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Inverse sum indeg index of graphs

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Abstract

The inverse sum indeg index $ISI(G)$ of a simple graph G is defined as the sum of the terms $\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)}$ over all edges uv of G, where $d_G(u)$ denotes the degree of a vertex u of G. In this paper, we present several upper and lower bounds on the inverse sum indeg index in terms of some molecular structural parameters and relate this index to various well-known molecular descriptors.

Keywords: Zagreb index; Inverse sum indeg index; Composite graph

1. Introduction

Molecular descriptors, results of functions mapping molecule's chemical information into a number [1], have found applications in modeling many physicochemical properties in QSAR and QSPR studies [2,3]. A particularly common type of molecular descriptors are those that are defined as functions of the structure of the underlying molecular graph, such as the Wiener index [4], the Zagreb indices [5], the Randić index [6] or the Balaban J-index [7]. Damir Vukicević and Marija Gasperov [8] observed that many of these descriptors are defined simply as the sum of individual bond contributions.

Among the 148 discrete Adriatic indices studied in [8], whose predictive properties were evaluated against the benchmark datasets of the International Academy of Mathematical Chemistry [9], 20 indices were selected as significant predictors of physicochemical properties. In this connection, Sedlar et al. [10] studied the properties of the inverse sum indeg index, the descriptor that was selected in [8] as a significant predictor of total surface area of octane isomers and for which the extremal graphs obtained with the help of Math. Chem. have a particularly simple and elegant structure. The *inverse sum indeg index* is defined as

$$ISI(G) = \sum_{uv \in E(G)} \frac{1}{\frac{1}{d_G(u)} + \frac{1}{d_G(v)}} = \sum_{uv \in E(G)} \frac{d_G(u)d_G(v)}{d_G(u) + d_G(v)}.$$

Extremal values of inverse sum indeg index across several graph classes, including connected graphs, chemical graphs, trees and chemical trees were determined in [10]. The bounds of a descriptor are important information of

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a molecular graph in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters. In [11], some sharp bounds for the inverse sum indeg index of connected graphs are given. The inverse sum indeg index of some nanotubes is computed in [12]. In this connection, we present several upper and lower bounds on the inverse sum indeg index in terms of some molecular structural parameters and relate this index to various well-known molecular descriptors.

The Zagreb indices are among the oldest topological indices, and were introduced by Gutman and Trinajstić [5] in 1972. These indices have since been used to study molecular complexity, chirality, ZE-ismerism and hetero-systems. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively, and defined as $M_1(G) = \sum_{v\in V(G)}(d_G(v))^2 = \sum_{uv\in E(G)}(d_G(u) + d_G(v))$ and $M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$.

In 1975, Milan Randić [6] proposed a structural descriptor, based on the end-vertex degrees of edges in a graph, called the branching index that later became the well-known Randić connectivity index. The *Randić index* $R(G)$ of G is defined as $R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$. The Randić index is one of the most successful molecular descriptors in QSPR and QSAR studies, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons.

Another variant of the Randić connectivity index named the harmonic index was introduced by Fajtlowicz [13] in 1987. The *harmonic index* $H(G)$ of G is defined as $H(G) = \sum_{uv\in E(G)} \frac{1}{d(u)+d(v)}$.

The eccentric connectivity index was introduced by Sharma et al. [14] in 1997. The *eccentric connectivity index* $\xi^c(G)$ of G is defined as $\xi^c(G) = \sum_{uv\in E(G)} d(u)\epsilon_u$. The eccentric connectivity index can also be expressed as a sum over edges of G, $\xi^c(G) = \sum_{uv\in E(G)}(\epsilon_u + \epsilon_v)$, where the eccentricity ϵ_u of a vertex u is the largest distance between u and any other vertex of G.

The *Zagreb eccentricity indices* were introduced by VukiceviĹc and Graovac [15] in 2010. These indices are defined in analogy with the Zagreb indices by replacing the vertex degrees with the vertex eccentricities. Thus, the first and second Zagreb eccentricity indices of G are defined as

$$\xi_1(G) = \sum_{u\in V(G)} \epsilon_u^2 \quad \text{and} \quad \xi_2(G) = \sum_{uv\in E(G)} \epsilon_u\epsilon_v.$$

Recently, Shirdel et al. [16] introduced a variant of the first Zagreb index called hyper-Zagreb index. The *hyper-Zagreb index* of G is denoted by $HM(G)$ and defined as $HM(G) = \sum_{uv\in E(G)}(d(u) + d(v))^2$.

2. Bounds on *ISI*-index of connected graphs

In this section, we obtain the upper and lower bounds for the inverse sum indeg index of a connected graph. We denote by Δ and δ the maximum and minimum vertex degrees of G, respectively.

Lemma 2.1 ([17]). *Suppose a_i and b_i, $1 \le i \le n$ are positive real numbers, then*

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \le \alpha(n)(A-a)(B-b),$$

where a, b, A and B are real constants, that for each i, $1 \le i \le n, a \le a_i \le A$ and $b \le b_i \le B$. Further, $\alpha(n) = n\left\lceil\frac{n}{2}\right\rceil\left(1 - \frac{1}{n}\left\lceil\frac{n}{2}\right\rceil\right)$. ■

Theorem 2.2. *Let G be a graph on n vertices and m edges. Then $ISI(G) \le \frac{\alpha(m)(\delta-\Delta)(\Delta^2-\delta^2)}{2m\delta\Delta} + \frac{H(G)M_2(G)}{2m}$, where $\alpha(m) = m\left\lceil\frac{m}{2}\right\rceil\left(1 - \frac{1}{m}\left\lceil\frac{m}{2}\right\rceil\right)$ with equality if and only if G is regular.*

Proof. We choose $a_i = \frac{1}{d_G(u)+d_G(v)}$, $b_i = d_G(u)d_G(v)$, $a = \frac{1}{2\delta}$, $A = \frac{1}{2\Delta}$, $b = \delta^2$ and $B = \Delta^2$, in Lemma 2.1, we obtain

$$\left| m\sum_{uv\in E(G)} \frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)} - \sum_{uv\in E(G)} \frac{1}{d_G(u)+d_G(v)} \sum_{uv\in E(G)} d_G(u)d_G(v) \right| \le \alpha(m)\Big(\frac{1}{\Delta} - \frac{1}{\delta}\Big)(\Delta^2 - \delta^2).$$

From the definitions of *ISI* and harmonic index, we have

$$mISI(G) - \frac{H(G)}{2}M_2(G) \le \alpha(m)\Big(\frac{\delta-\Delta}{2\delta\Delta}\Big)(\Delta^2 - \delta^2).$$

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