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From the Connectivity Index to Various Randić-Type Descriptors*

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Abstract

The Randić index was proposed by Randić in 1975 and has been widely studied in different areas. We briefly review the Randić index and various Randić-type descriptors from 1975 to date, including higher-order Randić indices, zeroth order Randić indices, D-L-S generalization, sum-connectivity indices, geometric–arithmetic indices, harmonic index, atom–bond connectivity index, Balaban index, Randić matrix, Randić spectrum, Randić energy, etc. We also point out some important applications of the various Randić–type indices.

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1 Introduction

In theoretical chemistry and biology, molecular structure descriptors have been used for quantifying information on molecules. This relates to characterizing physico-chemical, toxicologic, pharmacologic, biological and other properties of chemical compounds by utilizing molecular indices. The so-called topological indices are an important class thereof. Actually, thousands of topological indices have been introduced in order to describe physical and chemical properties of molecules. Those indices can be divided into several classes, namely degree–based indices [74], distance–based indices [74, 140], eigenvalue–based indices [106] and mixed indices (e.g., [47]).

Various mathematical properties of topological indices have been investigated. As topological indices have been defined for quantifying information of graphs, this area could be classified into the so-called quantitative graph theory [39]. There is no doubt that the Randić index is the most studied, most often applied, and most popular graph measure among all. Numerous papers and a few books have been contributed when exploring this structural descriptor.

As a technical remark, we stipulate the graphs in this paper to be connected and simple. For details, we refer to [14, 81].

The Randić index R was proposed by Milan Randić in 1975 [124]. Already Randić noticed that there is a good correlation between R and several physico-chemical properties of alkanes, namely boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc. In subsequent years countless applications of R were reported, most of them concerned with exploring medicinal and pharmacological issues. A turning point in the mathematical examination of the Randić and general Randić index happened in the second half of the 1990s, when a significant and ever growing research field on this matter started, resulting in numerous publications. In this context, especially the contributions [9,10] due to Erdős should be mentioned.

After the Randić index was introduced, based on its definition various Randić–type invariants have been proposed and studied. This kind of research includes investigating higher-order Randić indices, zeroth-order Randić indices, its D-L-S generalization, sum-connectivity indices, geometric–arithmetic indices, harmonic index, atom–bond connectivity index, Balaban index, Randić matrix, Randić spectrum, Randić energy. In this

paper, we are going to survey the Randić index and various Randić–type invariants.

2 Randić index

Randić [124] defined the topological index

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

under the name "*connectivity index*", "*branching index*", and considered it as suitable for measuring the extent of branching of the carbon–atom skeleton of saturated hydrocarbons. Now it is well-known as *Randić index*. For more chemical applications of the Randić index, we refer to [90, 91]. Caporossi et al. [21] gave another description of the Randić index by using linear programming.

Theorem 2.1. *Let G be a graph with n vertices. Then*

$$R(G) = \frac{n - n_0}{2} - \frac{1}{2} \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \right)^2 . \tag{2}$$

If G is without isolated vertices, i.e., $n_0 = 0$, then Eq. (2) is simplified as

$$R(G) = \frac{n}{2} - \frac{1}{2} \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \right)^2 . \tag{3}$$

From Eq. (3), it is easy to see that regular graphs are the graphs with the maximum value of the Randić index among all connected graphs with n vertices. If the graph G of order n is not connected, and has no isolated vertices, then $R(G)$ is maximal, equal to $n/2$, if all components of G are regular graphs, not necessarily of the same order.

Later, Bollobás and Erdős [9] generalized this index by replacing $-1/2$ with any real number α,

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u\, d_v)^\alpha . \tag{4}$$

It has been called the *general Randić index*. This index was also widely investigated by mathematicians [7,10]. The case of $\alpha = -1$ is also of special interest [24,25,29]. Actually, in [10], the Randić index of hypergraphs has been investigated.

In order to characterize extremal values of Randić indices and the corresponding extremal graphs, many kinds of methods have been introduced, including graph–theoretical

methods, graph operations, linear and non-linear programming, integer programming, etc. The relations between the Randić index and other graph invariants (like the chromatic number [104], diameter and average distance [48, 105], etc) have been widely explored, see [133]. Especially, many conjectures and open problems have been stated by using the AutoGraphiX 2 software [3,20,22,23,84,85] and Graffiti [59–61]. A comprehensive summary and study of these mathematical results can be found in the monograph of Li and Gutman [102] and the survey of Li and Shi [103, 107]. To study chemical properties of the Randić index, see the three surveys written by Randić [125–127] as well as the book [128].

3 Higher-order Randić indices

The higher-order connectivity indices manifest an extension of the notion of the bond additive connectivity index to path additive indices, generalizing Platt's "influence of neighbour bonds on additive bond properties" [122].

For $m \geq 1$, one defines the m-Randić index (or m-th order Randić index) [91] by

$$ {}^{m}R(G) = \sum_{i_1 i_2 \ldots i_{m+1}} \frac{1}{\sqrt{d_{i_1}\, d_{i_2} \cdots d_{i_{m+1}}}} \,. $$

The summation runs over all trails $i_1 i_2 \ldots i_{m+1}$ of length m, contained in G. Note that in a trail an edge appears exactly once, but a vertex can appear more than once. Other researchers studied this index on "paths", instead of "trails". But it should be noted that in this case, the meaning is different. For more results on the higher–order Randić indices, we refer to [4, 55, 100, 103, 123, 141, 143].

4 Zeroth-order Randić indices

The zeroth-order Randić index, defined by Kier and Hall [92], is

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

Later Li and Zheng in [108] defined the zeroth-order general Randić index ${}^{0}R_{\alpha}(G)$ of a graph G by

$$ {}^{0}R_{\alpha}(G) = \sum_{v \in V(G)} d(u)^{\alpha} \qquad (5) $$

for general real numbers α. It should be noted that the same quantity has sometimes been referred to as the *general first Zagreb index* [90,91], in view of the fact that $\sum_u (d_u)^2$ is usually called *the first Zagreb index* [6,120]. If we set $\alpha = 1$ in Eq. (4), then $R_\alpha(G)$ is also called the *second Zagreb index*. For $\alpha = 3$ in Eq. (5), ${}^0R_\alpha(G)$ is also called the *forgotten topological index* or shortly the *F-index* [64]. The relation between the first Zagreb index and the second Zagreb index was also studied [109]. In fact, many studies of the Zagreb indices have been performed leading to useful applications in information theory and network reliability [19,27].

As a graph invariant, the sum of degree powers (zeroth-order general Randić index) has received considerable attention in graph theory and extremal graph theory, which is related to the famous Ramsey problems [67]. For more results, we refer to [1,11,12,67,72].

5 Generalizations of Randić indices

There exist many kinds of generalizations of the Randić index, where all those represent degree–based topological indices.

5.1 D-L-S generalization

In order to simplify the arguments on the relation between Randić index and the diameter, Dvořák et al. [48] introduced a modified version,

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

Based on this, very recently, Knor et al. [95] introduced two generalizations:

$$R'_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{\min\{d_u^\alpha, d_v^\alpha\}} \qquad \text{and} \qquad R''_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_u^\alpha, d_v^\alpha\}}$$

for any real number α. Clearly, the former is a lower bound for the general Randić index, and the latter is its upper bound. For more results on this index, see [95,134].

5.2 Sum–connectivity indices

Zhou and Trinajstić [145] generalized the connectivity index to the sum version. The *sum-connectivity index* of a graph $G = (V, E)$ is defined by

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

Similarly, the *general sum-connectivity index* is defined by [146]:

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

where α is an arbitrary real number.

5.3 Geometric–arithmetic indices

In [139], Vukičević and Furtula introduced a degree based topological index, which has been called the geometric–arithmetic index. The *geometric–arithmetic index* of a graph $G = (V, E)$ is defined by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u\, d_v}}{d_u + d_v} .$$

For more results on geometric–arithmetic indices, we refer to the survey paper [31].

5.4 Atom–bond connectivity index

Estrada et al. proposed a new index, nowadays known as the atom–bond connectivity (ABC) index [56]. This index is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u\, d_v}} .$$

Recently, The ABC index attracted much attention of mathematicians which resulted in vey many published papers. Especially much was studied the problem of finding the connected graph(s) of order n, having the smallest ABC-value. It is easy to show that such graphs must be trees, but the structure of these trees remained obscure. For details see [44–46] and the references cited therein.

Graovac and Ghorbani [68] came up with a new version of the ABC index, which recently has been named the *Graovac–Ghorbani index* [62]. Recently, Estrada [54] introduced the concept of ABC matrix and then study some indices related to the eigenvalues of the ABC matrices, such as the ABC energy and the ABC Estrada index.

Trying to boost the predictive power of the ABC index, Furtula et al. [63] put forward its modified version, named *augmented Zagreb index*. It has been defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u \, d_v}{d_u + d_v - 2} \right)^3 .$$

5.5 Harmonic index

In [144], Zhong studied the harmonic index, which first appeared in [59] and recently is widely studied. For a graph G, the *harmonic index* is defined as

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

The relation between the harmonic index and the ABC index was investigated in [82].

5.6 Balaban index

The main weakness of the Randić index, as well as of other vertex–degree–based molecular descriptors, is its unacceptably low isomer discriminative power. In 1992, Balaban tried to overcome this problem by introducing an extension of the Randić index [5]. Nowadays this topological index is named after its inventor. The Balaban index is regarded as one of the topological descriptors with the highest discriminative power.

In order to define the Balaban index, some graph theoretical terms need to be properly introduced. The distance $dist(u, v)$ between the vertices u and v in a graph is equal to the number of edges in a shortest path that connects them. The transmission of a vertex u in a graph is

$$\sigma(u) = \sum_{v \in V(G)} dist(u, v) .$$

The Balaban index [5] is then defined as

$$J(G) = \frac{m}{m - n + 2} \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma(u) \, \sigma(v)}} \tag{6}$$

where m and n are the number of edges and vertices in a graph G, respectively. The term $\frac{1}{\sqrt{\sigma(u) \, \sigma(v)}}$ in the definition of $J(G)$ is evidently a replica of the analogous term in the definition of the Randić index $R(G)$, Eq. (1). The multiplier $m/(m - n + 2)$ in the

definition of the Balaban index serves to normalize its numerical value, i.e., to prevent that it increases with the increasing size of the molecular graph.

The main feature of the Balaban index is its extremely high isomer discriminating power.

Initially, this topological invariant was investigated exclusively as a molecular descriptor in various QSPR/QSAR researches. Twenty years after its creation, this index has also started to appear in mathematically oriented articles. Nowadays, there is a vast literature considering this structural molecular descriptor. For more details consult the recent papers [28, 57, 58, 93, 94, 96–98].

6 Randić matrix

The concept of Randić matrix was introduced in 2005 by Rodríguez [130], but the name "*Randić matrix*" was first used by Bozkurt et al. [15, 16]. The Randić matrix of a graph $G = (V, E)$, denoted by $\mathbf{R}(G)$, is a matrix whose rows and columns are indexed by the vertices of G and possess the following entries

$$R_{ij} = \begin{cases} \frac{1}{\sqrt{d_i\, d_j}} & \text{if } ij \in E(G) \\ 0 & \text{otherwise.} \end{cases}$$

For a graph G without isolated vertices, the Randić matrix can be written as [15, 16]

$$\mathbf{R}(G) = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} \tag{7}$$

where $\mathbf{A}$ is the adjacency matrix and $\mathbf{D}$ is the diagonal matrix of vertex degrees. Observe that this matrix is symmetric and non-negative. The connection between the Randić matrix and the Randić index is obvious; the sum of all elements of $\mathbf{R}(G)$ is equal to $2R_{-1/2}(G)$. As a consequence of Eq. (7), for graphs without isolated vertices, the Randić matrix of G has the same inertia as its adjacency matrix $\mathbf{A}$. The Randić matrix plays an outstanding role in the theory of Laplacian graph spectra, see [16].

In recent days, the Randić matrix became more popular leading to numerous results, see, e.g., [8]. In [41], Dehmer et al. defined novel graph measures based on the zeros of the characteristic polynomial by using the Randić matrix. Based on these eigenvalues, they obtained graph measures with high discrimination power [41]. In addition, Estrada [52] introduced the Randić polynomial in 1999.

Recently, the general Randić matrix [70], Randić incidence matrix [69], and the Randić Laplacian matrix and Randić signless Laplacian matrix [110] have been also defined and investigated.

7 Randić spectrum and Randić energy

The *Randić spectrum* of a graph G is the spectrum of the Randić matrix $\mathbf{R}(G)$. Let $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ be the eigenvalues of the Randić matrix $\mathbf{R}(G)$. The greatest eigenvalue ρ_1, the Randić spectral radius, is equal to 1 for all graphs. In [65, 66], the concept of Randić spread of a graph G, $sR(G)$, was defined as

$$sR(G) = \rho_2 - \rho_n$$

For more results on Randić spectrum and Randić spread, we refer to [2, 15, 16].

The energy $\mathcal{E}(G)$ of a graph G is defined as the sum of the absolute values of its eigenvalues. Based on different kinds of graph matrices, various graph energies are defined and investigated. Graph energies are well-studied and for details on graph energy, see the reviews [73, 75, 76, 78, 79, 106]. The respective *Randić energy* was defined in [16] as

$$RE(G) = \sum_{i=1}^{n} |\rho_i| .$$

For more results on Randić energy, we refer to [80] and the survey paper [33].

Recently, the concepts of general Randić energy [70], Randić incidence energy [69], skew Randić matrix, skew Randić energy [71], Hermitian–Randić matrix, and Hermitian–Randić energy [113] were introduced and investigated.

8 Applications of Randić indices

Except for its applications in chemistry, the Randić index has many applications in other areas, such as information theory [77, 99], network similarity [121], protein alignment [127]. For example, the Randić index can be used to study network heterogeneity [53, 83] and network robustness [34]. In this section, we mention two of them, namely network similarity and graph entropy. For more applications, we refer the readers to [125–127].

8.1 Network similarity

Methods to determine the structural similarity or distance between networks or graphs have been applied in many areas of sciences. For example, in mathematics [40, 136, 142], in biology [50, 89, 92], in chemistry [13, 135] and in chemoinformatics [137]. Other application–oriented areas where graph comparison techniques have been employed can be found in [40, 86, 114]. For more results on graph similarities, we refer to our recent survey [51].

The Randić index can be used in the study of chemical similarity [121]. Moreover, as a topological index, Randić index can be used to define a similarity measure, which is computed in a polynomial time. In [37], Dehmer et al. introduced a distance measure based on topological indices. Now we define the distance measure [131]

$$d(x,y) = 1 - e^{-\left(\frac{x-y}{\sigma}\right)^2} \tag{8}$$

which is a mapping $d : \mathbb{R} \times \mathbb{R} \longrightarrow \mathbb{R}_+$. Obviously it holds $d(x,x) = 0$, $d(x,y) \geq 0$, and $d(x,y) = d(y,x)$. In order to translate this concept to graphs, we employ topological indices [37] and obtain

$$d_I(G,H) := d(I(G), I(H)) = 1 - e^{-\left(\frac{I(G)-I(H)}{\sigma}\right)^2}.$$

If we let $I(G) = R(G)$, then we can calculate the similarity measure $d_R(G,H)$ easily. Actually, for graphs G and H from one class of graphs, the relations between d_R and d_W, d_{0^R}, $d_{\mathcal{E}}$ are studied in [37], where W, 0^R, and $\mathcal{E}$ denote the Wiener index, zeroth-order Randić index and graph energy, respectively. This measure is recently widely investigated [37, 38] and also is compared with graph edit distance [101].

8.2 Graph entropy

The study of entropy measures for exploring network-based systems emerged in the late fifties based on the seminal work due to Shannon [132]. Rashevsky [129] used the concept of graph entropy to measure the structural complexity of graphs. Mowshowitz [116–119] introduced the entropy of a graph as an information-theoretic quantity and interpreted it as the structural information content of a graph.

Definition 8.1. *Let $p = (p_1, p_2, \ldots, p_n)$ be a probability vector, namely, $0 \leq p_i \leq 1$ and $\sum_{i=1}^{n} p_i = 1$. The Shannon's entropy of p is defined as*

$$I(p) = -\sum_{i=1}^{n} p_i \log p_i \,.$$

In order to define information-theoretic graph measures, we will often consider a tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ of non-negative integers $\lambda_i \in \mathbb{N}$ [35]. This tuple forms a probability distribution $p = (p_1, p_2, \ldots, p_n)$, where

$$p_i = \frac{\lambda_i}{\sum_{j=1}^{n} \lambda_j} \quad , \quad i = 1, 2, \ldots, n \,.$$

Therefore, the entropy of the tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is given by

$$I(\lambda_1, \lambda_2, \ldots, \lambda_n) = -\sum_{i=1}^{n} p_i \log p_i = \log\left(\sum_{i=1}^{n} \lambda_i\right) - \sum_{i=1}^{n} \frac{\lambda_i}{\sum_{j=1}^{n} \lambda_j} \log \lambda_i \,.$$

In the literature, there are various ways to obtain the tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$, like the so-called magnitude-based information measures introduced by Bonchev and Trinajstić [13], or partition-independent graph entropies, introduced by Dehmer [35,43], which are based on information functionals.

We are now ready to define the entropy of a graph due to Dehmer [35] by using information functionals.

Definition 8.2. *Let $G = (V, E)$ be a connected graph. For a vertex $v_i \in V$, we define*

$$p(v_i) := \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)}$$

where f represents an arbitrary information functional.

Observe that $\sum_{i=1}^{|V|} p(v_i) = 1$. Hence, we can interpret the quantities $p(v_i)$ as vertex probabilities.

Now we immediately obtain one definition of a graph entropy.

Definition 8.3. *Let $G = (V, E)$ be a connected graph and f be an arbitrary information functional. The entropy of G is defined as*

$$\begin{aligned} I_f(G) &= -\sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log\left(\frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)}\right) \\ &= \log\left(\sum_{i=1}^{|V|} f(v_i)\right) - \sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log f(v_i) \,. \end{aligned} \tag{9}$$

In [19], Cao et al. define a novel information functional which is based on degree powers of graphs. Define the information functional as:

$$f := d_i^\alpha$$

where d_i is the degree of the vertex v_i and α is an arbitrary real number. Therefore, by applying the definition and Eq. (9), we obtain the special graph entropy

$$I_f(G) = -\sum_{i=1}^{n} \frac{d_i^\alpha}{\sum_{j=1}^{n} d_j^\alpha} \log\left(\frac{d_i^\alpha}{\sum_{j=1}^{n} d_j^\alpha}\right) = \log\left(\sum_{i=1}^{n} d_i^\alpha\right) - \sum_{i=1}^{n} \frac{d_i^\alpha}{\sum_{j=1}^{n} d_j^\alpha} \log d_i^\alpha \,.$$

After it was introduced, the entropy is widely studied and many related papers on theoretical aspects [17,18,27,30,32,87,111,112] and application aspects [88,115,138,147] are published.

In order to investigate the influence of the structure of social relations between individuals of community's economic development, Eagle et al. [49] developed two new metrics, social diversity and spatial diversity, to capture the social and spatial diversity of communication ties within a social network of each individual, by using the entropy for vertices. Following this, Chen et al. introduced the concept of graph entropy for weighted graphs [26], especially using the Randić weights.

For more results on network entropies, we refer the readers to the survey [42] and the recent edited book [36].

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