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Wiener index, Harary index and graph properties ☆

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ABSTRACT

Finding sufficient conditions for some properties of graphs in light of quantitative methods is an important problem. In this paper, in terms of the Wiener index or Harary index, we present several sufficient conditions for a graph to be k-connected, β-deficient, k-hamiltonian, k-path-coverable or k-edge-hamiltonian.

1. Introduction

Let $G = (V(G), E(G))$ be a connected graph with $|V(G)| = n$ and $|E(G)| = m$. We use $d(v)$ to denote the degree of a vertex v in G, $\delta(G)$ to denote the minimum degree of G. Let $d(u, v)$ denote the distance between two vertices u and v in G, i.e., the length of a shortest path connecting u and v in G.

The topological indices (also known as the molecular descriptors) had been received much attention in the past decades, and they have been found to be useful in structure–activity relationships (SAR) and pharmaceutical drug design in organic chemistry (see [16,17,31]). Many researchers also were devoted to study their graphical properties. Indeed, the topological index of a graph G can be viewed as a graph invariant under the isomorphism of graphs, that is, for some topological index TI, $TI(G) = TI(H)$ if $G \cong H$. Therefore, the results in this paper can also be seen as a topic in extremal graph theory.

One of the most thoroughly studied topological indices was the Wiener index which was proposed by Wiener in 1947 [34]. This index has been shown to possess close relation with the graph distance, which is an important concept in pure graph theory. It is also well correlated with many physical and chemical properties of a variety of classes of chemical compounds. Up to now, there is a tremendous amount of literature on the study of Wiener index and its modifications, see for example [7,10–12,14,22,23,28,30,37]. The *Wiener index* of a graph G, denoted by $W(G)$, is defined as

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

If we write $D(v) = \sum_{u \in V(G)} d(u, v)$, then the Wiener index can be rewritten as

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} D(v).$$

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From the above expression, it can be easily verified that

$$D(v) \geq d(v) + 2(n - 1 - d(v)).$$

In 1993, Plavšić et al. [17,29] introduced the reciprocal version of the Wiener index, which is now called the Harary index. The Harary index is also extensively studied for various graph classes, such as graphs with fixed matching number [8], graphs with fixed connectivity [24], trees with various parameters [15,33], bicyclic graphs [36], graphs with minimal Harary index [9]. For other related results, see [27,29]. For a connected graph G, its *Harary index*, denoted by $H(G)$, is defined as

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u, v)}.$$

If we write $\widehat{D}(v) = \sum_{u \in V(G)} \frac{1}{d(u,v)}$, then we can rewrite $H(G)$ as

$$H(G) = \frac{1}{2} \sum_{v \in V(G)} \widehat{D}(v).$$

From this expression, it can be easily verified that

$$\widehat{D}(v) \leq d(v) + \frac{1}{2}(n - 1 - d(v)).$$

For many graph invariants, their computational complexity is usually NP-complete. Thus, finding sufficient conditions for graphs possessing certain properties becomes meaningful in graph theory. For such topic, there are dozens of existing results, the most famous one is the so called the Dirac-type condition. For example, it is known that [2, page 4], if G is a simple graph of order $n \geq k + 1$, and if its minimum degree $\delta(G) \geq \frac{1}{2}(n + k - 2)$, then G is k-connected. In [5], it is obtained that for a graph G, if $\delta(G) \geq \frac{n+k}{2}$, then G is k-hamiltonian. In [4, page 15], it states that for a connected graph G, if $\delta(G) \geq n - \beta - 1$, then G contains a cycle of length at least $n - \beta$, and hence G has a matching of size at least $\frac{n-\beta}{2}$. However, there are only few such conditions in terms of the topological indices. As the Wiener and Harary indices are the two most popular and concise indices, several scholars tried to use them to do so. There are two reasons for using these two indices from mathematical and application-oriented aspects from my point of view. One reason is that investigating "distances in graphs" plays an important role in graph theory. The other reason is that these two indices have many applications in other disciplines such as organic chemistry and biology. A famous example is the gene networks, where the genes exchange information based on the shortest path connecting the two genes. Indeed, this is an example but triggers the hypothesis that distance-based quantities could be crucial for investigating those system. Along these lines, in [13], Hua and Wang gave a sufficient condition for a graph to be traceable by using the Harary index. In [35], Yang presented a sufficient condition for a graph to be traceable by using the Wiener index. The above results are further extended by Liu et al. [25,26]. Li [20,21] presented sufficient conditions in terms of the Harary index and Wiener index for a graph to be hamiltonian or hamilton-connected.

Our goal in this paper is, by utilizing the Wiener index, Harary index and the degree conditions, to derive some sufficient conditions for a wide variety of graph properties including k-connected, β-deficient, k-hamiltonian, k-path-coverable or k-edge-hamiltonian. These graph properties are also the concerns of plenty of graph theorists. So our results may be considered as new viewpoints for existing results.

2. Preliminaries

We first present some graph notations and terminologies.

Let K_n, S_n, P_n be the complete graph, the star and the path on n vertices, respectively. For two vertex-disjoint graphs G and H, we use $G \vee H$ to denote the join of G and H; $G \cup H$ to denote their union.

A connected graph G is said to be *k-connected* (or k-vertex connected) if it has more than k vertices and remains connected whenever fewer than k vertices are removed.

The *deficiency* of a graph G, denoted by def(G), is the number of vertices unmatched under a maximum matching in G. In particular, G has a 1-factor if and only if def$(G) = 0$. We call G β-deficient if def$(G) \leq \beta$. Thus a β-deficient graph G of order n has matching number $\frac{n-\beta}{2}$.

A graph G is *k-hamiltonian* if for all $|X| \leq k$, the subgraph induced by $V(G) \setminus X$ is hamiltonian. Thus 0-hamiltonian is the same as *hamiltonian*.

A graph is *traceable* if it contains a hamiltonian path. More generally, G is *k-path-coverable* if $V(G)$ can be covered by k or fewer vertex-disjoint paths. In particular, 1-path-coverable is the same as *traceable*.

A graph G is *k-edge-hamiltonian* if any collection of vertex-disjoint paths with at most k edges altogether belong to a hamiltonian cycle in G.

We use $\alpha(G)$ to denote the independence number of a graph G.

An integer sequence $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ is called *graphical* if there exists a graph G having π as its vertex degree sequence; in that case, G is called a *realization* of π. If P is a graph property, such as hamiltonian or k-connected, we call a graphical sequence π *forcibly* P if every realization of π has property P.

We next give some lemmas that will be used later.