Novel inequalities for generalized graph entropies – Graph energies and topological indices*

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(Received December 14, 2014; revised February 14, 2015)

A B S T R A C T

The entropy of a graph is an information–theoretic quantity for measuring the complexity of a graph. After Shannon introduced the entropy to information and communication, many generalizations of the entropy measure have been proposed, such as Rényi entropy and Daróczy entropy. In this article, we prove accurate connections (inequalities) between generalized graph entropies, graph energies, and topological indices. Additionally, we obtain some extremal properties of nine generalized graph entropies by employing graph energies and topological indices.

Keywords: Generalized graph entropies; Graph energies; Graph indices

1 Introduction

The entropy of a probability distribution can be interpreted not only as a measure of uncertainty, but also as a measure of information. As a matter of fact, the amount of information, which we get when we observe the result of an experiment, can be taken numerically equal to the amount of uncertainty concerning the outcome of the experiment

*Supported by the NSFC grant No. 11371205, "973" program No. 2013CB834204 and PCSIRT.

before carrying it out. Shannon first introduced the definition of entropy to information and communication. Moreover, studies of the information content of graphs and networks were initiated in the late 1950s [37, 44], following the publication of the widely cited paper [46] of Shannon. Later, entropy measures were developed by using various graph invariants [13]. Fortunately, such measures have been proved useful to investigate several important properties of a graph. The broad range of research on entropy measures and graphs is exemplified in [4, 5, 10, 13, 37, 48]. Early contributions in this field inspired researchers in various disciplines to apply entropy measures to the analysis of structures. Various information theoretic measures (and also non-information theoretic measures) and other techniques have been developed to determine the structural complexity of molecular structures and complex networks. An up-to-date review on graph entropy measures has recently been published by Dehmer and Mowshowitz [13].

It is worth mentioning that various graph entropy measures have been developed, see [4,13,37]. For example, partitions based on several graph invariants, such as vertices, edges and distances have been used to assign a probability distribution to a graph. In [5], Bonchev proposed the magnitude–based information indices, while the topological information content was developed by Rashevsky [44]. Moreover, so-called generalized graph entropies have been investigated due to Dehmer and Mowshowitz by applying generalized entropy measures, see [14]. The innovation represented by these generalized entropy measures is their dependence on the assignment of a probability distribution to a set of elements of a graph. Rather than determine a probability distribution from properties of a graph, one is imposed on the graph independently of its internal structure. Applying graph energy and spectral moments, Dehmer, Li and Shi [11] gave accurate connections between graph energy and generalized graph entropies, which were introduced by Dehmer and Mowshowitz [14]. Also, some extremal properties of the generalized graph entropies are described and proved in their article [11].

In this article, we focus on the mentioned generalized graph entropy measures and express these quantities using various graph energies and topological indices. At this point it is worth mentioning that there are many other fields where graph properties are important, such as evolutionary game theory [35,36], medicine [17], spread of epidemics [3,38,39], financing [18], and so on.

This article is organized as follows. Section 2 reviews existing entropies defined on graphs and generalized graph entropies. In Section 3, we obtain some extremal properties of nine generalized graph entropies by employing graph energies and topological indices. Moreover, we establish inequalities for generalized graph entropies. The paper ends with a short summary and conclusion.

2 Preliminaries

Graph entropies can be divided into two classes. The first class is based on an equivalence relation defined on the set X of elements of a graph, see [13, 37] while the second, introduced by Dehmer [10], is not based on partitions induced by equivalence relations. To define these measures, a probability value to each vertex $v_i \in V$ is assigned, and we obtain the following probability distribution

$$(p^f(v_1), p^f(v_2), \ldots, p^f(v_n)), \qquad |V| := n,$$

where [10]

$$p^f(v_i) := \frac{f(v_i)}{\sum\limits_{j=1}^{n} f(v_j)},$$

and f is an information function mapping graph elements (e.g., vertices) to the non-negative reals. The entropy of the underlying graph topology is here defined by [10]:

$$I_f(G) := -\sum_{i=1}^{n} \frac{f(v_i)}{\sum\limits_{j=1}^{n} f(v_j)} \log \frac{f(v_i)}{\sum\limits_{j=1}^{n} f(v_j)} .$$

Actually, many generalized entropies have been proposed after the seminal paper of Shannon [46]. Here, we mention two important examples of entropy measures: Rényi entropy [45] and Daróczy entropy [8]. The Rényi entropy is defined by

$$I_\alpha^r(P) := \frac{1}{1-\alpha} \log \left(\sum_{i=1}^{n} (p(v_i))^\alpha \right), \qquad \alpha > 0 \text{ and } \alpha \neq 1,$$

where $P := (p(v_1), p(v_2), \ldots, p(v_n))$. The Daróczy entropy is

$$H_n^\alpha(P) := \frac{\sum\limits_{i=1}^{n} ((p_i)^\alpha) - 1}{2^{1-\alpha} - 1}, \qquad \alpha > 0 \text{ and } \alpha \neq 1,$$

where $P := (p_1, p_2, \ldots, p_n)$. In [14], Dehmer and Mowshowitz introduced a new class of measures (here referred to as generalized measures) that derive from functions such as those defined by Rényi entropy, Daróczy entropy and the quadratic entropy function discussed by Arndt [1].

Definition 1. *Let G be a graph of order n. Then*

$$(i) \qquad I^1(G) = \sum_{i=1}^{n} \frac{f(v_i)}{\sum\limits_{j=1}^{n} f(v_i)} \left[1 - \frac{f(v_i)}{\sum\limits_{j=1}^{n} f(v_i)} \right];$$

$$(ii) \qquad I^2_\alpha(G) = \frac{1}{1-\alpha} \log \sum_{i=1}^{n} \left(\frac{f(v_i)}{\sum\limits_{j=1}^{n} f(v_i)} \right)^{\alpha},$$

$$(iii) \qquad I^3_\alpha(G) = \frac{1}{2^{1-\alpha}-1} \sum_{i=1}^{n} \left(\frac{f(v_i)}{\sum\limits_{j=1}^{n} f(v_i)} \right)^{\alpha} - 1, \quad \alpha \neq 1.$$

Let G be a graph of order n and M be a matrix related to it. Denote by $\mu_1, \mu_2, \ldots, \mu_n$ the eigenvalues of M (or the singular values in the case of the incidence matrix). If $f := |\lambda_i|$, then [15]

$$p^f(v_i) = \frac{|\mu_i|}{\sum\limits_{j=1}^{n} |\mu_i|}.$$

Therefore, the generalized graph entropies are defined as follows:

$$(i) \qquad I^1(G) = \sum_{i=1}^{n} \frac{|\mu_i|}{\sum\limits_{j=1}^{n} |\mu_j|} \left[1 - \frac{|\mu_i|}{\sum\limits_{j=1}^{n} |\mu_j|} \right]; \tag{1}$$

$$(ii) \qquad I^2_\alpha(G) = \frac{1}{1-\alpha} \log \sum_{i=1}^{n} \left(\frac{|\mu_i|}{\sum\limits_{j=1}^{n} |\mu_j|} \right)^{\alpha}, \quad \alpha \neq 1; \tag{2}$$

$$(iii) \qquad I^3_\alpha(G) = \frac{1}{2^{1-\alpha}-1} \sum_{i=1}^{n} \left(\frac{|\mu_i|}{\sum\limits_{j=1}^{n} |\mu_j|} \right)^{\alpha} - 1, \quad \alpha \neq 1. \tag{3}$$

Especially, for the first generalized graph entropy $I^1(G)$, we have

$$I^1(G) = \sum_{i=1}^{n} \frac{|\mu_i|}{\sum\limits_{j=1}^{n} |\mu_j|} \left[1 - \frac{|\mu_i|}{\sum\limits_{j=1}^{n} |\mu_j|} \right] = 1 - \left(\sum_{j=1}^{n} |\mu_j| \right)^{-2} \sum_{i=1}^{n} |\mu_i|^2 .$$

3 Extremal properties of generalized graph entropies

In this section, we introduce nine generalized graph entropies of distinct graph matrices. Accurate connections between the entropies and energies or topological indices are proved. Moreover, we examine the extremal properties of the above specified entropies.

1. Let $Q(G)$ be the signless Laplacian matrix of the graph G. Then $Q(G) = D(G) + A(G)$, where $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ denotes the diagonal matrix of vertex degrees of G and $A(G)$ is the adjacency matrix of G. Let $q_1, q_2, \ldots, q_n$ be the eigenvalues of $Q(G)$.

As well known, $q_i \geq 0$, $\sum\limits_{i=1}^{n} q_i = 2m$ and $\sum\limits_{i=1}^{n} q_i^2 = tr(Q^2(G)) = \sum\limits_{i=1}^{n} d_i^2 + \sum\limits_{i=1}^{n} d_i$. Then arrive at the following theorem.

Theorem 2. *Let G be a graph with n vertices and m edges. Then for $\alpha \neq 1$,*

$$(i) \qquad I_Q^1(G) = 1 - \frac{1}{4m^2}(M_1 + 2m), \tag{4}$$

$$(ii) \qquad I_\alpha^2(G) = \frac{1}{1-\alpha} \log \frac{M_\alpha^*}{(2m)^\alpha}, \tag{5}$$

$$(iii) \qquad I_\alpha^3(G) = \frac{1}{2^{1-\alpha} - 1}\left(\frac{M_\alpha^*}{(2m)^\alpha} - 1\right), \tag{6}$$

where M_1 denotes the first Zagreb index and $M_\alpha^* = \sum\limits_{i=1}^{n} |q_i|^\alpha$.

Proof. By substituting $\sum\limits_{i=1}^{n} q_i = 2m$ and $M_1 = \sum\limits_{i=1}^{n} q_i^2$ into equality (1), we get

$$\begin{aligned} I_Q^1(G) &= 1 - \left(\sum_{j=1}^{n} |q_j|\right)^{-2} \sum_{i=1}^{n} |q_i|^2 \\ &= 1 - \frac{1}{(2m)^2}\left(\sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i\right) = 1 - \frac{1}{4m^2}(M_1 + 2m). \end{aligned}$$

The other two equalities can be obtained by substituting $\sum\limits_{i=1}^{n} q_i = 2m$ and $M_\alpha^* = \sum\limits_{i=1}^{n} |q_i|^\alpha$ into equalities (2) and (3), respectively. □

Equality (4) provides an accurate relation between $I_Q^1(G)$ and the first Zagreb index M_1. Obviously, for a graph G, each upper (lower) bound of the first Zagreb index M_1 implies a lower (an upper) bound of $I_Q^1(G)$. Moreover, by employing some previously known bounds [29], we obtain the following extremal properties of the general graph entropy $I^1_Q(G)$.

Corollary 3. *i. For a graph G with n vertices and m edges,*

$$I^1_Q(G) \leq 1 - \frac{1}{2m} - \frac{1}{n}\,.$$

ii. Let G be a graph with n vertices and m edges. The minimum degree of G is δ and the maximum degree of G is Δ. Then

$$I^1_Q(G) \geq 1 - \frac{1}{2m} - \frac{1}{2n} - \frac{\Delta^2+\delta^2}{4n\Delta\delta},$$

with equality if and only if G is a regular graph, or G is a graph whose vertices have exactly two degrees Δ and δ such that $\Delta+\delta$ divides δn, and there are exactly $p = \frac{\delta n}{\delta+\Delta}$ vertices of degree Δ and $q = \frac{\Delta n}{\delta+\Delta}$ vertices of degree δ.

2. Let $\mathscr{L}(G)$ and $\mathcal{Q}(G)$ be, respectively, the normalized Laplacian matrix and the normalized signless Laplacian matrix. By definition, $\mathscr{L}(G) = D(G)^{-\frac{1}{2}}L(G)D(G)^{-\frac{1}{2}}$ and $\mathcal{Q}(G) = D(G)^{-\frac{1}{2}}Q(G)D(G)^{-\frac{1}{2}}$, where $D(G)$ is the diagonal matrix of vertex degrees, and $L(G) = D(G) - A(G)$, $Q(G) = D(G) + A(G)$ are, respectively, the Laplacian and the signless Laplacian matrices of the graph G. Denote the eigenvalues of $\mathscr{L}(G)$ and $\mathcal{Q}(G)$ by $\mu_1, \mu_2, \ldots, \mu_n$ and $q_1, q_2, \ldots, q_n$, respectively. Then $\mu_i \geq 0$, $q_i \geq 0$, $\sum_{i=1}^{n} \mu_i = \sum_{i=1}^{n} q_i = n$ and $\sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n} q_i^2 = n + 2\sum_{i\sim j} \frac{1}{d_i\, d_j}$. The equality relationship between the generalized graph entropy $I^1_{\mathscr{L}(\mathcal{Q})}(G)$ and general Randić index follows.

Theorem 4. *Let G be a graph with n vertices and m edges. Then for $\alpha \neq 1$,*

$$(i) \qquad I^1_{\mathscr{L}(\mathcal{Q})}(G) = 1 - \frac{1}{n^2}(n + 2R_{-1}(G))\,, \tag{7}$$

$$(ii) \qquad I^2_\alpha(G) = \frac{1}{1-\alpha}\log\frac{M^*_\alpha}{n^\alpha}\,, \tag{8}$$

$$(iii) \qquad I^3_\alpha(G) = \frac{1}{2^{1-\alpha}-1}\left(\frac{M^*_\alpha}{n^\alpha} - 1\right). \tag{9}$$

where $R_{-1}(G)$ denotes the general Randić index $R_\beta(G)$ of G with $\beta = -1$ and $M^*_\alpha = \sum_{i=1}^{n} |q_i|^\alpha$.

Proof. By substituting $\sum_{i=1}^{n}\mu_i=\sum_{i=1}^{n}q_i=n$ and $\sum_{i=1}^{n}\mu_i^2=\sum_{i=1}^{n}q_i^2=n+2\sum_{i\sim j}\frac{1}{d_i\,d_j}$ into equality (1), we have

$$I^1_{\mathscr{L}}(G)=1-\left(\sum_{j=1}^{n}|\mu_j|\right)^{-2}\sum_{i=1}^{n}|\mu_i|^2$$

$$=1-\frac{1}{n^2}\left(n+2\sum_{i\sim j}\frac{1}{d_i\,d_j}\right)=1-\frac{1}{n^2}(n+2R_{-1}(G)),$$

$$I^1_{\mathscr{Q}}(G)=1-\left(\sum_{j=1}^{n}|q_j|\right)^{-2}\sum_{i=1}^{n}|q_i|^2$$

$$=1-\frac{1}{n^2}\left(n+2\sum_{i\sim j}\frac{1}{d_i\,d_j}\right)=1-\frac{1}{n^2}(n+2R_{-1}(G))\,.$$

The other two equalities are obtained by substituting $\sum_{i=1}^{n}\mu_i=\sum_{i=1}^{n}q_i=2m$ and $M^*_\alpha=\sum_{i=1}^{n}|q_i|^\alpha$ into equalities (2) and (3), respectively. □

From equality (7), we can easily infer the relation of $I^1_{\mathscr{L}(\mathscr{Q})}(G)$ and the general Randić index $R_{-1}(G)$ of G. It implies that for a graph G, each upper (lower) bound of the general Randić index $R_{-1}(G)$ of G directly results in a lower (an upper) bound of $I^1_{\mathscr{L}(\mathscr{Q})}(G)$. It is easy to check the following extremal properties of $I^1_{\mathscr{L}(\mathscr{Q})}(G)$ by employing the bounds from [34, 47].

Corollary 5. *i. Let G be a graph with n vertices and m edges. If n is odd, then*

$$1-\frac{2}{n}+\frac{1}{n^2}\le I^1_{\mathscr{L}(\mathscr{Q})}(G)\le 1-\frac{1}{n-1}\,.$$

If n is even, then

$$1-\frac{2}{n}\le I^1_{\mathscr{L}(\mathscr{Q})}(G)\le 1-\frac{1}{n-1}$$

with right equality holding if and only if G is the complete graph, and with left equality holding if and only if G is the disjoint union of $\frac{n}{2}$ paths of length 1 if n is even, and is the disjoint union of $\frac{n-3}{2}$ paths of length 1 and a path of length 2 if n is odd.

ii. Let G be a graph with n vertices and m edges. Let the minimum and maximum degrees of G be δ and Δ, respectively. Then

$$1-\frac{1}{n}-\frac{1}{n\delta}\le I^1_{\mathscr{L}(\mathscr{Q})}(G)\le 1-\frac{1}{n}-\frac{1}{n\Delta}\,.$$

Equality occurs in both bounds if and only if G is a regular graph.

3. Let $I(G)$ be the incidence matrix of graph G. For a graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, the (i, j)-entry of $I(G)$ is 1 if the vertex v_i is incident to the edge e_j, and is 0 otherwise. As we know, $Q(G) = D(G) + A(G) = I(G) \cdot I^T(G)$. If the eigenvalues of $Q(G)$ are $q_1, q_2, \ldots, q_n$, then $\sqrt{q_1}, \sqrt{q_2}, \ldots, \sqrt{q_n}$ are the singular values of $I(G)$. In addition, the incidence energy of the graph G is defined as $IE(G) = \sum_{i=1}^{n} \sqrt{q_i}$. Similarly, we consider the connection between the generalized graph entropy $I_I^1(G)$ and the incidence energy $IE(G)$. We arrive at the following result.

Theorem 6. *Let G be a graph with n vertices and m edges. Then for $\alpha \neq 1$,*

$$(i) \qquad I_I^1(G) = 1 - \frac{2m}{IE^2(G)}, \tag{10}$$

$$(ii) \qquad I_\alpha^2(G) = \frac{1}{1-\alpha} \log \frac{M_\alpha^*}{IE^\alpha(G)}, \tag{11}$$

$$(iii) \qquad I_\alpha^3(G) = \frac{1}{2^{1-\alpha} - 1} \left(\frac{M_\alpha^*}{IE^\alpha(G)} - 1 \right) \tag{12}$$

where $IE(G)$ denotes the incidence energy of G and $M_\alpha^* = \sum_{i=1}^{n} (\sqrt{q_i})^\alpha$.

Proof. By substituting $IE(G) = \sum_{i=1}^{n} \sqrt{q_i}$ and $\sum_{i=1}^{n} q_i = tr(Q(G)) = 2m$ into equality (1), we get

$$\begin{aligned} I_I^1(G) &= 1 - \left(\sum_{j=1}^{n} |\sqrt{q_j}| \right)^{-2} \sum_{i=1}^{n} |\sqrt{q_i}|^2 \\ &= 1 - \frac{1}{IE^2(G)} \sum_{i=1}^{n} q_i = 1 - \frac{2m}{IE^2(G)} \, . \end{aligned}$$

The other two equalities can be obtained by substituting $M_\alpha^* = \sum_{i=1}^{n} \sqrt{q_i}^\alpha$ and $IE(G) = \sum_{i=1}^{n} \sqrt{q_i}$ into equalities (2) and (3), respectively. □

Equality (10) suggests that for a graph G, each upper (lower) bound of the incidence energy $IE(G)$ of G results in an upper (a lower) bound of $I_I^1(G)$. Applying some known bounds [25, 30], we obtain the following extremal properties of the general graph entropy $I_I^1(G)$.

Corollary 7. *i. For a graph G with n vertices and m edges,*

$$0 \leq I_I^1(G) \leq 1 - \frac{1}{n} \, .$$

The left equality holds if and only if $m \leq 1$, whereas the right equality holds if and only if $m = 0$.

ii. Let T be a tree of order n. Then

$$I_I^1(S_n) \leq I_I^1(T) \leq I_I^1(P_n)\,,$$

where S_n and P_n denote the star and path of order n, respectively.

4. Let G be a connected graph whose vertices are $v_1, v_2, \ldots, v_n$. The distance matrix of G is defined as $D(G) = [d_{ij}]$, where d_{ij} is the distance between the vertices v_i and v_j in G. We denote the eigenvalues of $D(G)$ by $\mu_1, \mu_2, \ldots, \mu_n$. It is easy to verify that $\sum_{i=1}^{n} \mu_i = 0$ and $\sum_{i=1}^{n} \mu_i^2 = 2 \sum_{1 \leq i < j \leq n} (d_{ij})^2$. The distance energy of the graph G is $DE(G) = \sum_{i=1}^{n} |\mu_i|$.

The k-th distance moment of G is defined as $W_k(G) = \sum_{1 \leq i < j \leq n} (d_{ij})^k$. In particular, $W(G) = W_1(G)$ and $WW(G) = \frac{1}{2}(W_2(G) + W_1(G))$, where $W(G)$ and $WW(G)$ respectively denote the Wiener index and hyper–Wiener index of G.

The following theorem describes the equality relationship between the generalized graph entropy $I_D^1(G)$ and $DE(G)$, $W(G)$, and $WW(G)$.

Theorem 8. *Let G be a graph with n vertices and m edges. Then for $\alpha \neq 1$,*

$$(i) \qquad I_D^1(G) = 1 - \frac{4}{DE^2(G)}(2WW(G) - W(G)), \tag{13}$$

$$(ii) \qquad I_\alpha^2(G) = \frac{1}{1-\alpha} \log \frac{M_\alpha^*}{DE^\alpha(G)}, \tag{14}$$

$$(iii) \qquad I_\alpha^3(G) = \frac{1}{2^{1-\alpha} - 1} \left(\frac{M_\alpha^*}{DE^\alpha(G)} - 1 \right) \tag{15}$$

where $M_\alpha^* = \sum_{i=1}^{n} |\mu_i|^\alpha$ and $DE(G)$ denotes the distance energy of G. Here $W(G)$ and $WW(G)$ are the Wiener index and hyper–Wiener index of G.

Proof. By substituting $DE(G) = \sum_{i=1}^{n} |\mu_i|$ and $W_2(G) = 2WW(G) - W(G)$ into equality (1), we obtain

$$I_D^1(G) = 1 - \left(\sum_{j=1}^{n} |\mu_j| \right)^{-2} \sum_{i=1}^{n} |\mu_i|^2$$

$$= 1 - \frac{1}{DE^2(G)} \sum_{i=1}^{n} \mu_i^2 = 1 - \frac{2}{DE^2(G)} \sum_{1 \leq i < j \leq n} (d_{ij})^2$$

$$= 1 - \frac{4W_2(G)}{DE^2(G)} = 1 - \frac{4}{DE^2(G)}(2WW(G) - W(G)).$$

The other two equalities can be obtained by substituting $M_\alpha^* = \sum_{i=1}^{n} |\mu_i|^\alpha$ and $DE(G) = \sum_{i=1}^{n} |\mu_i|$ into equalities (2) and (3), respectively. □

From equality (13), we easily infer the relation of $I_D^1(G)$ and the distance energy $DE(G)$ of G, the Wiener index and the hyper–Wiener index of G. Applying previously known bounds [41], we arrive at the following corollary on $I_D^1(G)$.

Corollary 9. *For a graph with n vertices and m edges,*

$$0 \leq I_D^1(G) \leq 1 - \frac{1}{n}.$$

5. Let G be a simple undirected graph, and G^σ be an oriented graph of G with the orientation σ. The skew adjacency matrix of G^σ is the $n \times n$ matrix $S(G^\sigma) = [s_{ij}]$, where $s_{ij} = 1$ and $s_{ji} = -1$ if $\langle v_i, v_j \rangle$ is an arc of G^σ, otherwise $s_{ij} = s_{ji} = 0$. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. It can be shown that $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all purely imaginary and that $\sum_{i=1}^{n} \lambda_i = 0$, $\sum_{i=1}^{n} \lambda_i^2 = -2m$. Then $\sum_{i=1}^{n} |\lambda_i|^2 = 2m$. The skew energy of G^σ is $SE(G^\sigma) = \sum_{i=1}^{n} |\lambda_i|$.

Now, we focus on the extremal properties of the generalized graph entropies $I_S^1(G)$, $I_\alpha^2(G)$ and $I_\alpha^3(G)$.

Theorem 10. *Let G^σ be an oriented graph with n vertices and m arcs. Then for $\alpha \neq 1$,*

$$(i) \qquad I_S^1(G^\sigma) = 1 - \frac{2m}{SE^2(G^\sigma)}, \tag{16}$$

$$(ii) \qquad I_\alpha^2(G^\sigma) = \frac{1}{1-\alpha} \log \frac{M_\alpha^*}{SE^\alpha(G^\sigma)}, \tag{17}$$

$$(iii) \qquad I_\alpha^3(G^\sigma) = \frac{1}{2^{1-\alpha} - 1} \left(\frac{M_\alpha^*}{SE^\alpha(G^\sigma)} - 1 \right) \tag{18}$$

where $SE(G^\sigma)$ denotes the skew energy of G^σ and $M_\alpha^* = \sum_{i=1}^{n} |\lambda_i|^\alpha$.

Proof. By substituting $SE(G^\sigma) = \sum_{i=1}^{n} |\lambda_i|$ and $\sum_{i=1}^{n} |\lambda_i|^2 = 2m$ into equality (1), we get

$$I_S^1(G^\sigma) = 1 - \left(\sum_{j=1}^{n} |\lambda_j| \right)^{-2} \sum_{i=1}^{n} |\lambda_i|^2 = 1 - \frac{2m}{SE^2(G^\sigma)}.$$

The other two equalities can be obtained by substituting $M_\alpha^* = \sum_{i=1}^{n} |\lambda_i|^\alpha$ and $SE(G^\sigma) = \sum_{i=1}^{n} |\lambda_i|$ into equalities (2) and (3), respectively. □

Obviously, the equality (16) implies that for an oriented graph G^σ, each upper (lower) bound of the skew energy $SE(G^\sigma)$ of G^σ results in an upper (a lower) bound of $I_S^1(G^\sigma)$. It is easy to check the following results, based on some previously known bounds [2].

Corollary 11. *i. For an oriented graph G^σ with n vertices, m arcs and maximum degree Δ,*

$$1 - \frac{2m}{2m + n(n-1)|\det(S(G^\sigma))|^{2/n}} \leq I_S^1(G^\sigma) \leq 1 - \frac{1}{n} \leq 1 - \frac{2m}{n^2\Delta}.$$

ii. Let T^σ be an oriented tree of order n. We have

$$I_S^1(S_n^\sigma) \leq I_S^1(T^\sigma) \leq I_S^1(P_n^\sigma),$$

where S_n^σ and P_n^σ denote, respectively, an oriented star and an oriented path of order n, with any orientation. Equality holds if and only if $T_n \cong S_n$ or $T_n \cong P_n$.

6. Let G be a simple graph. The Randić adjacency matrix of G is defined as $R(G) = [r_{ij}]$, where $r_{ij} = \frac{1}{\sqrt{d_i\, d_j}}$ if v_i and v_j are adjacent vertices of G, and $r_{ij} = 0$ otherwise. Denote by $\rho_1, \rho_2, \ldots, \rho_n$ its eigenvalues. Obviously, $\sum_{i=1}^{n} \rho_i = 0$ and $\sum_{i=1}^{n} \rho_i^2 = tr(R^2(G)) = 2\sum_{i\sim j} \frac{1}{d_i\, d_j}$. The Randić energy of the graph G is defined as $RE(G) = \sum_{i=1}^{n} |\rho_i|$.

Theorem 12. *Let G be a graph with n vertices and m edges. Then for $\alpha \neq 1$,*

$$(i) \qquad I_R^1(G) = 1 - \frac{2}{RE^2(G)} R_{-1}(G), \tag{19}$$

$$(ii) \qquad I_\alpha^2(G) = \frac{1}{1-\alpha} \log \frac{M_\alpha^*}{RE^\alpha(G)}, \tag{20}$$

$$(iii) \qquad I_\alpha^3(G) = \frac{1}{2^{1-\alpha} - 1} \left(\frac{M_\alpha^*}{RE^\alpha(G)} - 1 \right) \tag{21}$$

where $RE(G)$ denotes the Randić energy of G, and $R_{-1}(G)$ denotes the general Randić index $R_\beta(G)$ of G with $\beta = -1$ and $M_\alpha^* = \sum_{i=1}^{n} |\rho_i|^\alpha$.

Proof. By substituting $RE(G) = \sum_{i=1}^{n} |\rho_i|$ and $R_{-1}(G) = \sum_{i\sim j} \frac{1}{d_i\, d_j}$ into equality (1), we obtain

$$I_R^1(G) = 1 - \left(\sum_{j=1}^{n} |\rho_j| \right)^{-2} \sum_{i=1}^{n} |\rho_i|^2 = 1 - \frac{1}{RE^2(G)} \sum_{i=1}^{n} \rho_i^2$$

$$= 1 - \frac{2}{RE^2(G)} \sum_{i \sim j} \frac{1}{d_i\, d_j} = 1 - \frac{2}{RE^2(G)} R_{-1}(G)\,.$$

The other two equalities can be obtained by substituting $M_\alpha^* = \sum_{i=1}^{n} |\rho_i|^\alpha$ and $RE(G) = \sum_{i=1}^{n} |\rho_i|$ into equalities (2) and (3), respectively. □

Equality (19) provides a relation between $I_R^1(G)$ and the Randić energy $RE(G)$ and the general Randić index $R_{-1}(G)$ of G. Applying previously known bounds [7], we arrive at the following corollary on $I_R^1(G)$.

Corollary 13. *For a graph with n vertices and m edges,*

$$I_R^1(G) \leq 1 - \frac{1}{n}\,.$$

Equality is attained if and only if G is the graph without edges, or if all its vertices have degree one.

7. Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, and let d_i be the degree of vertex $v_i, i = 1, 2, \ldots, n$. Define an $n \times m$ matrix whose (i,j)-entry is $(d_i)^{-\frac{1}{2}}$ if v_i is incident to e_j and 0 otherwise. We call it the Randić incidence matrix of G and denote by $I_R(G)$. Obviously, $I_R(G) = D(G)^{-\frac{1}{2}} I(G)$. Let $\sigma_1, \sigma_2, \ldots, \sigma_n$ be its singular values. Now, $\sum_{i=1}^{n} \sigma_i$ is defined as the Randić incidence energy $I_R E(G)$ of the graph G.

Let U be the set of isolated vertices of G and $W = V(G) \setminus U$. Set $r = |W|$. Then we have $\sum_{i=1}^{n} \sigma_i^2 = r$. In particular, $\sum_{i=1}^{n} \sigma_i^2 = n$ if G has no isolated vertices.

Theorem 14. *Let G be a graph with n vertices and m edges. Let U be the set of isolated vertices of G and $W = V(G) \setminus U$. Set $r = |W|$. Then for $\alpha \neq 1$,*

$$(i) \qquad I_{I_R}^1(G) = 1 - \frac{r}{I_R E^2(G)}\,, \tag{22}$$

$$(ii) \qquad I_\alpha^2(G) = \frac{1}{1-\alpha} \log \frac{M_\alpha^*}{I_R E^\alpha(G)}\,, \tag{23}$$

$$(iii) \qquad I_\alpha^3(G) = \frac{1}{2^{1-\alpha} - 1} \left(\frac{M_\alpha^*}{I_R E^\alpha(G)} - 1 \right) \tag{24}$$

where $I_R E(G)$ denotes the Randić incidence energy of G and $M_\alpha^* = \sum_{i=1}^{n} |\sigma_i|^\alpha$.

Proof. By substituting $I_RE(G) = \sum_{i=1}^{n} |\sigma_i|$ and $\sum_{i=1}^{n} |\sigma_i|^2 = r$ into equality (1), we obtain

$$I^1_{I_R}(G) = 1 - \left(\sum_{j=1}^{n} |\sigma_j|\right)^{-2} \sum_{i=1}^{n} |\sigma_i|^2 = 1 - \frac{r}{I_RE^2(G)}\,.$$

The other two equalities can be obtained by substituting $M^*_\alpha = \sum_{i=1}^{n} |\sigma_i|^\alpha$ and $I_RE(G) = \sum_{i=1}^{n} |\sigma_i|$ into equalities (2) and (3), respectively. □

From equality (22), we easily infer the relation of $I^1_{I_R}(G)$ and the Randić incidence energy $I_RE(G)$ of G. This equality tells us that for a graph G, each upper (lower) bound of the skew energy $I_RE(G)$ of G implies an upper (a lower) bound of $I^1_{I_R}(G)$. Applying some previously known bounds [19], we obtain the following extremal properties of the generalized graph entropy $I^1_{I_R}(G)$.

Corollary 15. *i. For a graph G with n vertices and m edges,*

$$I^1_{I_R}(G) \geq 1 - \frac{r}{n}\,,$$

with equality holding if and only if $G \cong K_2$.

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

$$I^1_{I_R}(G) \leq 1 - \frac{r}{n^2 - 3n + 4 + 2\sqrt{2(n-1)(n-2)}},$$

and equality holds if and only if $G \cong K_n$.

iii. Let T be a tree of order n. We have

$$I^1_{I_R}(T) \leq I^1_{I_R}(S_n),$$

where S_n denotes the star graph of order n.

8. Let $R_\beta(G)$ be the general Randić matrix of graph G. Define $R_\beta(G) = [r_{ij}]$, where $r_{ij} = \frac{1}{(d_i\,d_j)^\beta}$ if v_i and v_j are adjacent vertices of G, and $r_{ij} = 0$ otherwise. Let $\gamma_1, \gamma_2, \ldots, \gamma_n$ be the eigenvalues of $R_\beta(G)$. By the definition of $R_\beta(G)$, we get $R_\beta(G) = D(G)^\beta A(G) D(G)^\beta$ and $\sum_{i=1}^{n} \gamma_i^2 = tr(R^2_\beta(G)) = 2\sum_{i\sim j}(d_i\,d_j)^{2\beta}$ directly. The general Randić energy is defined as $RE_\beta(G) = \sum_{i=1}^{n} |\gamma_i|$.

Theorem 16. *Let G be a graph with n vertices and m edges. Then for $\alpha \neq 1$,*

$$(i) \qquad I^1_{R_\beta}(G) = 1 - \frac{2}{RE^2_\beta(G)} R_{2\beta}(G)\,, \tag{25}$$

$$(ii) \qquad I^2_\alpha(G) = \frac{1}{1-\alpha} \log \frac{M^*_\alpha}{RE^\alpha_\beta(G)}\,, \tag{26}$$

$$(iii) \qquad I^3_\alpha(G) = \frac{1}{2^{1-\alpha}-1} \left(\frac{M^*_\alpha}{RE^\alpha_\beta(G)} - 1 \right) \tag{27}$$

where $RE_\beta(G)$ denotes the general Randić energy of G, and $R_{2\beta}(G)$ denotes the general Randić index of G and $M^*_\alpha = \sum\limits_{i=1}^{n} |\gamma_i|^\alpha$.

Proof. By substituting $RE_\beta(G) = \sum\limits_{i=1}^{n} |\gamma_i|$ and $\sum\limits_{i=1}^{n} |\gamma_i|^2 = 2 \sum\limits_{i \sim j} (d_i\, d_j)^{2\beta}$ into equality (1), we have

$$\begin{aligned} I^1_{R_\beta}(G) &= 1 - \left(\sum_{j=1}^{n} |\gamma_j| \right)^{-2} \sum_{i=1}^{n} |\gamma_i|^2 \\ &= 1 - \frac{2}{RE^2_\beta(G)} \sum_{i\sim j} (d_i\, d_j)^{2\beta} = 1 - \frac{2}{RE^2_\beta(G)} R_{2\beta}(G)\,. \end{aligned}$$

The other two equalities can be obtained by substituting $M^*_\alpha = \sum\limits_{i=1}^{n} |\gamma_i|^\alpha$ and $RE_\beta(G) = \sum\limits_{i=1}^{n} |\gamma_i|$ into equalities (2) and (3), respectively. □

9. Let G be a simple undirected graph, and G^σ be an oriented graph of G with the orientation σ. The skew Randić matrix of G^σ is the $n \times n$ matrix $R_s(G^\sigma) = [(r_s)_{ij}]$, where $(r_s)_{ij} = (d_i\, d_j)^{-\frac{1}{2}}$ and $(r_s)_{ji} = -(d_i\, d_j)^{-\frac{1}{2}}$ if $\langle v_i, v_j \rangle$ is an arc of G^σ, otherwise $(r_s)_{ij} = (r_s)_{ji} = 0$. Let $\rho_1, \rho_2, \ldots, \rho_n$ be the eigenvalues of $R_s(G^\sigma)$. It follows that $R_s(G^\sigma) = D(G)^{-\frac{1}{2}} S(G^\sigma) D(G)^{-\frac{1}{2}}$ and $\sum\limits_{i=1}^{n} \rho_i^2 = tr(R_s^2(G^\sigma)) = -2 \sum\limits_{i\sim j} \frac{1}{d_i\, d_j} = -2R_{-1}(G)$, which implies $\sum\limits_{i=1}^{n} |\rho_i|^2 = 2R_{-1}(G)$. The skew Randić energy is $RE_s(G^\sigma) = \sum\limits_{i=1}^{n} |\rho_i|$. We now establish an accurate relation among $RE_s(G^\sigma)$, $I^1_{R_s}(G^\sigma)$, $I^2_\alpha(G^\sigma)$ and $I^3_\alpha(G^\sigma)$.

Theorem 17. *Let G^σ be an oriented graph with n vertices and m arcs. Then for $\alpha \neq 1$,*

$$(i) \qquad I^1_{R_S}(G^\sigma) = 1 - \frac{2}{RE^2_S(G^\sigma)} R_{-1}(G)\,, \tag{28}$$

$$(ii) \qquad I^2_\alpha(G^\sigma) = \frac{1}{1-\alpha} \log \frac{M^*_\alpha}{RE^\alpha_S(G^\sigma)}\,, \tag{29}$$

$$(iii) \qquad I^3_\alpha(G^\sigma) = \frac{1}{2^{1-\alpha}-1}\left(\frac{M^*_\alpha}{RE^\alpha_S(G^\sigma)} - 1\right) \tag{30}$$

where $RE_S(G^\sigma)$ denotes the skew Randić energy of G^σ, and $R_{-1}(G)$ is the general Randić index of the underlying graph G with $\beta = -1$, and $M^*_\alpha = \sum_{i=1}^{n} |\rho_i|^\alpha$.

Proof. By substituting $RE_S(G^\sigma) = \sum_{i=1}^{n} |\rho_i|$ and $\sum_{i=1}^{n} |\rho_i|^2 = 2R_{-1}(G)$ into equality (1), we get

$$I^1_{R_s}(G^\sigma) = 1 - \left(\sum_{j=1}^{n} |\rho_j|\right)^{-2} \sum_{i=1}^{n} |\rho_i|^2 = 1 - \frac{2}{RE^2_s(G)} R_{-1}(G)\,.$$

The other two equalities can be obtained by substituting $M^*_\alpha = \sum_{i=1}^{n} |\rho_i|^\alpha$ and $RE_S(G^\sigma) = \sum_{i=1}^{n} |\rho_i|$ into equalities (2) and (3), respectively. □

The equality (28) establishes a relation between $I^1_{R_S}(G^\sigma)$ and the skew Randić energy $RE_S(G^\sigma)$ of G^σ and the general Randić index $R_{-1}(G)$ of G. Applying some previously known bounds [21], we arrive at the following extremal properties of the generalized graph entropy $I^1_{R_S}(G)$.

Corollary 18. *For an oriented graph G^σ with n vertices and m arcs,*

$$I^1_{R_S}(G^\sigma) \le 1 - \frac{1}{n}\,.$$

For the above nine different entropies, we present the following results on implicit information inequality, which can be obtained by the method from the paper [11].

Theorem 19. *i. If $0 < \alpha < 1$, then $I^2_\alpha < I^3_\alpha \cdot \ln 2$. If $\alpha > 1$, then $I^2_\alpha > \frac{(1-2^{1-\alpha})\ln 2}{\alpha-1} I^3_\alpha$.*

ii. If $\alpha \ge 2$ and $0 < \alpha < 1$, then $I^3_\alpha > I^1$. If $1 < \alpha < 2$, then $I^1 > (1 - 2^{1-\alpha}) I^3_\alpha$.

iii. If $\alpha \ge 2$, then

$$I^2_\alpha > \frac{(1 - 2^{1-\alpha}) \ln 2}{\alpha - 1} I^1$$

if $1 < \alpha < 2$, then

$$I^2_\alpha > \frac{(1 - 2^{1-\alpha})^2 \ln 2}{\alpha - 1} I^1$$

if $0 < \alpha < 1$, then $I^2_\alpha > I^1$.

4 Summary and Conclusion

In this paper, we examined graph entropies based on probability distributions defined in terms of eigenvalues or singular values of certain graph–theoretical matrices. Bearing in mind that the "*energy*" of a matrix is defined as the sum of its singular values [33, 40], which in the case of square matrices is the sum of absolute values of the eigenvalues, the graph entropies studied here are directly related with the corresponding graph energies. Graph energy and graph entropy are well-defined concepts that have been (independently) introduced by Gutman [22] and Mowshowitz [37], respectively. Graph entropy is an important method introduced by Mowshowitz [37] for determining the structural information content of graphs, that has been further developed by many authors such as Bonchev [4, 5], Körner [31] and Dehmer [10].

By means of the present approach, a new and somewhat unexpected application of the graph–energy concept is achieved. At the same time, the numerous results earlier obtained in the theory of graph energies, and the powerful mathematical apparatus of this theory [26, 33] are now becoming applicable in the theory of graph entropies [11]. In particular, as shown in this work, a variety of graph–energy results pertaining to extremal problems, e.g., [2, 6, 7, 9, 19, 26, 28], could now be used for designing inequalities for graph entropies.

In view of the large amount of existing graph measures, the problem of deriving inequalities pertaining to these measures has, so far, been investigated only to a limited extend. For example, earlier work on proving interrelations (inequalities) between graph entropies can be found in [10, 12]. We argue that by proving such inequalities, we better understand the measures themselves and their behavior. This may lead to novel applications and to the dissemination of the results towards other disciplines.

An equally remarkable fact is that by the approach presented in this work, interrelations between generalized graph entropies and a variety of topological indices are envisaged. Some of these topological indices (in particular, the Wiener [49], the first Zagreb [27] and the Randić [42]) are nowadays almost half-a-century old, and have been conceived and elaborated without any connection to graph entropy. Details on their theory can be found in the books and surveys: [**?**, 16, 48] (Wiener and other distance–based indices), [23, 48] (first Zagreb index) and [24, 32, 43, 48] (Randić and general Randić indices). The results outlined in this work may be understood as a new and significant application of these topological indices, and an additional justification for their use in chemistry.

References

[1] C. Arndt, Information Measures, Springer, Berlin, 2004.

[2] C. Adiga, R. Balakrishnan, W. So, The skew energy of a digraph, Linear Algebra Appl. 432 (2010) 1825–1835.

[3] A. L. Barabási, N. Gulbahce, J. Loscalzo, Network medicine: A network–based approach to human disease, Nature Rev. Genetics 12 (2011) 56–68.

[4] D. Bonchev, Information indices for atoms and molecules, MATCH Commun. Math. Comput. Chem. 7 (1979) 65–113.

[5] D. Bonchev, Information Theoretic Indices for Characterization of Chemical Structures, Research Studies Press, Chichester, 1983.

[6] Ş. B. Bozkurt, D. Bozkurt, On incidence energy, MATCH Commun. Math. Comput. Chem. 72 (2014) 215–225.

[7] Ş. B. Bozkurt, A. D. Güngör, I. Gutman, A. S. Çevik, Randić matirx and Randić energy, MATCH Commun. Math. Comput. Chem. 64 (2010) 239–250.

[8] Z. Daróczy, A. Jarai, On the measurable solutions of functional equations arising in information theory, Acta. Math. Acad. Sci. Hungar. 34 (1979) 105–116.

[9] K. C. Das, S. Sorgun, I. Gutman, On Randić energy, MATCH Commun. Math. Comput. Chem. 73 (2015) 81–92.

[10] M. Dehmer, Information processing in complex networks: Graph entropy and information functionals, Appl. Math. Comput. 201 (2008) 82–94.

[11] M. Dehmer, X. Li, Y. Shi, Connections between generalized graph entropies and graph theory, Complexity, in press, DOI: 10.1002/cplx.21539.

[12] M. Dehmer, V. Kraus, On extremal properties of graph entropies, MATCH Commun. Math. Comput. Chem. 68 (2012) 889–912

[13] M. Dehmer, A. Mowshowitz, A history of graph entropy measures, Inf. Sci. 181 (2011) 57–78.

[14] M. Dehmer, A. Mowshowitz, Generalized graph entropies, Complexity 17 (2011) 45–50.

[15] M. Dehmer, L. Sivakumar, K. Varmuza, Uniquely discriminating molecular structures using novel eigenvalue–based descriptors, MATCH Commun. Math. Comput. Chem. 67 (2012) 147–172.

[16] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001) 211–249.

[17] F. Emmert–Streib, The chronic fatigue syndrome: A comparative pathway analysis, J. Comput. Biol. 14 (2007) 961–972.

[18] F. Emmert–Streib, M. Dehmer, Identifying critical financial networks of the DJIA: Toward a network–based index, Complexity 16 (2010) 24–33.

[19] R. Gu, F. Huang, X. Li, Randić incidence energy of graphs, Trans. Combin. 3 (2014) 1–9.

[20] R. Gu, F. Huang, X. Li, General Randić matrix and general Randić energy, Trans. Combin. 3 (2014) 21–33.

[21] R. Gu, F. Huang, X. Li, Skew Randić matrix and skew Randić energy, arXiv:1406.1300v1.

[22] I. Gutman, The energy of a graph, Ber. Math.–Statist. Sekt. Forschungsz. Graz 103 (1978), 1–22.

[23] I. Gutman, Degree–based topological indices, Croat. Chem. Acta 86 (2013) 351–361.

[24] I. Gutman, B. Furtula (Eds.), Recent Results in the Theory of Randić Index, Univ. Kragujevac, Kragujevac, 2008.

[25] I. Gutman, D. Kiani, M. Mirzakhah, On incidence energy of graphs, MATCH Commun. Math. Comput. Chem. 62 (2009) 573–580.

[26] I. Gutman, X. Li, J. Zhang, Graph Energy, in: Analysis of Complex Networks: From Biology to Linguistics, M. Dehmer, F. Emmert–Streib (Eds.) Wiley–VCH, Wienhein 2009, pp. 145–174.

[27] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535–538.

[28] G. Huang, M. Kuang, H. Deng, Extremal graph with respect to matching energy for a random polyphenyl chain, MATCH Commun. Math. Comput. Chem. 73 (2015) 121–131.

[29] A. Ilić, M. Ilić, B. Liu, On the upper bounds for the first Zagreb index, Kragujevac J. Math. 35 (2011) 173–182.

[30] M. Jooyandeh, D. Kiani, M. Mirzakhah, Incidence energy of a graph, MATCH Commun. Math. Comput. Chem. 62 (2009) 561–572.

[31] J. Körner, Coding of an information source having ambiguous alphabet and the entropy of graphs, Transactions of the 6th Prague Conference on Information Theory (1973) 411–425.

[32] X. Li, I. Gutman, Mathematical Aspects of Randić–type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac, 2006.

[33] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.

[34] X. Li, Y. Yang, Sharp bounds for the general Randić index, MATCH Commun. Math. Comput. Chem. 51 (2004) 155–166.

[35] E. Lieberman, C. Hauert, M. A. Nowak, Evolutionary dynamics on graphs, Nature 433 (2005) 312–316.

[36] D. Lozovanu, S. Pickl, Discrete control and algorithms for solving antagonistic dynamic games on networks, Optimization 58 (2009) 665–683.

[37] A. Mowshowitz, Entropy and the complexity of the graphs I: An index of the relative complexity of a graph, Bull. Math. Biophys. 30 (1968) 175–204.

[38] S. Mukwembi, Effects of density of infected population to the spreading of HIV epidemic in communities, Physica A 390 (2011) 3915–3921.

[39] S. Mukwembi, B. G. Rodrigues, F. Nyabadza, Graph theoretic application to disease models, in: F.Nyabadza, M. Kgosimore, E. M. Lungu (Eds.), A Treatise of Biological Models, Nova, New York, 2012, pp. 97–126.

[40] V. Nikiforov, The energy of graphs and matrices, J. Math. Anal. Appl. 326 (2007) 1472–1475.

[41] H. S. Ramane, D. S. Revankar, I. Gutman, S. B. Rao, B. D. Acharya, H. B. Walikar, Bounds for the distance energy of a graph, Kragujevac J. Math. 31 (2008) 59–68.

[42] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609–6615.

[43] M. Randić, On history of the Randić index and emerging hostility toward chemical graph theory, MATCH Commun. Math. Comput. Chem. 59 (2008) 5–124.

[44] N. Rashevsky, Life, information theory and topology, Bull. Math. Biophys. 17 (1955) 229–235.

[45] P. Rényi, On measures of information and entropy, Proceedings of the 4th Berkeley Symposium on Mathematics, Statistics and Probability 1 (1967) 547–561.

[46] C. E. Shannon, W. Weaver, The Mathematical Theory of Communication, Univ. Illinois Press, 1949.

[47] L. Shi, Bounds on Randić indices, Discrete Math. 309 (2009) 5238–5241.

[48] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Wienheim, 2002.

[49] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.

[50] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance–based topological indices, MATCH Commun. Math. Comput. Chem. 71 (2014) 461–508.