Chapter 5
Inverse Sum Indeg Index of Subdivision, t–Subdivision Graphs, and Related Sums

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ABSTRACT

The inverse sum indeg (ISI) index of a graph G is defined as the sum of the weights dG(u)dG(v)/ dG(u)+dG(v) of all edges uv in G, where dG(u) is the degree of the vertex u in G. This index is found to be a significant predictor of total surface area of octane isomers. In this chapter, the authors present some lower and upper bounds for ISI index of subdivision graphs, t-subdivision graphs, s-sum and st -sum of graphs in terms of some graph parameters such as order, size, maximum degree, minimum degree, and the first Zagreb index. The extremal graphs are also characterized for their sharpness.

INTRODUCTION

A topological index (TI), also known as graph-based molecular descriptor, is a mapping $T : \Im \to \mathbb{R}$ from the collection of graphs $\Im$ to the set $\mathbb{R}$ of real numbers which characterizes numerically a topological structure of a molecular graph numerically. It is a graph invariant which does not depend on the labelling or the pictorial representation of a graph, i.e., $T\left(G\right) = T\left(H\right)$ iff the graphs *G* and *H* are isomorphic. The values of these indices are very helpful in predicting various physical and chemical properties of a molecular compound, among them boiling point, melting point, strain energy, stability, surface tension of isomers are to name a few. It studies quantitative structure–activity relationship (QSAR) and

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quantitative structure–property relationship (QSPR) which are used in predicting the biological activities and properties of the chemical compounds.

The first TI was defined by Wiener in the year 1947 (Wiener, 1947), named after his name as Wiener index which is a distance-based TI. Historically Zagreb indices can be considered as the first degree-based topological indices, which came into picture during the study of total π-electron energy of alternant hydrocarbons by Gutman and Trinajstić in 1972 (Gutman & Trinajstić, 1972). Since then many topological indices are proposed and studied based on degree, distance and other parameters of graph. Inverse sum indeg or simply ISI index is relatively a new addition to this wide list of degree based topological indices.

Formally the ISI index can be defined as

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

ISI index was selected by Vukičević and Gašperov (Vukičević & Gašperov, 2010) as a significant predictor of total surface area of octane isomers, and included in the list of 20 (twenty) indices which were selected as significant predictors of physico-chemical properties of a molecular compound out of a list of 148 discrete Adriatic indices considered in their study.

The study of ISI index for various operations of graphs is found to be limited in literature. Sedlar and Stevanović et al. determined extremal values of ISI index across several graph classes, including connected graphs, chemical graphs, trees and chemical trees (Sedlar, Stevanović, & Vasilyev, 2015). Some exact formulas for the inverse sum indeg index of some nanotubes is computed in (Falahati-Nezhad & Azari, 2016). In 2017, Falahati-Nezhad and Azari, et al. again published a paper (Falahati-Nezhad, Azari & Došlić, 2017) on ISI index in which several sharp upper and lower bounds for ISI index in terms of the order, size, radius, number of pendant vertices, minimal and maximal vertex degrees, and minimal non-pendent vertex degree are presented, and linked this index to various well-known TIs such as the Zagreb indices, Randić index, sum-connectivity index, modified Zagreb index, harmonic index, forgotten index, and eccentric connectivity index. Some extremal molecular graphs with the minimum and the maximum value of ISI index in $MG\left(i,n\right)$, where $MG\left(i,n\right)$ is the class of all *n*-vertex molecular graphs with minimum degree *i*, is proposed in Hasani (2017). In Pattabiraman (2018), several upper and lower bounds on the ISI index is presented in terms of some molecular structural parameters and linked this index to various well-known molecular descriptors. Some sharp bounds for ISI index of graphs with given matching number, independence number and vertex-connectivity are presented and characterized the extremal graphs for which the bounds are obtained in An and Xiong (2018). Chen and Deng derived some bounds for ISI index in terms of vertex (edge) connectivity, chromatic number, vertex bipartiteness etc. in Chen and Deng (2018). Gao and Jamil et al. computed ISI index of some chemical graphs (Gao, Jamil, Javed, Farahani, & Imran, 2018) by using the line graphs of subdivision of the graphs. In Gutman, Matejić, Milovanović, and Milovanović (2020) some lower bounds of ISI index reported in the literature are analysed and determined some new lower bounds for ISI index. Very recently, Gutman and Rodríguez et al. has established some linear and non-linear inequalities of ISI index in terms maximum degree, minimum degree, vertices and edges, and in terms of some well-known topological index in which some inequalities are also generalised (Gutman, Rodríguez, & Sigarreta 2019).