A Congruence Relation for the Wiener Index of Trees with 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 note, it is shown that if T and T' are two trees with P_r-factors on equal number of vertices, then $W(T) \equiv W(T') \pmod{r}$ for odd r and $W(T) \equiv W(T') \pmod{2r}$ for even r.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $deg_G(v)$ of a vertex v in G is the number of edges of G incident with v. A vertex of degree one is called a *pendent vertex*. A vertex v in a tree T is called a *branching vertex* if $deg_T(v) \geq 3$. A path with n vertices is denoted by P_n. A set of the independent edges in G which covers all the vertices in G is called a perfect matching 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

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

In organic chemistry, the Wiener index is one of the oldest distance-based structure descriptors which was first introduced by Wiener [16]. Numerous of its chemical applications and mathematical properties are well studied [2, 3, 10, 13].

Chemists are often interested in the Wiener index of certain trees which represent molecular structures. For detailed results on this topic, the readers may referred to [2]. Recently, some new properties of the Wiener index within some given classes of trees have been found. For instance, see [1] for trees with given matching number, [9, 15] for trees with given diameter, [7] for trees with given radius and [4, 5, 8, 12, 14, 17, 18] for trees with specific degree conditions.

In [6], Gutman and Rouvray established the following congruence relation for the Wiener index of trees with perfect matchings.

Theorem 1 ([6]) Let T and T' be two trees on equal number of vertices. If both T and T' have perfect matchings, then $W(T) \equiv W(T')$ (mod 4).

The following theorem, discovered by Doyle and Graver [3], is a well known result to compute the Wiener index of trees with few branching vertices.

Theorem 2 ([3]) Let T be a tree on n vertices. Then

$$W(T) = \binom{n+1}{3} - \sum_{u} \sum_{1 \leq i < j < k \leq deg_T(u)} n_i(u)n_j(u)n_k(u),$$

where the first summation goes over all branching vertices u of T, and $n_1(u)$, $n_2(u)$, ..., $n_{deg_T(u)}(u)$ are the number of vertices in each of the components of $T - u$.

A segment of a tree T is a path-subtree S whose terminal vertices are branching or pendent vertices of T. By using the Doyle-Graver formula stated as above and the concept of segments, Dobrynin, Entringer and Gutman [2] obtained a new congruence relation for the Wiener index in the class of $k-$proportional trees. Trees of this class have the same order and the lengths of all segments are proportional to the coefficient k, $k \geq 1$.

Theorem 3 ([2]) Let T and T' be two $k-$proportional trees. Then $W(T) \equiv W(T')$ (mod k^3).

In this note, we attempt to connect the theory of Wiener index with the theory of graph factors and establish some further congruence relations for the Wiener index within some classes of trees. To do so, we first introduce some terminologies and notations that appears in the theory of graph factors [11].

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 1. 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. Figure 1 illustrates an example of a P_4-factor (depicted by the thick lines) of a tree.
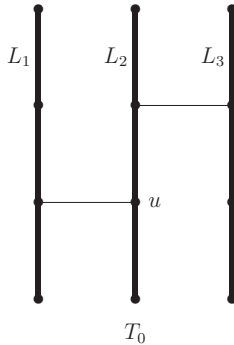

Fig. 1   A 12-vertex tree T_0 with a P_4-factor $F = L_1 \bigcup L_2 \bigcup L_3$

Now we can state our main result of this paper.

Theorem 4a If T is an $n-$vertex tree with a P_r-factor, then

$$W(T) \equiv \binom{n+1}{3} \pmod{r} \quad for\ odd\ r \tag{1}$$

and

$$W(T) \equiv \binom{n+1}{3} \pmod{2r} \quad for\ even\ r, \tag{2}$$

furthermore,

Theorem 4b If T and T' are two trees on equal number of vertices with P_r-factors, then

$$W(T) \equiv W(T') \pmod{r} \quad for\ odd\ r \tag{3}$$

and

$$W(T) \equiv W(T') \pmod{2r} \quad for\ even\ r. \tag{4}$$

.

Let us make several remarks here before proving the theorem.

Remark 2. By the definition of the P_r−factor, the well-known perfect matching (or 1-factor) is a P_2−factor. Theorem 4b thus is a natural generalization of Theorem 1.

Remark 3. The congruence relation in Theorem 4b is best possible in the following sense. If r is odd, then we cannot strengthen the relation (3) by replacing modulo r by modulo $2r$ or modulo r^2. Consider the 20-vertex trees T_1 and T_2 (shown in Figure 2) with P_5−factors (depicted by the thick lines), $W(T_1) = 1085$, $W(T_2) = 1090$, thus $W(T_2) - W(T_1) = 5 \equiv 0 \pmod{5}$. This example shows that if r is odd, then r is the largest value the divisor in relation (3) can take. Similarly, if r is even, then we cannot strengthen the relation (4) by replacing modulo $2r$ by modulo r^2 or other. Consider the 12-vertex trees T_3 and T_4 (shown in Figure 3) with P_4−factors (depicted by the thick lines), $W(T_3) = 238$, $W(T_4) = 246$, thus $W(T_4) - W(T_3) = 8 \equiv 0 \pmod{8}$. This example shows that if r is even, then $2r$ is the largest value the divisor in relation (4) can take.
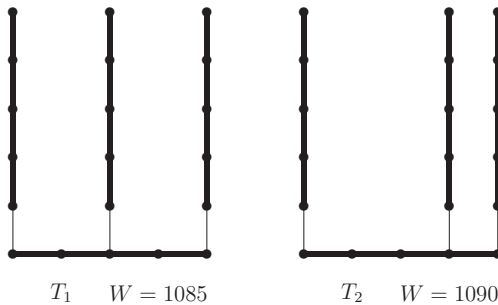

$$T_1 \quad W = 1085 \qquad T_2 \quad W = 1090$$

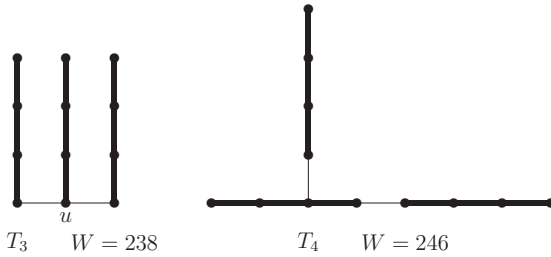**Fig. 2** Two 20-vertex trees with P_5-factors and their Wiener indices

Fig. 3 Two 12-vertex trees with P_4-factors and their Wiener indices

2 Proof of Theorem 4

Proof. It is obvious that Theorem 4b is an immediate corollary of Theorem 4a. Accordingly, it will be sufficient here to prove only the first statement.

Let T be an $n-$vertices tree with a P_r-factor.

If $T = P_n$, it is well known [2] that $W(P_n) = \binom{n+1}{3}$, Theorem 4a clearly holds in this case. So in the following, we always assume that $T \neq P_n$. Then T contains some branching vertices, we can compute the Wiener index of T in the following manner by Theorem 2:

$$W(T) = \binom{n+1}{3} - \sum_u \sum_{1 \leq i < j < k \leq deg_T(u)} n_i(u)n_j(u)n_k(u), \tag{5}$$

where the first summation goes over all branching vertices u of T.

Let u be an arbitrary branching vertex of T, and let $T_1, T_2, ..., T_p$ be the components of $T - u$, where $p = deg_T(u) \geq 3$. We call a component T_i of $T - u$ a k-component if $|V(T_i)|$ contains the factor k. Set $n_t(u) = |V(T_t)|$, $t = 1, 2, ..., p$.

By Remark 1, we know that there exist m ($m = |V(T)|/r$) vertex disjoint paths L_1, $L_2, ..., L_m$ of T such that $V(T) = V(L_1) \bigcup V(L_2) \bigcup ... \bigcup V(L_m)$ and each L_i is a path with r vertices. Thus u lies on exactly one path, say $L_q \in \{L_1, L_2, ..., L_m\}$, which implies that at most two components of $T - u$ contain some vertices of L_q. On the other hand, if a component of $T - u$ does not contain any vertex of L_q, then it again has a P_r-factor, and hence is a $r-$component of $T - u$.

By above discussion, we know that $T - u$ contains at least $(p - 2)$ $r-$components of $T - u$. This implies that each summand $n_i(u)n_j(u)n_k(u)$ in (5) contains the factor r. So

the relation (1) holds for any r with $r \geq 2$.

In particular, if r is even, as above, suppose that u lies on exactly one path, say $L_q \in \{L_1, L_2, ..., L_m\}$ and $T_1, T_2, ..., T_p$ are the components of $T - u$, where $p = deg_T(u) \geq 3$. Set $n_t(u) = |V(T_t)|$, $t = 1, 2, ..., p$.

In order to complete the proof, it is necessary to examine the following two cases.

Case 1. u is an end vertex of L_q (see the branching vertex u of the tree T_3 in Figure 3 for an example).

In this case, it is easily seen that $T - u$ contains $p - 1$ components, each of which does not contain any vertices of L_q and again has a P_r-factor, and hence is a $r-$component of $T - u$. This fact implies that each summand $n_i(u)n_j(u)n_k(u)$ in (5) contains the factor r^2, and hence the factor $2r$ (since r is even), so the relation (2) holds.

Case 2. u is an internal vertex of L_q (see the branching vertex u of the tree T_0 in Figure 1 for an example).

Then there are exactly two components of $T - u$, without loss of generality, say T_1 and T_2, each contains some vertices of L_q. Recall that $T_1, T_2, ..., T_p$ are the components of $T - u$, we easily get

$$|V(T_1)| + |V(T_2)| + |V(T_3)| + ... + |V(T_p)| = |V(T)| - 1 = mr - 1. \qquad (6)$$

Note that each of the components $T_3, ..., T_p$ does not contain any vertices of L_q and again has a P_r-factor, and hence is a $r-$component of $T - u$. Therefore, we may assume that $|V(T_3)| + ... + |V(T_p)| = sr$, where s is a positive integer. Now by (6), we arrive at $|V(T_1)| + |V(T_2)| = (m - s)r - 1$.

Since r is even, $(m - s)r - 1$ is an odd number. So $|V(T_1)|$ and $|V(T_2)|$ have different parities. Thus one of T_1, T_2 is a 2-component of $T - u$. Using this as well as the fact that r is even and $T_3, ..., T_p$ are $r-$components of $T - u$, we can conclude that each summand $n_i(u)n_j(u)n_k(u)$ in (5) contains the factor $2k$. So the relation (2) holds, and this completes the proof of the theorem. □

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