some function h, then

$$\begin{aligned} X_{\Pi,F_E}(G) &= \prod_{uv\in E(G)} F_E(d_u, d_v) = \prod_{uv\in E(G)} h(d_u)h(d_v) \\ &= \prod_{u\in V(G)} h(d_u)^{d_u} = X_{\Pi,F_V}(G). \end{aligned}$$

Hence, Proposition 2.1 gives

$$\begin{aligned} X_{\Pi,F_E}(G)^{1/n} = X_{\Pi,F_V}(G)^{1/n} &\le \frac{1}{n} X_{\Sigma,F_V}(G), \\ X_{\Pi,F_V}(G)^{1/m} = X_{\Pi,F_E}(G)^{1/m} &\le \frac{1}{m} X_{\Sigma,F_E}(G). \end{aligned}$$

□

Theorem 2.1. *Let G be a graph with m edges. Assume that $F_1(d_u, d_v) = h(d_u) + h(d_v)$ and $F_2(d_u, d_v) = h(d_u)h(d_v)$ for some function h. Then,*

$$X_{\Pi,F_2}(G) \le \Big(\frac{1}{2m} X_{\Sigma,F_1}(G)\Big)^{2m}.$$

Proof. Since the (weighted) geometric mean is at most the (weighted) arithmetic mean (by Jensen's inequality), the following inequality holds for every $x_i, w_i > 0$:

$$\Big(\prod_{i=1}^{n} x_i^{w_i}\Big)^{1/\sum_{i=1}^{n} w_i} \le \frac{1}{\sum_{i=1}^{n} w_i} \sum_{i=1}^{n} x_i\, w_i.$$

If we take $x_i = h(d_u)$ and $w_i = d_u$, then we get

$$\begin{aligned} \Big(\prod_{u\in V(G)} h(d_u)^{d_u}\Big)^{1/\sum_{u\in E(G)} d_u} &\le \frac{1}{\sum_{u\in V(G)} d_u} \sum_{u\in V(G)} d_u h(d_u), \\ \Big(\prod_{uv\in E(G)} h(d_u)h(d_v)\Big)^{1/(2m)} &\le \frac{1}{2m} \sum_{uv\in E(G)} (h(d_u) + h(d_v)), \\ X_{\Pi,F_2}(G) &\le \Big(\frac{1}{2m} X_{\Sigma,F_1}(G)\Big)^{2m}. \end{aligned}$$

□

This general result has as a particular consequence the following known inequality, see [9, Theorem 3.1].

Corollary 2.2. *Let G be a graph with m edges. Then,*

$$\Pi_2(G) \le \Big(\frac{1}{2m}\, M_1(G)\Big)^{2m}.$$

Proof. If we take $h(x) = x$, then $F_1(d_u, d_v) = d_u + d_v$, $F_2(d_u, d_v) = d_u d_v$, $X_{\Pi,F_2}(G) = \Pi_2(G)$, $X_{\Sigma,F_1}(G) = M_1(G)$, and Theorem 2.1 gives the desired inequality. □

In [22] appears the following Jensen-type inequality.

Theorem 2.2. *Let μ be a probability measure on the space X and $a \le b$ be real constants. If $f : X \to [a, b]$ is a measurable function and φ is a convex function on $[a, b]$, then f and $\varphi \circ f$ are μ-integrable functions, and*

$$\varphi\Big(a + b - \int_X f\, d\mu\Big) \le \varphi(a) + \varphi(b) - \int_X \varphi \circ f\, d\mu.$$

Theorem 2.2 allows one to find the following converse of Proposition 2.1, if we consider the normalized counting measure as μ.

Theorem 2.3. *Let G be a graph with n vertices and m edges, $a_V \le b_V$, $a_E \le b_E$ be real constants, and F_V, F_E be functions satisfying*

$$a_V \le F_V(d_u) \le b_V \quad \forall\, u \in V(G), \qquad a_E \le F_E(d_u, d_v) \le b_E \quad \forall\, uv \in E(G).$$

Then,

$$\frac{1}{n}\, X_{\Sigma,F_V}(G) \le e^{a_V} + e^{b_V} - e^{a_V+b_V} X_{\Pi,F_V}(G)^{-1/n},$$
$$\frac{1}{m}\, X_{\Sigma,F_E}(G) \le e^{a_E} + e^{b_E} - e^{a_E+b_E} X_{\Pi,F_E}(G)^{-1/m}.$$

Proof. Since $\varphi(x) = e^x$ is a convex function on $\mathbb{R}$, Theorem 2.2 gives

$$e^{a_V+b_V-\frac{1}{n}\sum_{u\in V(G)} \log F_V(d_u)} \le e^{a_V} + e^{b_V} - \frac{1}{n} \sum_{u\in V(G)} e^{\log F_V(d_u)},$$
$$e^{a_V+b_V} e^{\log(\Pi_{u\in V(G)} F_V(d_u))^{-1/n}} \le e^{a_V} + e^{b_V} - \frac{1}{n} \sum_{u\in V(G)} F_V(d_u),$$
$$e^{a_V+b_V} X_{\Pi,F_V}(G)^{-1/n} \le e^{a_V} + e^{b_V} - \frac{1}{n}\, X_{\Sigma,F_V}(G).$$

In a similar way,

$$e^{a_E+b_E-\frac{1}{m}\sum_{uv\in E(G)} \log F_E(d_u,d_v)} \le e^{a_E} + e^{b_E} - \frac{1}{m} \sum_{uv\in E(G)} e^{\log F_E(d_u,d_v)},$$
$$e^{a_E+b_E} e^{\log(\Pi_{uv\in E(G)} F_E(d_u,d_v))^{-1/m}} \le e^{a_E} + e^{b_E} - \frac{1}{m} \sum_{uv\in E(G)} F_E(d_u, d_v),$$
$$e^{a_E+b_E} X_{\Pi,F_E}(G)^{-1/m} \le e^{a_E} + e^{b_E} - \frac{1}{m}\, X_{\Sigma,F_E}(G).$$

□

Theorem 2.3 provides the following new lower bounds of Π_1 and Π_1^*.

Corollary 2.3. *Let G be a graph with n vertices and m edges, minimum degree δ, and maximum degree Δ. Then,*

$$\Pi_1(G) \ge \Big(e^{-\delta^2} + e^{-\Delta^2} - \frac{e^{-\delta^2-\Delta^2}}{n} M_1(G)\Big)^{-n},$$
$$\Pi_1^*(G) \ge \Big(e^{-2\delta} + e^{-2\Delta} - \frac{e^{-2\delta-2\Delta}}{m} M_1(G)\Big)^{-m}.$$

Proof. Since $\delta^2 \le d_u^2 \le \Delta^2$ and $2\delta \le d_u + d_v \le 2\Delta$, Theorem 2.3 implies

$$\frac{1}{n} M_1(G) \le e^{\delta^2} + e^{\Delta^2} - e^{\delta^2+\Delta^2} \Pi_1(G)^{-1/n},$$
$$\Pi_1(G) \ge \Big(e^{-\delta^2} + e^{-\Delta^2} - \frac{e^{-\delta^2-\Delta^2}}{n} M_1(G)\Big)^{-n},$$
$$\frac{1}{m} M_1(G) \le e^{2\delta} + e^{2\Delta} - e^{2\delta+2\Delta} \Pi_1^*(G)^{-1/m},$$
$$\Pi_1^*(G) \ge \Big(e^{-2\delta} + e^{-2\Delta} - \frac{e^{-2\delta-2\Delta}}{m} M_1(G)\Big)^{-m}.$$

□

The following Kober's inequalities in [23] (see also [24, Lemma 1]) are useful.

Lemma 2.1. *If $a_j > 0$ for $1 \le j \le k$, then*

$$\sum_{j=1}^{k} a_j + k(k-1)\Big(\prod_{j=1}^{k} a_j\Big)^{1/k} \le \Big(\sum_{j=1}^{k} \sqrt{a_j}\Big)^2 \le (k-1) \sum_{j=1}^{k} a_j + k\Big(\prod_{j=1}^{k} a_j\Big)^{1/k}.$$

Lemma 2.1 has the following consequence.

Theorem 2.4. *Let G be a graph with n vertices and m edges. Then,*

$$X_{\Sigma,F_V^2}(G) + n(n-1)X_{\Pi,F_V}(G)^{2/n} \le X_{\Sigma,F_V}(G)^2 \le (n-1)X_{\Sigma,F_V^2}(G) + nX_{\Pi,F_V}(G)^{2/n},$$
$$X_{\Sigma,F_E^2}(G) + m(m-1)X_{\Pi,F_E}(G)^{2/m} \le X_{\Sigma,F_E}(G)^2 \le (m-1)X_{\Sigma,F_E^2}(G) + mX_{\Pi,F_E}(G)^{2/m}.$$

Proof. Lemma 2.1 gives

$$\sum_{u\in V(G)} F_V(d_u)^2 + n(n-1)\Big(\prod_{u\in V(G)} F_V(d_u)^2\Big)^{1/n} \le \Big(\sum_{u\in V(G)} F_V(d_u)\Big)^2,$$
$$X_{\Sigma,F_V^2}(G) + n(n-1)X_{\Pi,F_V}(G)^{2/n} \le X_{\Sigma,F_V}(G)^2,$$

and

$$\Big(\sum_{u\in V(G)} F_V(d_u)\Big)^2 \le (n-1) \sum_{u\in V(G)} F_V(d_u)^2 + n\Big(\prod_{u\in V(G)} F_V(d_u)^2\Big)^{1/n},$$
$$X_{\Sigma,F_V}(G)^2 \le (n-1)X_{\Sigma,F_V^2}(G) + nX_{\Pi,F_V}(G)^{2/n}.$$

In a similar way, replacing $F_V(d_u)$ and n with $F_E(d_u, d_v)$ and m, respectively, we obtain

$$\sum_{uv\in E(G)} F_E(d_u, d_v)^2 + m(m-1)\Big(\prod_{uv\in E(G)} F_E(d_u, d_v)^2\Big)^{1/m} \le \Big(\sum_{uv\in E(G)} F_E(d_u, d_v)\Big)^2,$$
$$X_{\Sigma,F_E^2}(G) + m(m-1)X_{\Pi,F_E}(G)^{2/m} \le X_{\Sigma,F_E}(G)^2,$$

and

$$\Big(\sum_{uv\in E(G)} F_E(d_u, d_v)\Big)^2 \le (m-1)\sum_{uv\in E(G)} F_E(d_u, d_v)^2 + m\Big(\prod_{uv\in E(G)} F_E(d_u, d_v)^2\Big)^{1/m},$$
$$X_{\Sigma,F_E}(G)^2 \le (m-1)X_{\Sigma,F_E^2}(G) + mX_{\Pi,F_E}(G)^{2/m}.$$

□

Let us recall the following known Petrović inequality [25].

Theorem 2.5. *Let φ be a convex function on $[0, a]$, and $w_1, \dots, w_n \ge 0$. If $t_1, \dots, t_n \in [0, a]$ satisfy $\sum_{k=1}^n t_k w_k \in (0, a]$, and*

$$\sum_{k=1}^{n} t_k w_k \ge t_j, \qquad j = 1, \dots, n,$$

then

$$\sum_{k=1}^{n} \varphi(t_k) w_k \le \varphi\Big(\sum_{k=1}^{n} t_k w_k\Big) + \Big(\sum_{k=1}^{n} w_k - 1\Big)\varphi(0).$$

Theorem 2.5 has the following consequence.

Proposition 2.3. *Let φ be a convex function on $[0, a]$. If $t_1, \dots, t_n \in [0, a]$ satisfy $\sum_{k=1}^n t_k \in (0, a]$, then*

$$\sum_{k=1}^{n} \varphi(t_k) \le \varphi\Big(\sum_{k=1}^{n} t_k\Big) + (n-1)\varphi(0).$$

Proposition 2.3 allows for the proof of the following inequalities.

Theorem 2.6. *Let G be a graph with n vertices and m edges. Then,*

$$X_{\Sigma,F_V}(G) \le X_{\Pi,F_V}(G) + n - 1, \quad X_{\Sigma,F_E}(G) \le X_{\Pi,F_E}(G) + m - 1.$$

Proof. Let us consider the convex function $\varphi(x) = e^x$. Proposition 2.3 gives

$$\begin{aligned} X_{\Sigma,F_V}(G) &= \sum_{u\in V(G)} F_V(d_u) = \sum_{u\in V(G)} e^{\log F_V(d_u)} \\ &\le e^{\sum_{u\in V(G)} \log F_V(d_u)} + n - 1 = e^{\log \prod_{u\in V(G)} F_V(d_u)} + n - 1 \\ &= \prod\nolimits_{u\in V(G)} F_V(d_u) + n - 1 = X_{\Pi,F_V}(G) + n - 1. \end{aligned}$$

In a similar way,

$$\begin{aligned} X_{\Sigma,F_E}(G) &= \sum_{uv\in E(G)} F_E(d_u, d_v) = \sum_{uv\in E(G)} e^{\log F_E(d_u,d_v)} \\ &\le e^{\sum_{uv\in E(G)} \log F_E(d_u,d_v)} + m - 1 = e^{\log \prod_{uv\in E(G)} F_E(d_u,d_v)} + m - 1 \\ &= \prod\nolimits_{uv\in E(G)} F_E(d_u, d_v) + m - 1 = X_{\Pi,F_E}(G) + m - 1. \end{aligned}$$

□

Theorem 2.7. *Let G be a graph. Then,*

$$X_{\Pi,F_V}(G) \geq X_{\Sigma,\log F_V}(G) + 1, \qquad X_{\Pi,F_E}(G) \geq X_{\Sigma,\log F_E}(G) + 1.$$

Proof. The equality $e^x \geq x + 1$ holds for every $x \in \mathbb{R}$. This inequality gives

$$\begin{aligned} X_{\Pi,F_V}(G) &= e^{\log X_{\Pi,F_V}(G)} \geq \log X_{\Pi,F_V}(G) + 1 \\ &= \log\Big(\Pi_{u\in E(G)} F_V(d_u)\Big) + 1 = \sum_{u\in E(G)} \log F_V(d_u) + 1 \\ &= X_{\Sigma,\log F_V}(G) + 1. \end{aligned}$$

The same argument gives the second inequality. □

In [26], the Gutman-Milovanović index is defined as

$$M_{\alpha,\beta}(G) = \sum_{uv\in E(G)} (d_u d_v)^{\alpha} (d_u + d_v)^{\beta},$$

which is a natural generalization of Zagreb indices.

Next, we present an inequality relating some multiplicative indices and the Gutman-Milovanović index.

Theorem 2.8. *Let G be a graph with m edges, and $\alpha, \beta \in \mathbb{R}$. Then,*

$$M_{\alpha,\beta}(G) \geq m\, \Pi_2(G)^{\alpha/m}\, \Pi_1^*(G)^{\beta/m}.$$

The equality is attained for any α, β if G is regular.

Proof. Since the geometric mean is at most the arithmetic mean, we get

$$\begin{aligned} \frac{1}{m} M_{\alpha,\beta}(G) &= \frac{1}{m} \sum_{uv\in E(G)} (d_u d_v)^{\alpha} (d_u + d_v)^{\beta} \\ &\geq \Big(\prod_{uv\in E(G)} (d_u d_v)^{\alpha} (d_u + d_v)^{\beta} \Big)^{1/m} = \Pi_2(G)^{\alpha/m}\, \Pi_1^*(G)^{\beta/m}. \end{aligned}$$

Thus,

$$M_{\alpha,\beta}(G) \geq m\, \Pi_2(G)^{\alpha/m}\, \Pi_1^*(G)^{\beta/m}.$$

If the graph is δ-regular, then $M_{\alpha,\beta}(G) = 2^{\beta}\delta^{2\alpha+\beta} m$, $\Pi_2(G)^{\alpha/m} = (\delta^{2m})^{\alpha/m} = \delta^{2\alpha}$, $\Pi_1^*(G)^{\beta/m} = ((2\delta)^m)^{\beta/m} = 2^{\beta}\delta^{\beta}$, and the equality holds. □

We have some direct formulas for some multiplicative indices, e.g.,

$$\Pi_1(G) = NK(G)^2, \quad \Pi_2(G) = R_{\Pi}(G)^{-2},$$
$$\Pi_1^*(G) = 2^{-m} H_{\Pi}(G)^{-1}, \quad \Pi_1^*(G) = S_{\Pi}(G)^{-2}, \quad H_{\Pi}(G) = 2^m S_{\Pi}(G)^2,$$

for every graph G with m edges.

Let us show some inequalities relating different multiplicative indices.

Theorem 2.9. *Let G be a graph with m edges, maximum degree* Δ *and minimum degree* δ*. Then,*

$$\frac{2^m}{\Delta^m}\,\Pi_2(G) \le \Pi_1^*(G) \le \frac{2^m}{\delta^m}\,\Pi_2(G),$$
$$\Big(\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\Big)^m R_\Pi(G) \le H_\Pi(G) \le R_\Pi(G),$$
$$(2\delta^2)^m\,\Pi_2(G)^{-2} \le ID_\Pi(G) \le (2\Delta^2)^m\,\Pi_2(G)^{-2},$$
$$2^m\,\Pi_2(G)^{-1} \le ID_\Pi(G) \le \Big(\frac{\Delta^2+\delta^2}{\Delta\delta}\Big)^m\,\Pi_2(G)^{-1}.$$

Furthermore, the equality in each inequality is attained for every regular graph.

Proof. First of all, note that if

$$c \le \frac{F_E(x,y)^\alpha}{F'_E(x,y)^\beta} \le C$$

for every $\delta \le x, y \le \Delta$, then we have for every $uv \in E(G)$,

$$c\,F'_E(d_u,d_v)^\beta \le F_E(d_u,d_v)^\alpha \le C\,F'_E(d_u,d_v)^\beta,$$
$$c^m\Bigg(\prod_{uv\in E(G)} F'_E(d_u,d_v)\Bigg)^\beta \le \Bigg(\prod_{uv\in E(G)} F_E(d_u,d_v)\Bigg)^\alpha \le C^m\Bigg(\prod_{uv\in E(G)} F'_E(d_u,d_v)\Bigg)^\beta,$$
$$c^m X_{\Pi,F'_E}(G)^\beta \le X_{\Pi,F_E}(G)^\alpha \le C^m X_{\Pi,F'_E}(G)^\beta,$$

for every graph G with m edges, maximum degree Δ, and minimum degree δ.

Since

$$\frac{2}{\Delta} \le \frac{1}{x} + \frac{1}{y} = \frac{x+y}{xy} \le \frac{2}{\delta}\,,$$

we have

$$\frac{2^m}{\Delta^m}\,\Pi_2(G) \le \Pi_1^*(G) \le \frac{2^m}{\delta^m}\,\Pi_2(G).$$

Since

$$\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \le \frac{2\sqrt{xy}}{x+y} = \frac{\frac{2}{x+y}}{\frac{1}{\sqrt{xy}}} \le 1,$$

we have

$$\Big(\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\Big)^m R_\Pi(G) \le H_\Pi(G) \le R_\Pi(G).$$

Since

$$2\delta^2 \le x^2 + y^2 = \frac{\frac{1}{x^2}+\frac{1}{y^2}}{(xy)^{-2}} \le 2\Delta^2,$$

we have

$$(2\delta^2)^m\,\Pi_2(G)^{-2} \le ID_\Pi(G) \le (2\Delta^2)^m\,\Pi_2(G)^{-2}.$$

Let us consider the function

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

where

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

Since

$$f'(t) = 1 - \frac{1}{t^2} = \frac{t^2 - 1}{t^2}$$

f is decreasing on $(0, 1]$ and increasing on $[1, \infty)$. Since $f(1) = 2$, we conclude

$$2 \le A(x, y) \le \frac{\Delta^2 + \delta^2}{\Delta\delta}.$$

Hence,

$$2^m \, \Pi_2(G)^{-1} \le ID_\Pi(G) \le \Big(\frac{\Delta^2 + \delta^2}{\Delta\delta} \Big)^m \, \Pi_2(G)^{-1}.$$

Let G be a δ-regular graph. Hence,

$$\begin{aligned} &\Pi_2(G) = \delta^{2m}, \quad \Pi_1^*(G) = (2\delta)^m, \\ &R_\Pi(G) = \delta^{-m}, \quad H_\Pi(G) = \delta^{-m}, \quad ID_\Pi(G) = 2^m \delta^{-2m}, \\ &\frac{2\sqrt{\Delta\delta}}{\Delta + \delta} = 1, \quad \frac{\Delta^2 + \delta^2}{\Delta\delta} = 2. \end{aligned}$$

Therefore, the equality in each inequality is attained for every regular graph. □

Recall that 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. We say that a graph is (Δ, δ)-biregular if we want to write explicitly the maximum and minimum degrees.

Theorem 2.10. *If G is a graph with m edges, minimum degree δ, and maximum degree Δ, then*

$$2^{3m} \, \Pi_1^*(G)^{-2} \le ID_\Pi(G) \le (\Delta + \delta)^{2m} (\Delta^{-2} + \delta^{-2})^m \, \Pi_1^*(G)^{-2}.$$

The equality in the lower bound is attained if and only if each connected component of G is a regular graph. The equality in the upper bound is attained if and only if G is a regular or biregular graph.

Proof. Define

$$A(x, y) := \frac{x^{-2} + y^{-2}}{(x + y)^{-2}} = (x + y)^2 (x^{-2} + y^{-2}),$$

for $x, y \in [\delta, \Delta]$. Note that, in order to find the bounds of A, it suffices to consider the case $y \ge x$. We have

$$\begin{aligned} \frac{\partial A}{\partial y}(x, y) &= 2(x + y)(x^{-2} + y^{-2}) - 2(x + y)^2 y^{-3} \\ &= 2x^{-2} y^{-3} (x + y)(y^3 + x^2 y - x^3 - x^2 y) \\ &= 2x^{-2} y^{-3} (x + y)(y^3 - x^3) > 0, \end{aligned}$$

for every $y \in (x, \Delta]$. Hence, $A(x, x) \le A(x, y) \le A(x, \Delta)$. Note that $A(x, x) = 8$.

Define

$$B(x) = A(x, \Delta) = (x + \Delta)^2 (x^{-2} + \Delta^{-2}),$$

for $x \in [\delta, \Delta]$. We get

$$B'(x) = 2\Delta^{-2}x^{-3}(x+\Delta)(x^3-\Delta^3) < 0,$$

for every $x \in [\delta, \Delta)$. Therefore,

$$A(x,\Delta) = B(x) \le B(\delta) = (\Delta+\delta)^2(\Delta^{-2}+\delta^{-2}),$$

for $x \in [\delta, \Delta]$. Hence,

$$8 \le A(x,y) \le (\Delta+\delta)^2(\Delta^{-2}+\delta^{-2}),$$

and so,

$$2^{3m}\,\Pi_1^*(G)^{-2} \le ID_\Pi(G) \le (\Delta+\delta)^{2m}(\Delta^{-2}+\delta^{-2})^m\,\Pi_1^*(G)^{-2}.$$

The previous argument gives that the equality in the lower bound is attained if and only if $d_u = d_v$ for every $uv \in E(G)$, and this happens if and only if each connected component of G is a regular graph.

Also, the equality in the upper bound is attained if and only if $\{d_u, d_v\} = \{\Delta, \delta\}$ for every $uv \in E(G)$, and this happens if and only if G is a regular (if $\Delta = \delta$) or (Δ, δ)-biregular (if $\Delta \ne \delta$) graph. □

3. Statistical properties of multiplicative topological indices on random networks

The statistical properties of topological indices in random networks have been intensively studied, see, e.g., [27, 28]. Within this statistical approach, it has been recently shown that the average values of indices of the type $X_\Sigma(G)$, normalized to the order of the network n, scale with the average degree $\langle d\rangle$, see, e.g., [15–18]. That is, $\langle X_\Sigma(G)\rangle/n$ is a function of $\langle d\rangle$ only. Moreover, it was also found that $\langle X_\Sigma(G)\rangle$, for indices like $R(G)$ and $H(G)$, is highly correlated with the Shannon entropy of the eigenvectors of the adjacency matrix of random networks [19]. This is a notable result because it puts forward the application of topological indices beyond mathematical chemistry. Specifically, given the equivalence of the Hamiltonian of a tight-binding network (in the proper setup) and the corresponding network adjacency matrix, either $\langle R(G)\rangle$ or $\langle H(G)\rangle$ could be used to determine the eigenvector localization and delocalization regimes which in turn determine the insulator and metallic regimes of quantum transport.

Below, for the first time to our knowledge, we apply the MTIs of Eqs (1.9)–(1.16) on three models of random networks: Erdös-Rényi (ER) networks, random geometric (RG) graphs, and bipartite random (BR) networks.

ER networks [29–31] $G_{\rm ER}(n, p)$ are formed by n vertices connected independently with probability $p \in [0, 1]$. While RG graphs [32, 33] $G_{\rm RG}(n, r)$ consist of n vertices uniformly and independently distributed on the unit square, where two vertices are connected by an edge if their Euclidean distance is less than or equal to the connection radius $r \in [0, \sqrt{2}]$. In addition, we examine BR networks $G_{\rm BR}(n_1, n_2, p)$ composed of two disjoint sets, set 1 and set 2, with n_1 and n_2 vertices each such that there are no adjacent vertices within the same set, being $n = n_1 + n_2$ the total number of vertices in the bipartite network. The vertices of the two sets are connected randomly with probability $p \in [0, 1]$.

3.1. Multiplicative topological indices on Erdös-Rényi random networks

Before computing MTIs on ER random networks, we note that in the dense limit, i.e., when $\langle d\rangle \gg 1$, we can approximate $d_u \approx d_v \approx \langle d\rangle$ in Eqs (1.9)–(1.16), with

$$\langle d\rangle = (n-1)p. \tag{3.1}$$

Thus, for example, when $np \gg 1$, we can approximate $NK_{\Pi}(G_{\text{ER}})$ as

$$NK(G_{\text{ER}}) = \prod_{u \in V(G)} d_u \approx \prod_{u \in V(G)} \langle d \rangle \approx \langle d \rangle^n ,$$

which leads us to

$$\ln NK(G_{\text{ER}}) \approx n \ln \langle d \rangle$$

or

$$\frac{\ln NK(G_{\text{ER}})}{n} \approx \ln \langle d \rangle . \tag{3.2}$$

A similar approximation gives

$$\frac{\ln \Pi_1(G_{\text{ER}})}{n} \approx 2 \ln \langle d \rangle . \tag{3.3}$$

Also, for $\Pi_2(G_{\text{ER}})$, we have that

$$\Pi_2(G_{\text{ER}}) = \prod_{uv \in E(G)} d_u d_v \approx \prod_{uv \in E(G)} \langle d \rangle \langle d \rangle = \prod_{uv \in E(G)} \langle d \rangle^2 \approx \langle d \rangle^{n \langle d \rangle}$$

where we have used $| E(G_{\text{ER}}) |= n \langle d \rangle /2$. Therefore,

$$\ln \Pi_2(G_{\text{ER}}) \approx n \langle d \rangle \ln \langle d \rangle$$

or

$$\frac{\ln \Pi_2(G_{\text{ER}})}{n} \approx \langle d \rangle \ln \langle d \rangle . \tag{3.4}$$

Following this procedure, for the rest of the MTIs of Eqs (1.12)–(1.16) we get:

$$\frac{\ln \Pi_1^*(G_{\text{ER}})}{n} \approx \frac{1}{2} \langle d \rangle \ln(2 \langle d \rangle), \tag{3.5}$$

$$\frac{\ln R_{\Pi}(G_{\text{ER}})}{n} \approx -\frac{1}{2} \langle d \rangle \ln \langle d \rangle , \tag{3.6}$$

$$\frac{\ln H_{\Pi}(G_{\text{ER}})}{n} \approx -\frac{1}{2} \langle d \rangle \ln \langle d \rangle , \tag{3.7}$$

$$\frac{\ln \chi_{\Pi}(G_{\text{ER}})}{n} \approx -\frac{\ln 2}{4} \langle d \rangle - \frac{1}{4} \langle d \rangle \ln \langle d \rangle , \tag{3.8}$$

and

$$\frac{\ln ID_{\Pi}(G_{\text{ER}})}{n} \approx \frac{\ln 2}{2} \langle d \rangle - \langle d \rangle \ln \langle d \rangle . \tag{3.9}$$

From the approximate expressions above we note that the logarithm of the MTIs on ER random networks, normalized to the network size n, does not depend on n. That is, in the dense limit, we expect $\ln X_{\Pi}(G_{\text{ER}})/n$ to depend on $\langle d \rangle$ only; here, X_{Π} represents all the MTIs of Eqs (1.9)–(1.16).

With Eqs (3.2)–(3.9) as a guide, in what follows we compute the average values of the logarithm of the MTIs listed in Eqs (1.9)–(1.16). All averages are computed over ensembles of $10^7/n$ ER networks characterized by the parameter pair (n, p).

In Figure 1 we present the average logarithm of the eight MTIs of Eqs (1.9)–(1.16) as a function of the probability p of ER networks of sizes $n = \{125, 250, 500, 1000\}$. Since $\langle \ln X_{\Pi}(G_{\text{ER}}) \rangle < 0$, for R_{Π},

H_Π, and χ_Π we conveniently plotted $-\langle \ln X_\Pi(G_{ER})\rangle$ in log scale to have a detailed view of the data for small p, see Figure 1(e–g). Thus, we observe that $\langle \ln X_\Pi(G_{ER})\rangle$ for NK, $\Pi_{1,2}$, and Π_1^* [for R_Π, H_Π, and χ_Π] is a monotonically increasing [monotonically decreasing] function of p. In contrast, $\langle \ln ID_\Pi(G_{ER})\rangle$ is a nonmonotonic function of p, see Figure 1(h).

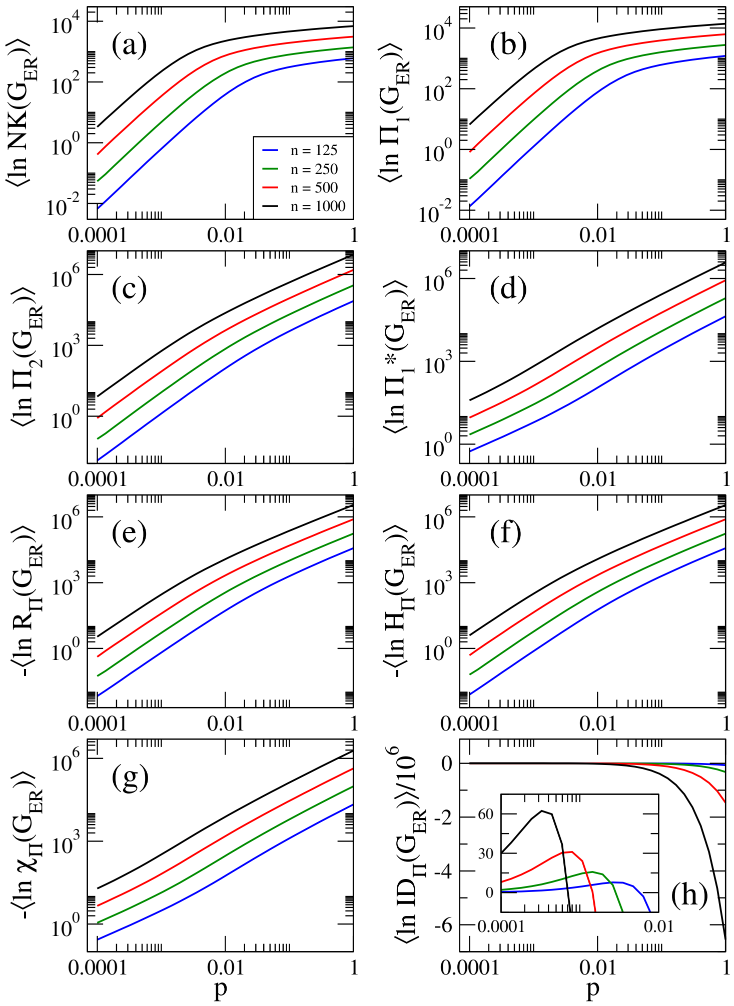

Figure 1. Average logarithm of the multiplicative topological indices of Eqs (1.9)–(1.16) as a function of the probability p of Erdös-Rényi networks of size n. The inset in (h) is an enlargement for small p.

Then, following Eqs (3.2)–(3.9), in Figure 2 we show again the average logarithm of the MTIs, but now normalized to the network size, $\langle \ln X_\Pi(G_{ER})\rangle /n$, as a function of $\langle d\rangle$. As can be clearly observed in this figure, the curves $\langle \ln X_\Pi(G_{ER})\rangle /n$ versus $\langle d\rangle$ fall one on top of the other for different network sizes; so, these indices are properly scaled where $\langle d\rangle$ works as the scaling parameter. That is, $\langle d\rangle$ is the parameter that fixes the average values of the normalized MTIs on ER networks. It is remarkable that the scaling of $\langle \ln X_\Pi(G_{ER})\rangle /n$ with $\langle d\rangle$, expected for $\langle d\rangle \gg 1$ according to Eqs (3.2)–(3.9), works perfectly well for all values of $\langle d\rangle$; even for $\langle d\rangle \ll 1$. Since the topological properties of random graphs and networks, when characterized by indices of the form $X_\Sigma(G)$, have been shown to scale with $\langle d\rangle$ for all values of $\langle d\rangle$ (see e.g., [15–19]), we should expect other topological measures to also scale with $\langle d\rangle$, such as the MTIs studied here. Also, in Figure 2, we show that Eqs (3.2)–(3.9) (orange-dashed lines) indeed describe well the data (thick full curves) for $\langle d \rangle \geq 10$, which can be regarded as the dense limit of the ER model.

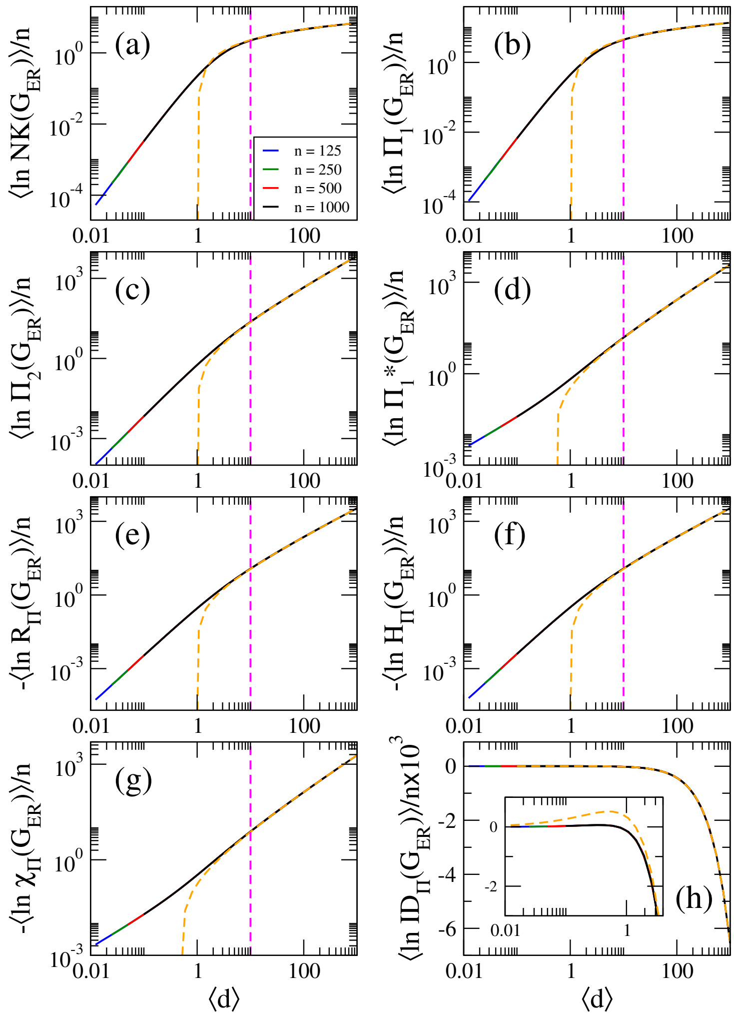

Figure 2. Average logarithm of the multiplicative topological indices of Eqs (1.9)–(1.16), normalized to the network size n, as a function of the average degree $\langle d \rangle$ of Erdös-Rényi networks. Orange dashed lines in (a-h) are Eqs (3.2)–(3.9), respectively. The vertical magenta dashed lines indicate $\langle d \rangle = 10$. The inset in (h) is an enlargement for small $\langle d \rangle$.

3.2. Multiplicative topological indices on random geometric graphs

As in the previous Subsection, here we start by exploring the dense limit. Indeed, for RG graphs in the dense limit, i.e., when $\langle d \rangle \gg 1$, we can approximate $d_u \approx d_v \approx \langle d \rangle$, where

$$\langle d \rangle = (n - 1)g(r) \tag{3.10}$$

and [34]

$$g(r) = \begin{cases} r^2\left[\pi - \frac{8}{3}r + \frac{1}{2}r^2\right], & 0 \le r \le 1\,, \\ \frac{1}{3} - 2r^2\left[1 - \arcsin(1/r) + \arccos(1/r)\right] & \\ \qquad +\frac{4}{3}(2r^2+1)\sqrt{r^2-1} - \frac{1}{2}r^4, & 1 \le r \le \sqrt{2}\,. \end{cases} \tag{3.11}$$

Thus, we obtain

$$\frac{\ln NK(G_{\mathrm{RG}})}{n} \approx \ln\langle d\rangle\,, \tag{3.12}$$

$$\frac{\ln \Pi_1(G_{\mathrm{RG}})}{n} \approx 2\ln\langle d\rangle\,, \tag{3.13}$$

$$\frac{\ln \Pi_2(G_{\mathrm{RG}})}{n} \approx \langle d\rangle\ln\langle d\rangle\,, \tag{3.14}$$

$$\frac{\ln \Pi_1^*(G_{\mathrm{RG}})}{n} \approx \frac{1}{2}\langle d\rangle\ln(2\langle d\rangle), \tag{3.15}$$

$$\frac{\ln R_\Pi(G_{\mathrm{RG}})}{n} \approx -\frac{1}{2}\langle d\rangle\ln\langle d\rangle\,, \tag{3.16}$$

$$\frac{\ln H_\Pi(G_{\mathrm{RG}})}{n} \approx -\frac{1}{2}\langle d\rangle\ln\langle d\rangle\,, \tag{3.17}$$

$$\frac{\ln \chi_\Pi(G_{\mathrm{RG}})}{n} \approx -\frac{\ln 2}{4}\langle d\rangle - \frac{1}{4}\langle d\rangle\ln\langle d\rangle\,, \tag{3.18}$$

and

$$\frac{\ln ID_\Pi(G_{\mathrm{RG}})}{n} \approx \frac{\ln 2}{2}\langle d\rangle - \langle d\rangle\ln\langle d\rangle\,. \tag{3.19}$$

Remarkably, the approximate Eqs (3.12)–(3.19) for RG graphs are exactly the same as the corresponding equations for ER graphs, see Eqs (3.2)–(3.9); however, note that the definition of $\langle d\rangle$ is different for both models, i.e., compare Eqs (3.1), (3.10), and (3.11).

Then, in Figure 3 we present the average logarithm of the eight MTIs of Eqs (1.9)–(1.16) as a function of the connection radius r of RG graphs of sizes $n = \{125, 250, 500, 1000\}$. All averages are computed over ensembles of $10^7/n$ random graphs, and each ensemble is characterized by a fixed parameter pair (n, r).

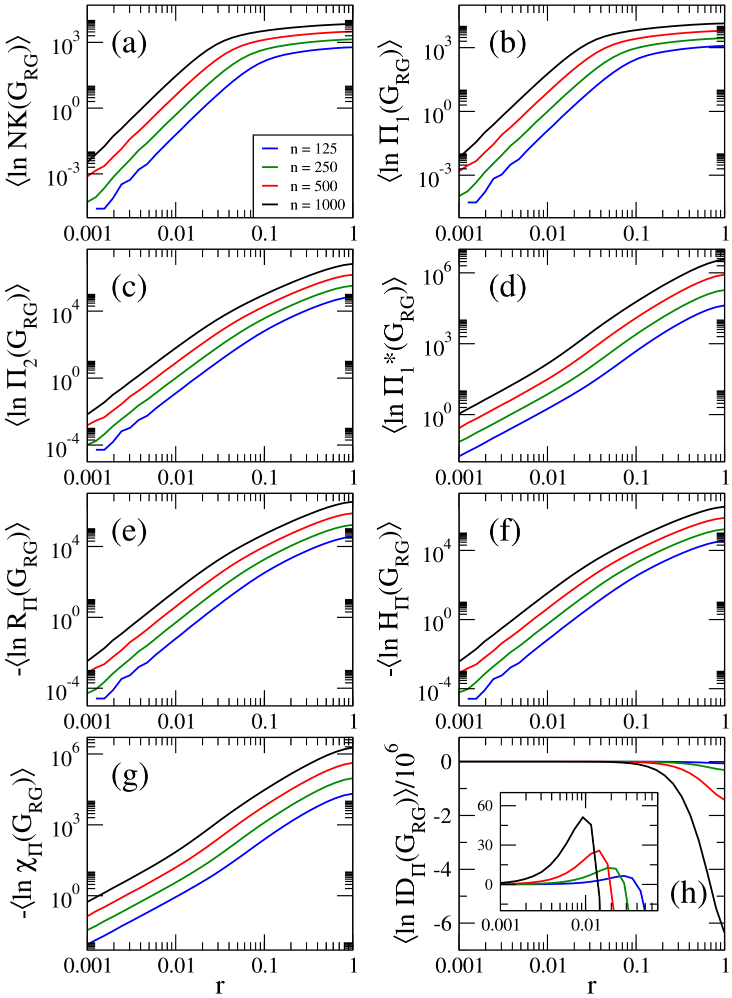

Figure 3. Average logarithm of the multiplicative topological indices of Eqs (1.9)–(1.16) as a function of the connection radius r of random geometric graphs of size n. The inset in (h) is an enlargement for small r.

For comparison purposes, Figure 1 for ER networks and Figure 3 for RG graphs have the same format and contents. In fact, all the observations made in the previous Subsection for ER networks are also valid for RG graphs by replacing $G_{\rm ER} \to G_{\rm RG}$ and $p \to g(r)$. Therefore, in Figure 4 we plot $\langle \ln X_\Pi(G_{\rm RG}) \rangle /n$ as a function of $\langle d \rangle$ showing that all curves are properly scaled; that is, curves for different graph sizes fall on top of each other. Also, in Figure 4 we show that Eqs (3.12)–(3.19) (orange-dashed lines) indeed describe the data well (thick full curves) for $\langle d \rangle \geq 10$, which can be regarded as the dense limit of RG graphs.

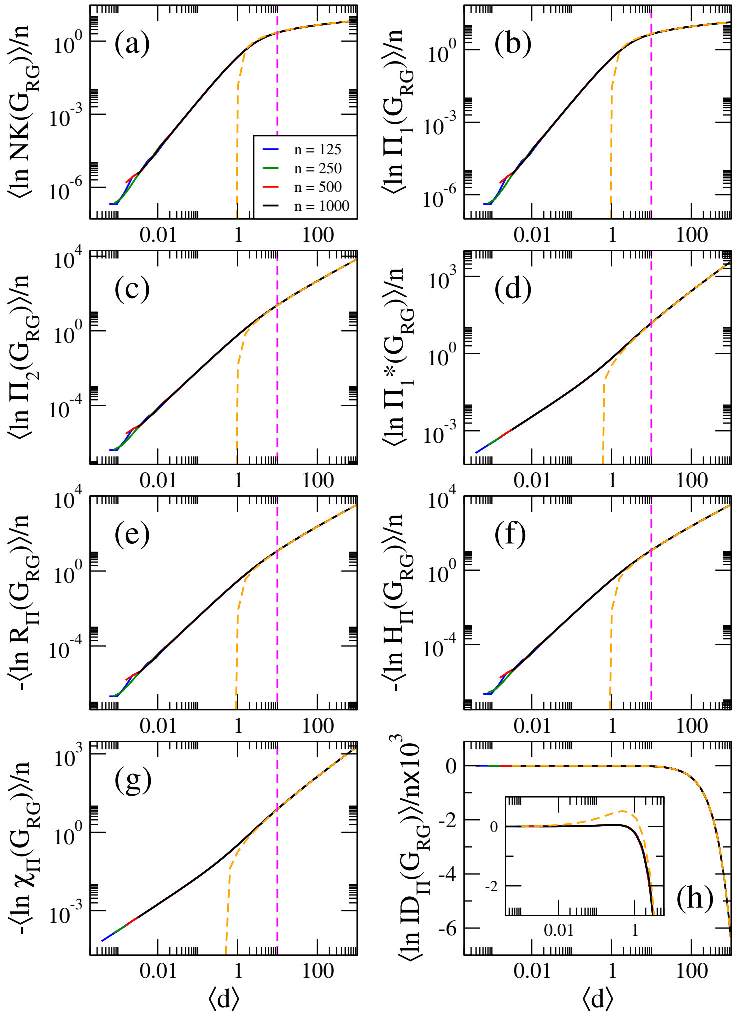

Figure 4. Average logarithm of the multiplicative topological indices of Eqs (1.9)–(1.16), normalized to the graph size n, as a function of the average degree $\langle d \rangle$ of random geometric graphs. Orange dashed lines in (a-h) are Eqs (3.12)–(3.19), respectively. The vertical magenta dashed lines indicate $\langle d \rangle = 10$. The inset in (h) is an enlargement for small $\langle d \rangle$.

3.3. Multiplicative topological indices on bipartite random networks

We start by writing approximate expressions for the MTIs on BR networks in the dense limit. Moreover, since edges in a bipartite network join vertices of different sets, and we are labeling here the sets as set 1 and set 2, we replace d_u by d_1 and d_v by d_2 in the expression for the MTIs. Thus, when $n_1 p \gg 1$ and $n_2 p \gg 1$, we can approximate $d_u = d_1 \approx \langle d_1 \rangle$ and $d_v = d_2 \approx \langle d_2 \rangle$ in Eqs (1.9)–(1.16), with

$$\langle d_{1,2} \rangle = n_{2,1} p. \tag{3.20}$$

Therefore, in the dense limit, the MTIs of Eqs (1.11)–(1.16) on BR networks are well approximated by

$$\frac{\ln \Pi_2(G_{\rm BR})}{n_{1,2}} \approx \langle d_{1,2} \rangle \ln(\langle d_1 \rangle \langle d_2 \rangle), \tag{3.21}$$

$$\frac{\ln \Pi_1^*(G_{\rm BR})}{n_{1,2}} \approx \langle d_{1,2}\rangle \ln(\langle d_1\rangle + \langle d_2\rangle), \tag{3.22}$$

$$\frac{\ln R_\Pi(G_{\rm BR})}{n_{1,2}} \approx -\frac{1}{2}\langle d_{1,2}\rangle \ln\left(\langle d_1\rangle \langle d_2\rangle\right), \tag{3.23}$$

$$\frac{\ln H_\Pi(G_{\rm BR})}{n_{1,2}} \approx \langle d_{1,2}\rangle \left[\ln 2 - \ln\left(\langle d_1\rangle + \langle d_2\rangle\right)\right], \tag{3.24}$$

$$\frac{\ln \chi_\Pi(G_{\rm BR})}{n_{1,2}} \approx -\frac{1}{2}\langle d_{1,2}\rangle \ln\left(\langle d_1\rangle + \langle d_2\rangle\right), \tag{3.25}$$

and

$$\frac{\ln ID_\Pi(G_{\rm BR})}{n_{1,2}} \approx \langle d_{1,2}\rangle \ln\left(\frac{1}{\langle d_1\rangle^2} + \frac{1}{\langle d_2\rangle^2}\right). \tag{3.26}$$

Above we used $\mid E(G_{\rm BR}) \mid = n_1 n_2 p = n_{1,2}\langle d_{1,2}\rangle$. We note that we are not providing approximate expressions for neither $NK(G_{\rm BR})$ nor $\Pi_1(G_{\rm BR})$.

Now we compute MTIs on ensembles of $10^7/n$ BR networks. In contrast to ER and RG networks, now the BR network ensembles are characterized by three parameters: n_1, n_2, and p. For simplicity, but without lost of generality, in our numerical calculations we consider $n_1 = n_2$. It is remarkable to notice that, in the case of $n_1 = n_2 = n/2$, where $\langle d_1\rangle = \langle d_2\rangle = \langle d\rangle = np/2$, Eqs (3.21)–(3.26) reproduce Eqs (3.4)–(3.9).

Then, in Figure 5 we present the average logarithm of the eight MTIs of Eqs (1.9)–(1.16) as a function of the probability p of BR networks of sizes $n_1 = n_2 = \{125, 250, 500, 1000\}$. Therefore, by plotting $\langle \ln X_\Pi(G_{\rm BR})\rangle / n$ as a function of $\langle d\rangle$ (see Figure 6), we confirm that the curves of the MTIs on BR networks are properly scaled, as predicted by Eqs (3.21)–(3.26); see the orange dashed lines in Figure 6 (c–h). Here, we can also say that $\langle d\rangle \geq 10$ can be regarded as de dense limit of BR networks. We have verified (not shown here) that we arrive at equivalent conclusions when $n_1 \neq n_2$.

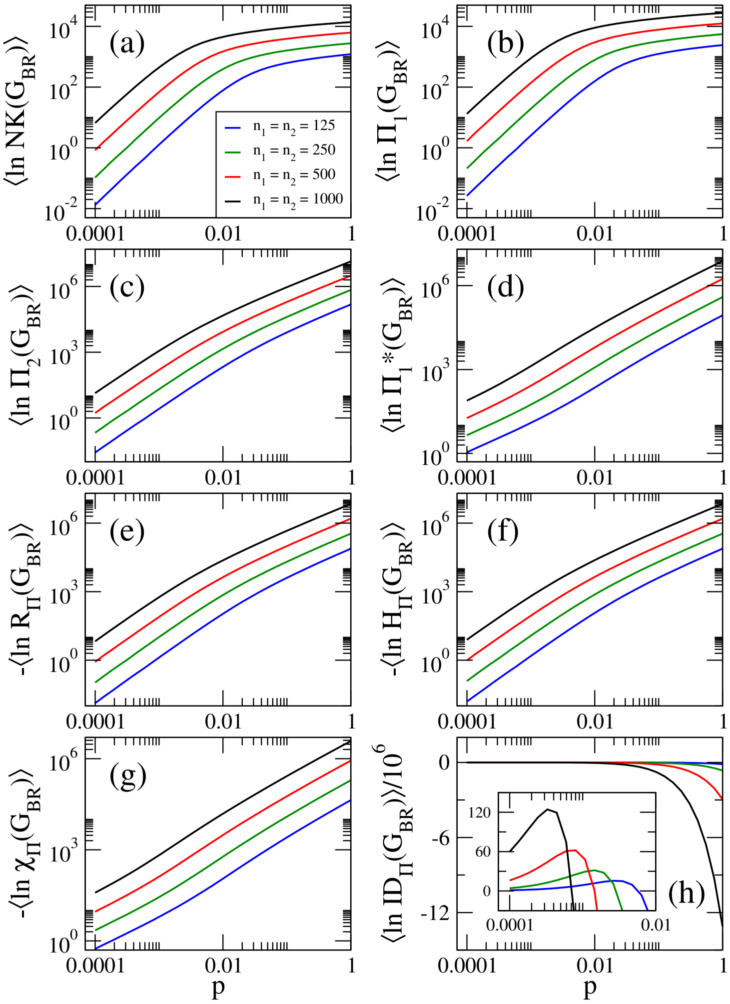

Figure 5. Average logarithm of the multiplicative topological indices of Eqs (1.9)–(1.16) as a function of the probability p of bipartite random networks of sizes n_1 and n_2. In all panels, $n_1 = n_2 = \{125, 250, 500, 1000\}$. The inset in (h) is an enlargement for small p.

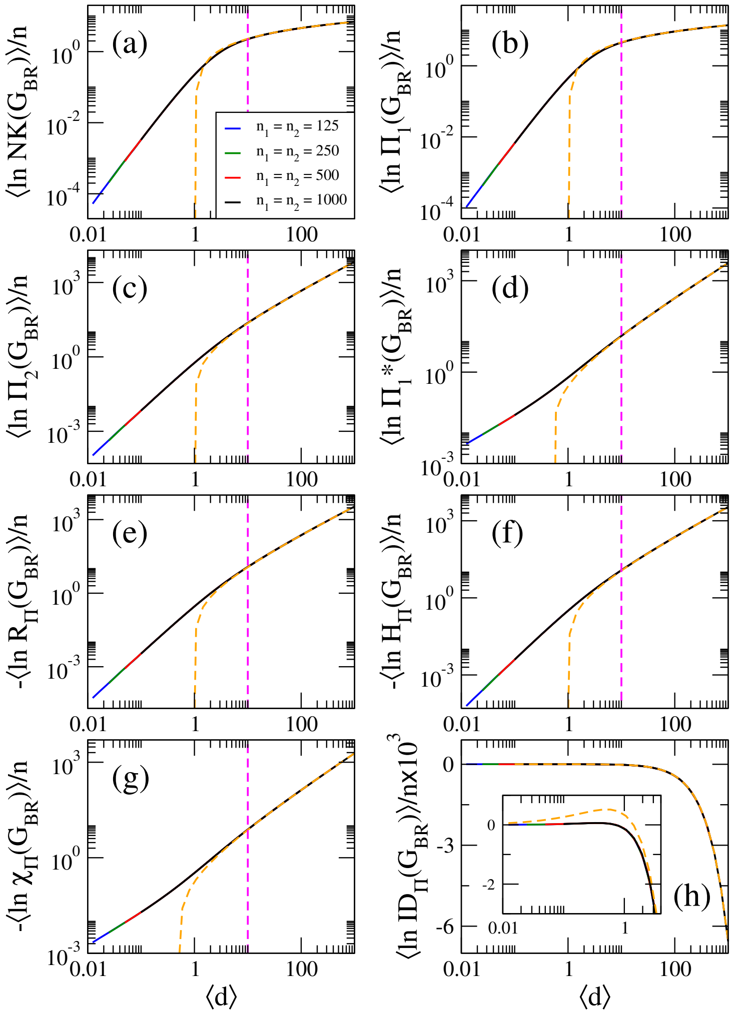

Figure 6. Average logarithm of the multiplicative topological indices of Eqs (1.9)–(1.16), normalized to the network size n, as a function of the average degree $\langle d \rangle$ of bipartite random networks of sizes n_1 and n_2. In all panels, $n_1 = n_2 = \{125, 250, 500, 1000\}$. Orange dashed lines in (a,b) are Eqs (3.2) and (3.3), respectively. Orange dashed lines in (c–h) are Eqs (3.21)–(3.26), respectively. The vertical magenta dashed lines indicate $\langle d \rangle = 10$. The inset in (h) is an enlargement for small $\langle d \rangle$.

Note that in panels (a,b) of Figure 6 we included Eqs (3.2) and (3.3) as orange dashed lines. Those equations were obtained for ER networks, however they reproduce perfectly well both $NK(G_{\rm BR})$ and $\Pi_1(G_{\rm BR})$ when $\langle d \rangle \geq 10$ since we are considering $n_1 = n_2 = n/2$.

4. Discussion and conclusions

In this work we have performed a thorough analytical and statistical study of multiplicative topological indices (MTIs) X_Π.

From an analytical viewpoint, we found several inequalities that relate MTIs among themselves as well as to their additive versions X_Σ. To find inequalities between different indices is a classical topic in the study of topological indices.

Within a statistical approach we computed MTIs on random networks. Some previous works deal with the statistical analysis of (non-multiplicative) topological indices. As models of random networks we have used Erdös-Rényi (ER) networks, random geometric (RG) graphs, and bipartite random (BR) networks. We showed that the average logarithm of the MTIs, $\langle \ln X_\Pi(G)\rangle$, normalized to the order of the network, scale with the network average degree $\langle d\rangle$. Thus, we conclude that $\langle d\rangle$ is the parameter that fixes the average values of the logarithm of the MTIs on random networks. Moreover, the equivalence among Eqs (3.2)–(3.9) for ER networks, Eqs (3.12)–(3.19) for RG graphs, and Eqs (3.21)–(3.26) for BR networks (when the subsets are equal in size) allows us to state a scaling law that connects the three graph models. That is, given the MTI X_Π, the average of its logarithm divided by the network size is the same function of the average degree regardless the network model:

$$\frac{\langle \ln X_\Pi(G_{\rm ER})\rangle}{n} \approx \frac{\langle \ln X_\Pi(G_{\rm RG})\rangle}{n} \approx \frac{\langle \ln X_\Pi(G_{\rm BR})\rangle}{n} \approx f(\langle d\rangle). \tag{4.1}$$

To validate Eq (4.1), without loss of generality we choose three MTIs: the Narumi-Katayama index, the multiplicative sum-connectivity index, and the multiplicative inverse degree index. We apply these indices to ER networks, RG graphs, and BR networks and plot $\langle \ln NK_\Pi(G)\rangle/n$, $-\langle \ln \chi_\Pi(G)\rangle/n$ and $\langle \ln ID_\Pi(G)\rangle/n$ in Figure 7. There, for each index, we can clearly see that the curves corresponding to the three network models fall one on top of the other, thus validating Eq (4.1). Also, notice that we are using networks of different sizes to stress the scaling law in Eq (4.1). We observe the same scaling behavior in all the other MTIs of Eqs (1.10)–(1.14) (not shown here).

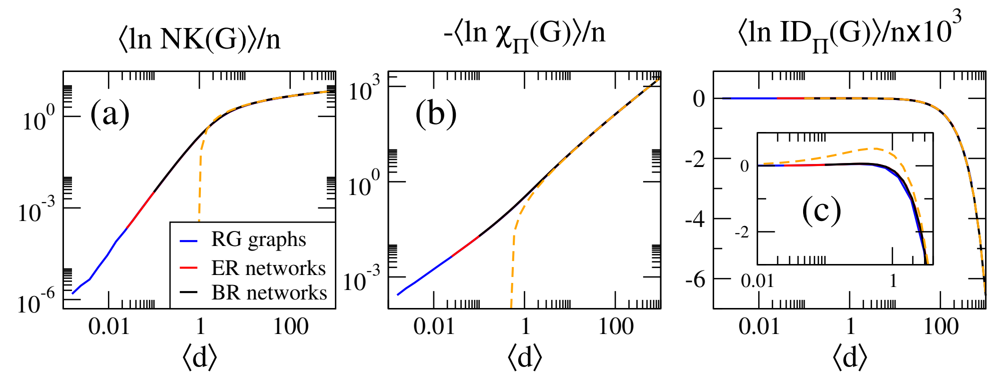

Figure 7. Average logarithm of (a) $NK(G)$, (b) $\chi_\Pi(G)$, and (c) $ID_\Pi(G)$, normalized to the network size n, as a function of the average degree $\langle d\rangle$ of random geometric graphs of size $n = 500$, Erdös-Rényi networks of size $n = 250$ and bipartite random networks of size $n = 2n_1 = 2n_2 = 2000$. Orange dashed lines are (a) Eq (3.2), (b) Eq (3.8), and (c) Eq (3.9). The inset in (c) is an enlargement for small $\langle d\rangle$.

Finally, it is fair to mention that we found that the multiplicative version of the geometric-arithmetic index $GA_\Pi(G)$ on random networks does not scale with the average degree. This situation is quite unexpected for us since all other MTIs we study here scale with $\langle d\rangle$. In addition, our previous statistical and theoretical studies of topological indices of the form $X_\Sigma(G)$ (see Eq (1.1)), showed that the normalized geometric-arithmetic index $GA_\Sigma(G)$ scales with $\langle d\rangle$ [16]. Thus, we believe that the multiplicative index $GA_\Pi(G)$ on random graphs requires further analysis.

Augmented Reality (AR) algorithms have shown rapid development in recent years when applied to the study of different networks, such as neural and communication networks (see e.g., [35, 36]). Therefore, it would be interesting to apply AR techniques in the analysis of random networks.

We hope that our work may motivate further analytical and computational studies of MTIs.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

Acknowledgments

This publication is part of the grant PID2019-106433GB-I00 funded by Agencia Estatal de Investigación MCIN/AEI/ 10.13039/501100011033. J.A.M.-B. thanks support from CONACyT (Grant No. 286633), CONACyT-Fronteras (Grant No. 425854), and VIEP-BUAP (Grant No. 100405811-VIEP2023), Mexico. J.M.R. was supported by the Madrid Government (Comunidad de Madrid-Spain) under the Multiannual Agreement with UC3M in the line of Excellence of University Professors (EPUC3M23), and in the context of the V PRICIT (Regional Programme of Research and Technological Innovation).

We would like to thank the referees for their comments which have improved the presentation of the paper.

Conflict of interest

Prof. Jose M. Rodriguez is the Guest Editor of special issue "Graph theory and its applications" for AIMS Mathematics. Prof. Jose M. Rodriguez was not involved in the editorial review and the decision to publish this article.

All authors declare no conflicts of interest in this paper.

References

1. I. Gutman, Degree-based topological indices, *Croat. Chem. Acta*, **86** (2013), 351–361. https://doi.org/10.5562/cca2294
2. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17** (1972), 535–538. https://doi.org/10.1016/0009-2614(72)85099-1
3. M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.*, **97** (1975), 6609–6615. https://doi.org/10.1021/ja00856a001
4. S. Fajtlowicz, On conjectures of Graffiti–II, *Congr. Numer.*, **60** (1987), 187–197.
5. B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.*, **46** (2009), 1252–1270. https://doi.org/10.1007/s10910-008-9515-z
6. G. Dustigeer, H. Ali, M. I. Khan, Y. M. Chu, On multiplicative degree based topological indices for planar octahedron networks, *Main Group Metal Chem.*, **40** (2020), 219–228. https://doi.org/10.1515/mgmc-2020-0026

7. W. Gao, M. K. Jamil, M. R. Farahani, The hyper-Zagreb index and some graph operations, *J. Appl. Math. Comput.*, **54** (2017), 263–275. https://doi.org/10.1007/s12190-016-1008-9

8. M. Ghorbani, S. Zangi, N. Amraei, New results on symmetric division deg index, *J. Appl. Math. Comput.*, **65** (2021), 161–176. https://doi.org/10.1007/s12190-020-01386-9

9. J. Liu, Q. Zhang, Sharp upper bounds for multiplicative Zagreb indices, *MATCH Commun. Math. Comput. Chem.*, **68** (2012), 231–240.

10. E. Mehdi, A. Iranmanesha, I. Gutman, Multiplicative versions of first Zagreb index, *MATCH Commun. Math. Comput. Chem.*, **68** (2012), 217–230.

11. S. Mondal, K. C. Das. Zagreb connection indices in structure property modelling, *J. Appl. Math. Comput.*, **69** (2023), 3005–3020. https://doi.org/10.1007/s12190-023-01869-5

12. M. C. Shanmukha, N. S. Basavarajappa, A. Usha, K. C. Shilpa, Novel neighbourhood redefined first and second Zagreb indices on carborundum structures, *J. Appl. Math. Comput.*, **66** (2021), 263–276. https://doi.org/10.1007/s12190-020-01435-3

13. H. Narumi, M. Katayama, Simple topological index. A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons, *Mem. Fac. Engin. Hokkaido Univ.*, **16** (1984), 209–214.

14. R. Todeschini, V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees, *MATCH Commun. Math. Comput. Chem.*, **64** (2010), 359–372.

15. C. T. Martínez-Martínez, J. A. Mendez-Bermudez, J. M. Rodríguez, J. M. Sigarreta, Computational and analytical studies of the Randić index in Erdös-Rényi models, *Appl. Math. Comput.*, **377** (2020), 125–137. https://doi.org/10.1016/j.amc.2020.125137

16. R. Aguilar-Sanchez, I. F. Herrera-Gonzalez, J. A. Mendez-Bermudez, J. M. Sigarreta, Computational properties of general indices on random networks, *Symmetry*, **12** (2020), 1341. https://doi.org/10.3390/sym12081341

17. C. T. Martínez-Martínez, J. A. Mendez-Bermudez, J. M. Rodríguez, J. M. Sigarreta, Computational and analytical studies of the harmonic index in Erdös-Rényi models, *MATCH Commun. Math. Comput. Chem.*, **85** (2021), 395–426.

18. R. Aguilar-Sanchez, J. A. Mendez-Bermudez, J. M. Rodríguez, J. M. Sigarreta, Normalized Sombor indices as complexity measures of random networks, *Entropy*, **23** (2021), 976. https://doi.org/10.3390/e23080976

19. R. Aguilar-Sanchez, J. A. Mendez-Bermudez, F. A. Rodrigues, J. M. Sigarreta-Almira, Topological versus spectral properties of random geometric graphs, *Phys. Rev. E*, **102** (2020), 042306. https://doi.org/10.1103/PhysRevE.102.042306

20. I. Gutman, I. Milovanović, E. Milovanović, Relations between ordinary and multiplicative degree-based topological indices, *Filomat*, **32** (2018), 3031–3042. https://doi.org/10.2298/FIL1808031G

21. T. Réti, I. Gutman, Relations between ordinary and multiplicative Zagreb indices, *Bull. Inter. Math. Virtual Inst.*, **2** (2012), 133–140.

22. P. Bosch, Y. Quintana, J. M. Rodríguez, J. M. Sigarreta, Jensen-type inequalities for m-convex functions, *Open Math.*, **20** (2022), 946–958. https://doi.org/10.1515/math-2022-0061

23. H. Kober, On the arithmetic and geometric means and on Hölder's inequality, *Proc. Amer. Math. Soc.*, **9** (1958), 452–459. https://doi.org/10.1090/S0002-9939-1958-0093564-7

24. B. Zhou, I. Gutman, T. Aleksić, A note on Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.*, **60** (2008), 441–446.

25. M. Petrović, Sur une fonctionnelle, *Publ. Math. Univ. Belgrade*, **1** (1932), 146–149.

26. I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graphs Comb.*, **17** (2020), 74–85. https://doi.org/10.1016/j.akcej.2018.05.002

27. Z. Raza, S. Akhter, Y. Shang, Expected value of first Zagreb connection index in random cyclooctatetraene chain, random polyphenyls chain, and random chain network, *Front. Chem.*, **10** (2023), 1067874. https://doi.org/10.3389/fchem.2022.1067874

28. Y. Shang, Sombor index and degree-related properties of simplicial networks, *Appl. Math. Comput.*, **419** (2022), 126881. https://doi.org/10.1016/j.amc.2021.126881

29. R. Solomonoff, A. Rapoport, Connectivity of random nets, *Bull. Math. Biophys.*, **13** (1951), 107–117. https://doi.org/10.1007/BF02478357

30. P. Erdös, A. Rényi, On random graphs, *Publ. Math. (Debrecen)*, **6** (1959), 290–297.

31. P. Erdös, A. Rényi, On the strength of connectedness of a random graph, *Acta Math. Hungarica*, **12** (1961), 261–267. https://doi.org/10.1007/BF02066689

32. J. Dall, M. Christensen, Random geometric graphs, *Phys. Rev. E*, **66** (2002), 016121. https://doi.org/10.1103/PhysRevE.66.016121

33. M. Penrose, *Random geometric graphs*, Oxford: Oxford University Press, 2003.

34. E. Estrada, M. Sheerin, Random rectangular graphs, *Phys. Rev. E*, **91** (2015), 042805. https://doi.org/10.1103/PhysRevE.91.042805

35. S. Narayanan, S. Doss, Augmented reality using artificial neural networks - a review, *Int. J. Eng. Techn.*, **8** (2019), 603–610. https://doi.org/10.14419/ijet.v8i4.29981

36. P. Cipresso, I. A. C. Giglioli, I. Raya, G. Riva, The past, present, and future of virtual and augmented reality research: A network and cluster analysis of the literature, *Front. Psych.*, **9** (2011), 2086. https://doi.org/10.3389/fpsyg.2018.02086

AIMS Press