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Extremal Wiener Index of Trees with Prescribed Path Factors*

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Abstract

The Wiener index of a connected graph is defined as the sum of distances between all unordered pairs of its vertices. A graph G is said to have a P_r-factor if G contains a spanning subgraph F of G such that every component of F is a path with r vertices. In this paper, we characterize the trees which minimize and maximize the Wiener index among all trees on kr vertices ($k \geq 2$, $r \geq 2$) with a P_r-factor respectively. This generalizes an early result concerning the minimum Wiener index of tree with perfect matchings, which was independently obtained by Du and Zhou (Minimum Wiener indices of trees and unicyclic graphs of given matching number, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 101–112) as well as Lin, Wang, Xu and Wu (Ordering trees with perfect matchings by their Wiener indices, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 337-345).

1 Introduction

All graphs considered in this paper are simple, connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The distance of a vertex v, denoted by $d_G(v)$, is the sum of distances between v and all other vertices of G. The distance between vertices u and v of G is denoted by $d_G(u,v)$. The Wiener index of a connected graph G is defined as

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

The Wiener index belongs among the oldest graph-based structure descriptors (topological indices) which was first introduced by Wiener [15] and has been extensively studied in literature. Chemists are often interested in the Wiener index of certain trees which represent some acyclic molecular structures. Some extremal results of Wiener index of trees can be found in [1, 9-14] and references cited therein. For more details, the reader may see the survey by Dobrynin et al. [2] and the survey by Xu et al. [16].

Denote by $K_{1,n-1}$ and P_n the star and the path with n vertices, respectively. A subgraph F of a graph G is called a *factor* of G if F is a spanning subgraph of G. A *path factor* of a graph G is a factor of G such that each component of the factor is a path, in particular, if each component of the factor is required to be a path with exactly r vertices, such a factor is called a P_r*-factor* of G.

Remark A. According to this definition, if a graph G has a P_r-factor, then there exist m ($m = |V(G)|/r$) vertex disjoint paths L_1, L_2, ..., L_m such that

$$V(G) = V(L_1) \bigcup V(L_2) \bigcup ... \bigcup V(L_m)$$

and each L_i is a path with r vertices. In this sense, the well-known perfect matchings (or 1-factor) is a P_2-factor.

In [5], Gutman and Rouvray proved that if T and T' are two trees with perfect matchings on equal number of vertices. then $W(T) \equiv W(T') \pmod 4$. This result was generalized by the author of present paper [9] to trees with P_r-factor and further generalized by Gutman, Xu and Liu [6] to even much larger class of graphs. In [7], K. Hriňáková, M. Konr, R. Škrekovski and A. Tepeh continued to generalized it to a large families of graphs with a tree-like structure.

The aim of this paper is to investigate the extremal Wiener index of trees with a P_r-factor. Let $\mathbb{F}_{P_r,k}$ be the set of trees of order kr with a P_r-factor, $k \geq 2$, $r \geq 2$. A tree T belonging to the set $\mathbb{F}_{P_4,4}$ is shown in Figure 1.

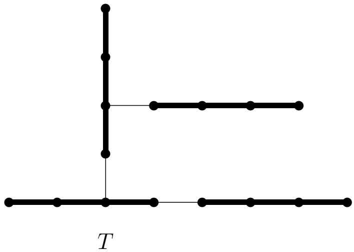

Figure 1. A 16-vertex tree T with a P_4-factor.

The *eccentricity* of a vertex v of a connected graph G, denoted by $ECC_G(v)$, is defined by $ECC_G(v) = max_{w \in V(G)} d_G(v, w)$. The *center* of G, denoted by $Cr(G)$, is the set of vertices with minimum eccentricity. It is well known that the center of a tree consists of a single vertex or two adjacent vertices [2].

Let T^*_{kr} be the tree (depicted Figure 2) obtained from k vertex disjoint $r-$vertex paths L_1, L_2, ..., L_k by joining u_1 to each of the vertices u_2, u_3, ..., u_k, where $u_i \in Cr(L_i)$ for each $i = 1, 2, ..., k$. Clearly, $T^*_{kr} \in \mathbb{F}_{P_r,k}$.

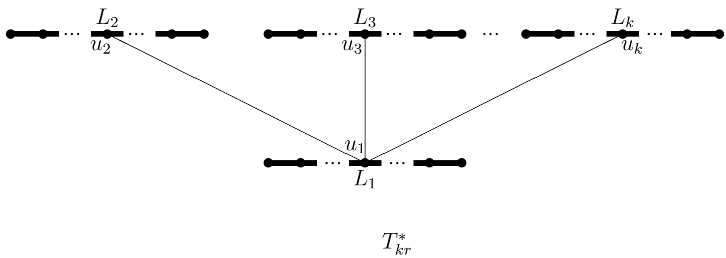

Figure 2. The tree T^*_{kr} .

With above notations, the main result of this paper can be stated as follows.

Theorem 1. Let $T \in \mathbb{F}_{P_r,k}$ where $r \geq 2$ and $k \geq 2$. Then

$$W(T^*_{kr}) \leq W(T) \leq \binom{kr+1}{3},$$

with left equality if and only if $T = T^*_{kr}$ and with right equality if and only if $T = P_{kr}$.

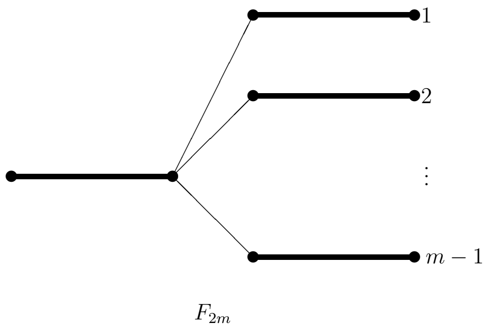

Figure 3. The tree F_{2m}.

Let $\mathbb{T}_{2m}$ be the set of $2m-$vertex trees with perfect matchings and let F_{2m} be the tree shown in Figure 3. Clearly, $F_{2m} \in \mathbb{T}_{2m}$. The following result is contained in Theorem 1 of [3] and Theorem 4.1 of [12].

Theorem 2. Let $T \in \mathbb{T}_{2m}$, where $m \geq 2$. Then

$$W(T) \geq W(F_{2m}),$$

with equality if and only if $T = F_{2m}$.

Remark B. By the definition of the P_r-factor, the perfect matching is a P_2-factor. Note that any vertex of the path P_2 belongs to $Cr(P_2)$, namely $V(P_2) = Cr(P_2)$, thus the set $\mathbb{T}_{2m}$ is just the set $\mathbb{F}_{P_2,m}$, and hence Theorem 1 is a natural generalization of Theorem 2.

The rest of this paper is organized as follows. In Section 2, we provide some useful notations and results which will help to prove our main result. We close this paper in Section 3 by proving Theorem 1 and proposing some new problems for research.

2 Preliminaries

Entringer et al. [4] proved the following result which bounds the Wiener index of a tree in term of its order.

Theorem 3 ([4]). Let T be a tree on n vertices, then

$$(n-1)^2 \leq W(T) \leq \binom{n+1}{3},$$

the lower bound is achieved if and only if $T = K_{1,n-1}$ and the upper bound is achieved if and only if $T = P_n$.

A maximal subtree containing a vertex v of a tree T as a pendent vertex will be called a *branch of T at v*. The *weight of a branch B*, denoted by $BW_T(B)$ is the number of edges in it. The *branch weight of a vertex v*, denoted by $BW_T(v)$ is the maximum of the weights of the branches at v. The *centroid* of a tree T , denoted by $Cd(T)$, is the set of vertices of T with minimum branch weight. Jordan [8] characterized the centroid of a tree (see Section 3 of [2]).

Theorem 4 ([8]). The centroid of a tree consists of a single vertex or two adjacent vertices.

Zelinka [17] observed that the set of vertices with minimum distance in a tree T coincides with $Cd(T)$ (see Section 3 of [2]).

Theorem 5 ([17]). The set of vertices with minimum distance in a tree T is the centroid of T.

Remark C. For a tree T, it should be noticed that $Cr(T)$ may not coincide with $Cd(T)$. Let T be the tree as shown in Figure 4, then $Cr(T) = \{c_1, c_2\}$. A direct calculation gives that $d_T(u) = 22$, $d_T(c_1) = 24$, $d_T(c_2) = 28$, $d_T(v_1) = 40$, $d_T(v_2) = 30$, $d_T(v_3) = d_T(v_4) = d_T(v_5) = d_T(v_6) = 26$, $d_T(v_7) = 34$, $d_T(v_8) = 42$ and $d_T(v_9) = 52$. Thus, $Cd(T) = \{u\}$ and $Cd(T) \cap Cr(T) = \emptyset$. The center and centroid play special roles with respect to the Wiener index of trees, the reader may see Section 3 of [2] for a general introduction.

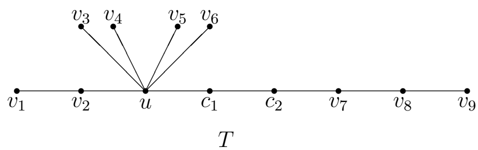

Figure 4. The tree T.

If we restrict trees to be paths, the following result is a simple observation from Theorem 4 and Theorem 5.

Lemma 6. Let P be a path, then $Cd(P) = Cr(P)$.

Lemma 7 ([2, P227]). Let T be obtained from arbitrary trees T_1 and T_2 of order n_1 and n_2, respectively, and $v_1 \in V(T_1)$, $v_2 \in V(T_2)$. If v_1 and v_2 are joined by an edge, then

$$W(T) = W(T_1) + W(T_2) + n_1 d_{T_2}(v_2) + n_2 d_{T_1}(v_1) + n_1 n_2 \ .$$

3 Proof of Theorem 1 and discussion

Note that $P_{kr} \in \mathbb{F}_{P_r,k}$, thus by Theorem 3, we have $W(T) \leq \binom{kr+1}{3}$ with equality if and only if $T = P_{kr}$.

Now we turn to prove the lower bound of $W(T)$ by induction on k.

If $k = 2$, Let T be the tree obtained from two vertex disjoint $r-$vertex paths L_1 and L_2 by joining v_1 to v_2, where $v_1 \in V(L_1)$ and $v_2 \in V(L_2)$. From Lemma 7,

$W(T) = W(L_1) + W(L_2) + rd_{L_1}(v_1) + rd_{L_2}(v_2) + r^2$

$=2W(P_r) + r^2 + r[d_{L_1}(v_1) + d_{L_2}(v_2)]$.

By Lemma 6, if $v_1 \in Cr(L_1)$ and $v_2 \in Cr(L_2)$, then the tree $T = T^*_{2r}$ and T attains the maximum Wiener index in $\mathbb{F}_{P_r,2}$. The statement of theorem clearly holds in this case.

Suppose now that $T^*_{(k-1)r}$, $k \geq 3$, uniquely attains the minimum Wiener index in $\mathbb{F}_{P_r,k-1}$ and let T be any tree in $\mathbb{F}_{P_r,k}$. In the following, we shall prove that $W(T) \geq W(T^*_{kr})$ with equality if and only if $T = T^*_{kr}$.

Let T_1 be the tree obtained from T^*_{kr} (as shown in Figure 2) by deleting the vertices in $V(L_k)$ together with all edges adjacent to these vertices. Then by Lemma 7,

$$W(T^*_{kr}) = W(T_1) + W(L_k) + (k-1)rd_{L_k}(u_k) + rd_{T_1}(u_1) + (k-1)r^2 \ .$$

Note that $T_1 = T^*_{(k-1)r}$, $L_k = P_r$, so

$$W(T^*_{kr}) = W(T^*_{(k-1)r}) + W(P_r) + (k-1)rd_{L_k}(u_k) + rd_{T^*_{(k-1)r}}(u_1) + (k-1)r^2. \qquad (1)$$

Since T has a P_r-factor, according to Remark A, there exist k vertex disjoint paths L'_1, L'_2, ..., L'_k such that $V(T) = V(L'_1) \bigcup V(L'_2) \bigcup ... \bigcup V(L'_k)$ and each L'_i is a path with r vertices. According to this structure, there exist two paths in $\{L'_1, L'_2, ..., L'_k\}$, without loss of generalization, say L'_1 and L'_k, such that L'_1 and L'_k are joined by an edge $u'_1 u'_k$, $u'_1 \in V(L'_1)$, $u'_k \in V(L'_k)$, and after deleting all vertices in $V(L'_k)$ together with all edges adjacent to these vertices will result in a subtree, say T'_1 of T. Again by Lemma 7,

$$W(T) = W(T'_1) + W(L'_k) + (k-1)rd_{L'_k}(u'_k) + rd_{T'_1}(u'_1) + (k-1)r^2 \ .$$

Note that $L'_k = P_r$, so

$$W(T) = W(T'_1) + W(P_r) + (k-1)rd_{L'_k}(u'_k) + rd_{T'_1}(u'_1) + (k-1)r^2 \qquad (2)$$

Note that T'_1 again has P_r-factor, $T'_1 \in \mathbb{F}_{P_r,k-1}$, by the induction hypothesis

$$W(T'_1) \geq W(T^*_{(k-1)r}), \qquad (3)$$

with equality if and only if $T'_1 = T^*_{(k-1)r}$.

Both L_k and L'_k are $r-$vertex paths, it is obvious that

$$d_{L'_k}(u'_k) \geq d_{L_k}(u_k), \tag{4}$$

with equality if and only if $u'_k \in Cd(L'_k)$.

Since T^*_{kr} has structure which is specified in Figure 2, then for any vertex $x \in V(L_i)$, $i \in \{2, 3, ..., k-1\}$, the unique path in T_1 joining x and u_1 must contain the edge u_1u_i. With this observation, it is easy to see that

$$\begin{aligned} d_{T^*_{(k-1)r}}(u_1) &= d_{L_1}(u_1) + \sum_{i=2}^{k-1} \left[\sum_{x \in V(L_i)} d_{T^*_{(k-1)r}}(u_1, x) \right] \\ &= d_{L_1}(u_1) + \sum_{i=2}^{k-1} \left[\sum_{x \in V(L_i)} \left(d_{T^*_{(k-1)r}}(u_1, u_i) + d_{T^*_{(k-1)r}}(u_i, x) \right) \right] . \end{aligned}$$

Note that $d_{T^*_{(k-1)r}}(u_1, u_i) = 1$, $d_{T^*_{(k-1)r}}(u_i, x) = d_{L_i}(u_i, x)$, therefore

$$d_{T^*_{(k-1)r}}(u_1) = d_{L_1}(u_1) + \sum_{i=2}^{k-1} \left[\sum_{x \in V(L_i)} (1 + d_{L_i}(u_i, x)) \right] = d_{L_1}(u_1) + \sum_{i=2}^{k-1} [r + d_{L_i}(u_i)] .$$

On the other hand, for the tree T'_1, with the similar discussion, one can get that

$$\begin{aligned} d_{T'_1}(u'_1) &= d_{L'_1}(u'_1) + \sum_{i=2}^{k-1} \left[\sum_{y \in V(L'_i)} d_{T'_1}(u'_1, y) \right] \\ &= d_{L'_1}(u'_1) + \sum_{i=2}^{k-1} \left[\sum_{y \in V(L'_i)} \left(d_{T'_1}(u'_1, y'_i) + d_{L'_i}(y, y'_i) \right) \right] , \end{aligned}$$

where y'_i is the first vertex encountered in L'_i when one goes from u'_1 to y.

Clearly,

$$d_{L'_1}(u'_1) \geq d_{L_1}(u_1), \sum_{y \in V(L'_i)} d_{L'_i}(y, y'_i) \geq d_{L'_i}(u'_i), \text{ (since } u'_i \in Cd(L'_i))$$

and

$$\sum_{y \in V(L'_i)} d_{T'_1}(u'_1, y'_i) \geq r ,$$

with three equalities holding simultaneously if and only if $u'_1 \in Cd(L'_1)$ and $y'_i \in Cd(L'_i)$.

So we have

$$d_{T_1'}(u_1') \geq d_{T^*_{(k-1)r}}(u_1), \tag{5}$$

with the equality if and only if $T_1' = T^*_{(k-1)r}$.

Now from the relations (1)-(5) and above discussion, we arrive at

$$W(T) \geq W(T^*_{kr}),$$

with the equality if and only if $T = T^*_{kr}$.

This completes the proof the Theorem 1. ■

Theorem 1 generalizes Theorem 2, it is interesting that it might be generalized to even much large class of trees.

Let R be the forest consisting of k disjoint trees T_1, T_2, ..., T_k. Let $\mathbb{F}_{T_1,T_2,...,T_k}$ $(k \geq 2)$ be the set of trees with R as a factor. Clearly, if for each $i = 1, 2, ..., k$, $T_i = P_r$, then $\mathbb{F}_{T_1,T_2,...,T_k} = \mathbb{F}_{P_r,k}$.

Given a set $\mathbb{F}_{T_1,T_2,...,T_k}$, without loss of generality , we may assume that the Wiener indices of trees T_1, T_2, ..., T_k have the following order

$$W(T_1) \geq W(T_2) \geq ... \geq W(T_k).$$

Let T_1^* be the tree obtained from k vertex disjoint trees T_1, T_2, ..., T_k by joining u_1 to each of the vertices u_2, u_3, ..., u_k, where $u_i \in Cd(T_i)$ for each $i = 1, 2, ..., m$. Clearly, if for each $i = 1, 2, ..., k$, $T_i = P_r$, then $T_1^* = T^*_{kr}$ (depicted in Figure 2). Let T_2^* be the tree with the structure illustrated in Figure 5, where v_1 is a vertex with the largest distance in the tree T_1 and v_2 is a vertex with the largest distance in the tree T_2. Clearly, $T_1^* \in \mathbb{F}_{T_1,T_2,...,T_k}$ and $T_2^* \in \mathbb{F}_{T_1,T_2,...,T_k}$. Roughly speaking, T_1^* has a star-like structure and T_2^* has a chain-like structure.

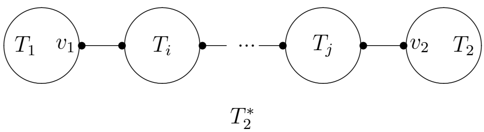

Figure 5. The tree T_2^*.

Numerical testing of trees in $\mathbb{F}_{T_1,T_2,...,T_k}$ with a small value of k reveals that T_1^* attains the minimum Wiener index and T_2^* attains the maximum Wiener index. So it might be worthwhile to consider the following problem.

Problem A. Let T be any tree in $\mathbb{F}_{T_1,T_2,\ldots,T_k}$, $k \geq 2$, does the following relation hold

$$W(T_1^*) \leq W(T) \leq W(T_2^*) \ .$$

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