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On the extremal graphs with respect to bond incident degree indices

Akbar Ali [a], Darko Dimitrov [b,c,*]

[a] Department of Mathematics, University of Management & Technology, Sialkot, Pakistan
[b] Hochschule für Technik und Wirtschaft Berlin, Germany
[c] Faculty of Information Studies, Novo mesto, Slovenia

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ABSTRACT

Many existing degree based topological indices can be classified as bond incident degree (BID) indices, whose general form is $\mathrm{BID}(G) = \sum_{uv\in E(G)} f(d_u, d_v)$, where uv is the edge connecting vertices u, v of the graph G, $E(G)$ is the edge set of G, d_u is the degree of a vertex u and f is a non-negative real valued (symmetric) function of d_u and d_v. Firstly, here an intuitively expected result is proven, which states that an extremal (n, m)-graph with respect to the BID index (corresponding to f) must contain at least one vertex of degree $n-1$ if f satisfies certain conditions. It is shown that these certain conditions are satisfied for the general sum-connectivity index (whose special cases are the first Zagreb index and the Hyper Zagreb index), for the general Platt index (whose special cases are the first reformulated Zagreb index and the Platt index) and for the variable sum exdeg index. With help of the aforementioned result of existence of at least one vertex of degree $n-1$ and further analysis, graphs with maximum values of the above mentioned BID indices among tree, unicyclic, bicyclic, tricyclic and tetracyclic graphs are characterized. Some of these results are new and the already existing results are proven in a shorter and more unified way.

1. Introduction

It is well known fact that molecules can be represented by graphs in which vertices correspond to the atoms while edges represent the covalent bonds between atoms [10,32]. Predicting physicochemical properties of molecules is considered to be a fascinating issue in theoretical chemistry. Many predictive methods have been developed for correlating molecular structures with their physicochemical properties. One of the simplest such methods involves topological indices [4]. Topological indices are numerical quantities of a graph which are invariant under graph isomorphism. The Wiener index (a distance based topological index) is the oldest topological index, which was devised in 1947 for predicting the boiling points of paraffins [37]. The Platt index (Pl), proposed for predicting paraffin properties [25], belongs to the oldest degree based topological indices:

$$Pl(G) = \sum_{uv\in E(G)} (d_u + d_v - 2),$$

where uv is the edge connecting the vertices u, v of the graph G, $E(G)$ is the edge set of G and d_u is the degree of the vertex u. Several authors (see for example [5,9]) used the notation F for representing the Platt index. However, this notation is being

* Corresponding author at: Hochschule für Technik und Wirtschaft Berlin, Germany.
E-mail addresses: akbar.ali@skt.umt.edu.pk (A. Ali), dimitrov@htw-berlin.de (D. Dimitrov).

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also used for the forgotten topological index [11]. Thereby, we use Pl, instead of F, for representing the Platt index. It is worth mentioning here that the Platt index can be written as $Pl(G) = M_1(G) - 2m$ where m is the size of G and M_1 is the first Zagreb index, appeared in 1972 within the study of total π-electron energy [15], which can be defined as:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

Because of the relation $Pl(G) = M_1(G) - 2m$ and the following lemma, it is clear that the Platt index is also related to the size of $L(G)$, the line graph of G:

Lemma 1.1 (*[16]*). *If G is an (n, m)-graph then the size of $L(G)$ is $\frac{M_1(G)}{2} - m$.*

Gutman and Estrada [14] proposed line-graph-based topological indices: if $I(G)$ is a topological index that can be computed from a graph G, then there is another topological index $i(G)$ such that $i(G) = I(L(G))$. Applying this idea to first general Zagreb index (also known as zeroth-order general Randić index) [23], gives general Platt index:

$$Pl_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)^\alpha,$$

$\alpha \in \mathbb{R} \setminus \{0\}$. It needs to be mentioned here that Pl_2 coincides with the first reformulated Zagreb index [24].

Zhou and Trinajstić [39] introduced the general sum-connectivity index:

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

$\alpha \in \mathbb{R} \setminus \{0\}$. Note that χ_1 is the first Zagreb index and χ_2 is the Hyper-Zagreb index [27]. Details about general sum-connectivity index can be found in the recent papers [1,7,29–31,40] and related references cited therein.

In 2011, Vukičević [34] proposed the following topological index (and named it as the variable sum exdeg index) for predicting the octanol–water partition coefficient of certain chemical compounds:

$$SEI_a = \sum_{uv \in E(G)} (a^{d_u} + a^{d_v}),$$

$a \in \mathbb{R}^+ \setminus \{1\}$. Details about variable sum exdeg index can be found in the papers [13,33,38].

So far, numerous topological indices have been and are being introduced. A considerable amount of existing degree based topological indices (such as the (general) Platt index, first Zagreb index, variable sum exdeg index, generalized sum-connectivity index, etc.) can be written [17,36] in the following form:

$$\mathrm{BID}(G) = \sum_{uv \in E(G)} f(d_u, d_v), \tag{1}$$

where f is a non-negative real valued (symmetric) function of d_u and d_v. The topological indices which have the form (1) are called *bond incident degree indices* [35] (BID indices in short). BID indices form a subset of the set of all *vertex-degree-based topological indices* [6,26]. Higher order Randić indices [22] are the examples of vertex-degree-based topological indices, which are not BID indices. The problem of characterizing extremal graphs with respect to certain BID indices among the set of all n-vertex tree, unicyclic, bicyclic, tricyclic and tetracyclic graphs is one of the most studied problems in chemical graph theory. In many cases, the extremal graphs for different BID indices are same or have some common properties. The main purpose of the present note is to attack the aforementioned problem for general BID indices. Here, it is proved that if a BID index satisfy some certain conditions then the extremal (n, m)-graph with respect to the BID index (under consideration) must contain at least one vertex having degree $n - 1$. Using this result, graphs having maximum general sum-connectivity index, general Platt index and variable sum exdeg index in the collections of all n-vertex tree, unicyclic, bicyclic, tricyclic and tetracyclic graphs are characterized and several existing results [12,13,18,20,21,28,40] are obtained as corollaries.

All the graphs considered in the present study are finite, undirected, simple and connected. An (n, m)-graph (connected) is said to be a tree, unicyclic graph, bicyclic graph, tricyclic graph, tetracyclic graph if $m = n - 1$, $m = n$, $m = n + 1$, $m = n + 2$, $m = n + 3$ respectively. For a vertex $u \in V(G)$, the set of all vertices adjacent with u is denoted by $N_G(u)$ (the neighborhood of u). A vertex $v \in V(G)$ of degree 1 is called pendent vertex. A vertex, which is not pendent is called as non-pendent vertex. As usual, the n-vertex star graph is denoted by S_n. The unique n-vertex unicyclic graph obtained from S_n by adding an edge is denoted by S_n^+. Undefined notations and terminologies from (chemical) graph theory can be found in [10,16,32].

2. Preliminaries

In order to obtain the main results, we need to establish some preliminary results. Firstly, we present the following lemma, related to the function f introduced in (1).

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