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On the Steiner hyper-Wiener index of a graph

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ABSTRACT

In this paper, we study the Steiner hyper-Wiener index of a graph, which is obtained from the standard hyper-Wiener index by replacing the classical graph distance with the Steiner distance. It is shown how this index is related to the Steiner Hosoya polynomial, which generalizes similar result for the standard hyper-Wiener index. Next, we show how the Steiner 3-hyper-Wiener index of a modular graph can be expressed by using the classical graph distances. As the main result, a method for computing this index for median graphs is developed. Our method makes computation of the Steiner 3-hyper-Wiener index much more efficient. Finally, the method is used to obtain the closed formulas for the Steiner 3-Wiener index and the Steiner 3-hyper-Wiener index of grid graphs.

1. Introduction

The Wiener index and the hyper-Wiener index are distance-based graph invariants, used as structure descriptors for predicting physicochemical properties of organic compounds (often those significant for chemistry, pharmacology, agriculture, environment-protection etc.). Their history goes back to 1947, when H. Wiener used the distances in the molecular graphs of alkanes to calculate their boiling points [40]. This research has led to the Wiener index, which is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

for any connected graph G. The origins and applications of the Wiener index are discussed in [36], while some recent research related to this index can be found in [3,23–25].

The hyper-Wiener index was introduced in 1993 by Randić [35] and has been extensively studied in many papers (see, for example, [6,20,43]). Randić's original definition of the hyper-Wiener index was applicable just to trees and therefore, the hyper-Wiener index was later defined for any connected graph G [21] as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v)^2.$$

The hyper-Wiener index is related to the Hosoya polynomial [14], which is defined as

$$H(G,x) = \sum_{m \geq 0} d(G,m) x^m,$$

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where $d(G, m)$ is the number of unordered pairs of vertices at distance m. In [4] the following relation was shown:

$$WW(G) = H'(G,1) + \frac{1}{2}H''(G,1).$$

Distance-based topological indices were extensively investigated and also the edge versions were studied [39]. Many methods for computing these indices more efficiently were proposed and the most famous between them is the cut method [18]. This method is commonly used on benzenoid systems [8,38] or on partial cubes [7], which constitute a large class of graphs with a lot of applications and includes, for example, many families of chemical graphs (benzenoid systems, trees, phenylenes, cyclic phenylenes, polyphenylenes). In particular, methods for computing the hyper-Wiener index and the edge-hyper-Wiener index were introduced in [17,37].

The Steiner distance of a graph, introduced by Chartrand et. al. in 1989 [5], is a natural and nice generalization of the concept of classical graph distance. For a set $S \subseteq V(G)$, the Steiner distance $d(S)$ among the vertices of S is the minimum size among all connected subgraphs whose vertex sets contain S. The Steiner distance in a graph was considered in many papers, for some relevant investigations see [2,11,33,34,41] and a survey paper [28]. On the other hand, the Steiner tree problem requires a tree T with minimum number of edges such that $S \subseteq V(T)$. In general, this problem is known to be NP-complete [15]. The Steiner distance and the Steiner tree problem have a lot of applications in real-word problems, for example in circuit layout, network design and in modeling of biomolecular structures [32].

If in the definition of the Wiener index the classical graph distance is replaced by the Steiner distance, the Steiner Wiener index is obtained [26]. In particular, if we replace the distances between pairs of vertices by the distances of all subsets with cardinality k, we obtain the Steiner k-Wiener index. It was shown in [13] that for some molecules the combination of the Steiner Wiener index and the Wiener index has even better correlation with the boiling points than the Wiener index. For some recent investigations on the Steiner Wiener index see [27,29,31]. However, a closely similar concept was already studied in the past under the name average Steiner distance [9,10]. Moreover, the Steiner degree distance [12,30] and other analogous generalizations of distance-based molecular descriptors (where the classical distance is replaced by the Steiner distance) were introduced [28].

In [26] the relation between the Steiner 3-Wiener index and the Wiener index was shown for trees and later for modular graphs [22] (see the definition in the preliminaries). In this paper, we first prove the relation between the Steiner hyper-Wiener index and the Steiner Hosoya polynomial. Next, we show how the Steiner 3-hyper-Wiener index of a modular graph can be expressed by using the classical graph distances. Furthermore, if G is a partial cube, we develop a cut method for computing the Steiner 3-hyper-Wiener index, which enables us to compute the index very efficiently and also to find the closed formulas for some families of graphs. Finally, our method is used to obtain the closed formulas for the Steiner 3-Wiener index and the Steiner 3-hyper-Wiener index of grid graphs.

2. Preliminaries

Unless stated otherwise, the graphs considered in this paper are simple and finite. For a graph G we say that $|V(G)|$ is the *order* of G and that $|E(G)|$ is its *size*. Moreover, we define $d_G(x, y)$ (or simply $d(x, y)$) to be the usual shortest-path distance between vertices $x, y \in V(G)$.

For a connected graph G and an non-empty set $S \subseteq V(G)$, the *Steiner distance* among the vertices of S, denoted by $d_G(S)$ or simply by $d(S)$, is the minimum size among all connected subgraphs whose vertex sets contain S. Note that if H is a connected subgraph of G such that $S \subseteq V(H)$ and $|E(H)| = d(S)$, then H is a tree. An *S-Steiner tree* or a *Steiner tree for S* is a subgraph T of G such that T is a tree and $S \subseteq V(T)$. Moreover, if T is a Steiner tree for S such that $|E(T)| = d(S)$, then T is called a *minimum Steiner tree for S*. It is obvious that for a set $S = \{x, y\}$, $x \neq y$, it holds $d(S) = d(x, y)$.

Let G be a connected graph and k a positive integer such that $k \leq |V(G)|$. The *Steiner k-Wiener index* of G, denoted by $SW_k(G)$, is defined as

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S).$$

The *Steiner k-hyper-Wiener index* of G, denoted by $SWW_k(G)$, is defined as

$$SWW_k(G) = \frac{1}{2}\sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S) + \frac{1}{2}\sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S)^2.$$

The *Steiner k-Hosoya polynomial* of G, denoted by $SH_k(G, x)$, is defined as

$$SH_k(G,x) = \sum_{m \geq 0} d_k(G,m)x^m,$$

where $d_k(G, m)$ denotes the number of subsets $S \subseteq V(G)$ with $|S| = k$ and $d(S) = m$.

Two edges $e_1 = u_1v_1$ and $e_2 = u_2v_2$ of a connected graph G are in relation Θ, $e_1 \Theta e_2$, if

$$d_G(u_1,u_2) + d_G(v_1,v_2) \neq d_G(u_1,v_2) + d_G(u_1,v_2).$$