Chapter 4
A Novel Weighted First Zagreb Index of Graph

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ABSTRACT

The Zagreb indices are the oldest among all degree-based topological indices. For a connected graph G, the first Zagreb index $M_1(G)$ is the sum of the term $d_G(u)+d_G(v)$ corresponding to each edge uv in G, that is, $M_1(G)=\sum_{UV\in E(G)}[(d_{G(u)}+d_{G(v)})]$, where $d_G(u)$ is degree of the vertex u in G. In this chapter, the authors propose a weighted first Zagreb index and calculate its values for some standard graphs. Also, the authors study its correlations with various physico-chemical properties of octane isomers. It is found that this novel index has strong correlation with acentric factor and entropy of octane isomers as compared to other existing topological indices.

INTRODUCTION

The introduction of topological index or molecular structure descriptor in literature is a great success as it can correlate various physical properties, biological reactivity or chemical activity of molecules without undergoing actual experimentation. A topological index is a real number that can be associated to a molecule based on its molecular graph. A molecular graph is a simple graph corresponding to a molecule in which vertices represents atoms and edges represents various chemical bonds between them. For historical background of the topological index interested reader can go through (Trinajstić, 2011). The success of this simple mathematical quantity is because of the fact that the properties of a chemical compound is highly related to its molecular structure and we calculate the indices directly from the molecular graph of a molecule using various graph theoretic notions (e.g. degree, distance, etc). Some of the topological indices may be found in (Das & Tinajstić, 2010; Gutman, 2013; Estrada, 2000; Gutman, Milovanović & et al., 2018) and the references therein.

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Throughout the chapter only undirected, finite and simple connected graphs are considered. The degree of a vertex u in a graph G is the number of vertices incident on u and it is denoted as $d_G(u)$ or simply as $d(u)$ if there is no scope for confusion. The notation $uv \in E(G)$ represents any edge between two vertices u and v in a graph G. $d(u,v)$ is used to denote the distance between vertices u and v which is nothing but the length of the shortest path between u and v. The status of a vertex u in a graph G is denoted by $\sigma_G(u)$ or simply $\sigma(u)$ and is defined as the sum of distances of all other vertices from u in G.

Among all the degree based topological indices that exist in literature, the Zagreb indices are the oldest (Gutman, 2013). The Zagreb indices are defined by Gutman and Trinajstić in 1972 during their study of the total π electron energy of alternant hydrocarbons (Gutmam & Trinajstić, 1972). They have defined these indices as

$$M_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right] \text{and } M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v),$$

where M_1 is called first Zagreb index and M_2 is called the second Zagreb index. Some of the research works on these indices can be seen in (Deng, Sarala & et al., 2016; Da Fonseca & Stevanović, 2014; Gutman & et al., 2015; Khalifeh, Yousefi-Azari & et al., 2009) and references cited therein. In 2016 Ramane & et al. defined a status based topological index and called it as Harmonic status index (HS). For a connected graph G, HS is given as

$$HS(G) = \sum_{uv \in E(G)} \frac{2}{\sigma(u) + \sigma(v)}.$$

In the next section, the authors propose a new topological index which is basically a weighted version of first Zagreb index. Then, the values of this newly proposed index for some of the popular graphs are provided. Further a study of the correlation of this novel index with various physicochemical properties of octane isomers is also reported in this chapter and at the end of the chapter, the conclusions are made.

WEIGHTED FIRST ZAGREB INDEX

In Llić & Milosavljević (2017) the authors introduced a new topological index and named it as *Weighted Szeged index*. This index is defined as

$$wSz(G) = \sum_{uv \in E(G)} \left[d(u) + d(v)\right].n_u(e).n_v(e)$$

where $n_u(e)$ is cardinality of the set

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