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On the generalized Wiener polarity index of trees with a given diameter

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ABSTRACT

The generalized Wiener polarity index of a graph G, denoted by $W_k(G)$, is the number of unordered pairs of vertices that are at distance k in G. In this paper, we characterize the extremal trees with respect to the index among all trees of order n and diameter d, which partially answers a question of Bollobás and Tyomkyn (2012) and also generalizes some results of Deng et al. (2010).

1. Introduction

Throughout this paper, all graphs considered are finite, simple and undirected. Let G be a connected graph. The distance between two vertices u and v in G, denoted by $d_G(u, v)$, is the length of a shortest path between u and v in G. The Wiener polarity index of a graph G is the number of unordered pairs of vertices $\{u, v\}$ of G such that $d_G(u, v) = 3$. The name "Wiener polarity index" was introduced by Wiener [32] in 1947. Wiener himself conceived the index only for acyclic molecules and defined it in a slightly different – yet equivalent – manner. In the same paper, Wiener also introduced another index for acyclic molecules, called *Wiener index* or *Wiener distance index* and defined by $W(G) := \sum_{\{u,v\}\subseteq V} d_G(u, v)$. The Wiener index $W(G)$ is popular in both chemical and mathematical literatures. For more results on Wiener index of trees, we refer to the survey paper [16] written by Dobrynin et al.

The Wiener polarity index is used to demonstrate quantitative structure–property relationships in a series of acyclic and cycle-containing hydrocarbons by Lukovits and Linert [26]. Hosoya [19] found a physical–chemical interpretation of the Wiener polarity index. Du et al. [17] described a linear time algorithm APT for computing the Wiener polarity index of trees, and characterized the trees maximizing the Wiener polarity index among all trees of given order. The extremal Wiener polarity index of (chemical) trees with given different parameters (e.g. order, diameter, maximum degree, the number of pendants, etc.) was studied, see [11,12,14,23–25]. Moreover, the unicyclic graphs minimizing (resp. maximizing) the Wiener polarity index among all unicyclic graphs of order n were given in [20]. For other classes of graphs, we refer to [1,7,8,13,27,28]. Recently, there are some new results of the Wiener polarity index of the graph operations and the relations with other indexes, such as [21,29,34]. In addition, the more results are described in a recent survey [33].

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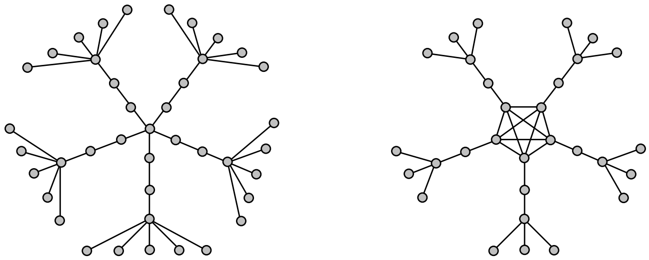

Fig. 1. A 5-broom for $k = 8$ and a 5-broom for $k = 7$.

In [22], Ilić and Ilić gave the generalized Wiener polarity index $W_k(G)$ as the number of unordered pairs of vertices $\{u, v\}$ of G such that $d_G(u, v) = k$ (this is actually the kth coefficient in the Wiener polynomial), i.e.,

$$W_k(G) := |\{\{u, v\}|d_G(u, v) = k,\ u, v \in V(G)\}|.$$

Actually, the Wiener polarity index is exactly $W_3(G)$. In [31], Tyomkyn and Uzzell independently investigated the same problem from the extremal aspect. However, there are a few results about the generalized Wiener polarity index. In [5], Bollobás and Tyomkyn proved that if T is a tree, then $W_k(T)$ is maximal when T is a t-broom for some t. And they also asked the following problem.

Problem. How to determine the minimal and maximal number of paths of length k in a tree T on n vertices, subject to additional parameters? For example, one could only consider trees of diameter at least $d(n, k)$ or maximal degree at most $\Delta(n, l)$ for appropriately chosen functions d and Δ.

In 2007, Peña et al. [10] published the conjecture that the maximum of the Estrada index [18] on trees of order n is attained on a star, and its minimum is attained on a path. And then Nikiforov [30] proposed a stronger conjecture that for a fixed value of k the number of closed walks of length k on trees of order n attains its extreme values on the same graphs. Recently, Nikiforov's conjecture was proved by Csikv́ari [9]. All the above study focus on the walks. However, paths of a given length were investigated by Bollobás et al. [2–5]. Observe that in trees, the number of paths with length k is equal to the number of unordered pairs of vertices with distance k.

In this paper, we will study W_k of a tree on n vertices with a given diameter d. Extremal trees with respect to the index W_k among all trees of order n and diameter d are characterized, which partially answers the above problem and also generalizes some results of Deng et al. [14].

2. Preliminaries

In this section, we first start with some basic concepts and definitions. And then we list some known results, which will be used in the following sections. For notation and terminology not given here, see [6,15].

Given a connected graph G. The greatest distance between any two vertices in G is the diameter of G, denoted by $diam(G)$. For any $v \in V(G)$, the set of vertices, whose distance is i from v, is denoted by $N^i_G(v)$, where $i \in \{1, 2, 3, \ldots, diam(G)\}$. Let $d^i_G(v) = |N^i_G(v)|$ denote the i-degree of v. We use $N_G(v)$ (resp. $d_G(v)$) instead of $N^1_G(v)$ (resp. $d^1_G(v)$) for short when $i = 1$. If $d_G(v) = 1$ for $v \in V(G)$, then we call v a pendant vertex of G (also call v a leaf if G is a tree). Suppose that V' is a nonempty subset of V. The subgraph of G whose vertex set is V' and whose edge set is the set of those edges of G that have both ends in V' is called the subgraph of G induced by V', denoted by $G[V']$; we say that $G[V']$ is an induced subgraph of G. For a positive integer k, let $[k] := \{1, 2, \ldots, k\}$.

Given a positive integer $k \geq 3$, we define a t-*broom* ($t \geq 2$) as follows. For even $k \geq 4$, define a t-broom to be a graph consisting of a central vertex v with t 'brooms' attached, each consisting of a path of length $(k - 2)/2$ with leaves attached to the ends opposite v. In this way, the leaves of different brooms will be at distance k. For odd $k \geq 3$, to define a t-broom, take a copy of K_t and attach a broom to each vertex, adjusting the length of the path (See Fig. 1).

In [5], Bollobás and Tyomkyn proved that if T is a tree, then $W_k(T)$ is maximal when T is a t-broom for some t.

Theorem 2.1. *Let $n \geq k \geq 3$. If T is a tree on n vertices, then $W_k(T)$ is maximal when T is a t-broom. If k is odd, then $t = 2$. If k is even, then t is within 1 of*

$$\frac{1}{4} + \sqrt{\frac{1}{16} + \frac{n-1}{k-2}}.$$

Let $T(r, t)$ be the graph which is obtained from a path $P_d = v_0v_1 \ldots v_d$ of length d by adding r pendant vertices to v_1 and t pendant vertices to v_{d-1}, where $r + t = n - d - 1$. Let $CT_n(x_1, x_2, \ldots, x_{d-3})$ be a capillary tree which is obtained from a path $P_d = v_0v_1 \ldots v_d$ of length d by adding x_i pendant vertices to v_{i+1} for $1 \leq i \leq d - 3$, where $x_1 + x_2 + \cdots + x_{d-3} = n - d - 1$.

For the special case $k = 3$, Deng et al. [14] gave the following results.