

The hyper-Wiener index of trees with given parameters *

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Abstract

Let G be a connected graph. The hyper-Wiener index $WW(G)$ is defined as $WW(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u,v) + \frac{1}{2} \sum_{u,v \in V(G)} d^2(u,v)$, with the summation going over all pairs of vertices in G and $d(u,v)$ denotes the distance between u and v of G . In this paper, we determine the upper or lower bounds on hyper-Wiener index of trees with given number of pendent vertices, matching number, independence number, domination number, diameter, radius and maximum degree.

Key words: hyper-Wiener index; tree; pendent vertices; matching number; diameter; maximum degree.

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1 Introduction

Throughout this work we consider simple connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. We denote by $d(x,y)$, $N(x)$ and $deg(x)$, the distance between vertices x and y , neighbors of vertex x and the degree of x , respectively.

The Wiener index, defined as $W(G) = \sum_{u,v \in V(G)} d(u,v)$, is perhaps the most studied topological index from application and theoretical viewpoints. The hyper-Wiener index of acyclic graphs was introduced by Milan

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Randić in 1993 [1] as an extension of the Wiener index. Then Klein et al. [2] generalized Randić's definition for cyclic structures. The *hyper-Wiener index* of a graph G is defined as

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

with the summation going over all pairs of vertices in G . By setting $S(G) = \sum_{u,v \in V(G)} d^2(u,v)$, we have $WW(G) = \frac{1}{2} W(G) + \frac{1}{2} S(G)$. If we denote by $D_G(u) = \sum_{v \in V(G)} d(u,v)$, $DD_G(u) = \sum_{v \in V(G)} d^2(u,v)$, then $W(G) = \frac{1}{2} \sum_{u \in V(G)} D_G(u)$, $S(G) = \frac{1}{2} \sum_{u \in V(G)} DD_G(u)$.

Up to now, a few results are obtained concerning the hyper-Wiener index. In [3], general expressions were derived for the hyper-Wiener index for several series of hydrocarbons, both benzenoid and non-benzenoid, including some two-dimensional networks. In [15], the authors presented the algorithm for calculation the hyper-Wiener index of benzenoid hydrocarbons. In [6] the authors discussed the discriminating ability of the hyper-Wiener index on a class of acyclic structures (trees) including the molecular graphs of alkanes. Gutman et al. in [12] determined the trees with minimal and maximal hyper-Wiener indices: among n -vertex trees, the minimum and maximum hyper-Wiener index is achieved exactly for the star S_n and the path P_n , respectively. Some relationships between hyper-Wiener index and Wiener index were investigated in [5], [10], [11], [13], [19]. The closed formulas for the hyper-Wiener index of C_4 nanotubes, C_4 nanotori, zigzag polyhex nanotorus were established in [7] and [14]. The present authors in [8] determined the extremal unicyclic graphs with n vertices and girth k having minimal and maximal hyper-Wiener index.

Let P_n and S_n denote the path and the star on n vertices, respectively. A *starlike tree* S_{n_1, n_2, \dots, n_k} is a tree with exactly one vertex v of degree at least 3, $S_{n_1, n_2, \dots, n_k} - v = P_{n_1} \cup P_{n_2} \cup \dots \cup P_{n_k}$, where $n_1 \geq n_2 \geq \dots \geq n_k \geq 1$ and $\sum_{i=1}^k n_i + 1 = n$. Clearly, n_1, n_2, \dots, n_k determine the starlike tree up to isomorphism. $BS_{n,k} \cong S_{n_1, n_2, \dots, n_k}$ is *balanced* if all paths have almost equal lengths, i.e., $|n_i - n_j| \leq 1$ for every $1 \leq i < j \leq k$.

Let $\mathfrak{T}_{n,k}$ ($2 \leq k \leq n-1$) be the set of trees on n vertices with k pendent vertices. If $k = 2$, then the set $\mathfrak{T}_{n,2}$ contains just the path P_n ; while if $k = n-1$, the set $\mathfrak{T}_{n,n-1}$ contains just the star S_n . So, we assume that $3 \leq k \leq n-2$ in the sequel.

Let G be a connected graph. Two distinct edges in a graph G are *independent* if they are not incident with a common vertex in G . A set of pairwise independent edges in G is called a *matching* in G . While a matching of maximum cardinality is a maximum matching in G . The *matching number* $\beta(G) = \beta$ of G is the cardinality of a maximum matching of G . It is well known that $\beta(G) \leq \frac{n}{2}$, with equality if and only if G has a perfect

matching. A subset $S \subseteq V(G)$ is called an *independent set* of G if no two vertices in S are adjacent in G . The *independence number* of G , denoted by $\alpha(G) = \alpha$, is the size of a maximum independent set of G . A subset $S \subseteq V(G)$ is called a *dominating set* of G if for every vertex $v \in V - S$, there exists a vertex $u \in S$, such that v is adjacent to u . The *domination number* of G , denoted by $\gamma(G) = \gamma$, is the minimum cardinality of a dominating set of G .

If $\frac{n-1}{2} < m \leq n-1$, then $A_{n,m}$ is the tree obtained from S_{m+1} by adding a pendent edge to each of $n - m - 1$ of the the pendent vertices of S_{m+1} . We call $A_{n,m}$ a spur. Clearly, $A_{n,m}$ has n vertices and m pendent vertices; the matching number, independence number and domination number of $A_{n,m}$ are $n - m$, m and $n - m$, respectively. Note that if $m > \frac{n-1}{2}$, then $A_{n,m} \cong BS_{n,m}$.

The eccentricity $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex, and the vertices of minimum eccentricity form the center. A tree has exactly one or two adjacent center vertices; in this latter case one speaks of a bicenter. The diameter $d(G)$ of a graph G is the maximum eccentricity over all vertices in a graph, and the radius $r(G)$ is the minimum eccentricity over all $v \in V(G)$. For a tree T with radius $r(T)$, it holds

$$d(T) = \begin{cases} 2r(T) - 1 & \text{if } T \text{ has a bicenter} \\ 2r(T) & \text{if } T \text{ has has a center.} \end{cases} \quad (1)$$

Let $C_{n,d}(p_1, p_2, \dots, p_{d-1})$ be a caterpillar on n vertices obtained from a path $P_{d+1} = v_0v_1 \dots v_{d-1}v_d$ by attaching $p_i \geq 0$ pendent vertices to v_i , $1 \leq i \leq d-1$, where $n = d+1 + \sum_{i=1}^{d-1} p_i$. Denote $C_{n,d,i} = C_{n,d}(\underbrace{0, \dots, 0}_{i-1}, n - d - 1, 0, \dots, 0)$. Obviously, $C_{n,d,i} = C_{n,d,n-i}$.

Denote by $\Delta(T)$ the maximum vertex degree of a tree T . The path P_n is the unique tree with $\Delta = 2$, while the star S_n is the unique tree with $\Delta = n - 1$. Therefore, we can assume that $3 \leq \Delta \leq n - 2$. The broom $B_{n,\Delta}$ is a tree consisting of a star $S_{\Delta+1}$ and a path of length $n - \Delta - 1$ attached to an arbitrary pendent vertex of the star.

In this paper, we deal with the hyper-Wiener index of trees with prescribed parameters such as the number of pendent vertices, matching number, independence number, domination number, diameter, radius and maximum degree. Furthermore, we introduce the ordering of starlike trees and determine the trees with the second smallest and largest hyper-Wiener index.

2 Preliminaries

Definition 2.1 Let v be a vertex of a tree T and $\deg(v) = m + 1$. Suppose that P_1, P_2, \dots, P_m are pendent paths incident with v , with the starting vertices of paths v_1, v_2, \dots, v_m , respectively and lengths $n_i \geq 1$ ($i = 1, 2, \dots, m$). Let w be the neighbor of v distinct from v_i . Let $T' = \delta(T, v)$ is a new tree obtained from T by removing the edges $vv_1, vv_2, \dots, vv_{m-1}$ and adding new edges $wv_1, wv_2, \dots, wv_{m-1}$. We say that T' is a δ -transformation of T .

This transformation preserves the number of leaves in a tree T .

Lemma 2.2 Let T be a tree rooted at the center vertex u with at least two vertices of degree at least 3. Let $v \in \{z \mid \deg(z) \geq 3, z \neq u\}$ be a vertex with the largest distance $d(u, v)$ from the center vertex. Then for the δ -transformation tree $T' = \delta(T, v)$ (as in Definition 2.1), it holds

$$WW(T) > WW(T'). \quad (2)$$

Proof. We follow the symbols in Definition 2.1. Let G be the component of $T - wv$ containing the vertex w . Let $M = \{P_1, P_2, \dots, P_{m-1}\}$. After δ transformation, the distances between vertices from G and M decreased by one, while the distance between vertices from M and $Q = P_m \cup \{v\}$ increased by one. By direct calculation, we have $WW(T') - WW(T) = \sum_{x \in G, y \in M} ((d(x, y) - 1) + (d(x, y) - 1)^2 - d(x, y) - d^2(x, y)) + \sum_{x \in Q, y \in M} ((d(x, y) + 1) + (d(x, y) + 1)^2 - d(x, y) - d^2(x, y)) = 2(\sum_{x \in Q, y \in M} (d(x, y) + 1) - \sum_{x \in G, y \in M} d(x, y))$.

According to the assumption, there is an induced path $P = ww_1w_2 \dots w_k$ passing through the center vertex u in G , with length at least $\max\{n_1, n_2, \dots, n_m\}$. For the path P_i , $1 \leq i \leq m - 1$, it follows $D_i = \sum_{x \in Q, y \in P_i} (d(x, y) + 1) - \sum_{x \in G, y \in P_i} d(x, y) < \sum_{x \in Q, y \in P_i} (d(x, y) + 1) - \sum_{x \in P, y \in P_i} d(x, y) \leq 0$.

Finally, we get $WW(T') - WW(T) = 2 \sum_{i=1}^{m-1} D_i < 0$, since T contains at least two vertices of degree at least 3, we have strict inequality. ■

From the above lemma, the hyper-Wiener index decreases if we move pendent paths P_i towards the center vertex u of T along the path P passing through u .

Lemma 2.3 Let G be a connected graph and $v \in V(G)$. The graph $G_{s,m}^*$ is obtained from G by attaching two paths $P = vv_1 \dots v_s$ and $Q = vv_1 \dots v_m$ of lengths s and m ($s \geq m \geq 1$) at v , respectively. Then $S(G_{s,m}^*) < S(G_{s+1,m-1}^*)$ and $WW(G_{s,m}^*) < WW(G_{s+1,m-1}^*)$.

Proof. The second conclusion is also obtained in [13], we present an alternative proof here. From the definition, we have

$$S(G_{s,m}^*) = \sum_{x,y \in V(G_{s,m-1}^*)} d^2(x,y) + \sum_{x \in V(G_{s,m-1}^*)} (d(x, u_{m-1}) + 1)^2.$$

$$S(G_{s+1,m-1}^*) = \sum_{x,y \in V(G_{s,m-1}^*)} d^2(x,y) + \sum_{x \in V(G_{s,m-1}^*)} (d(x, v_s) + 1)^2.$$

It follows that $S(G_{s,m}^*) - S(G_{s+1,m-1}^*) = \sum_{x \in V(G_{s,m-1}^*)} (d(x, u_{m-1}) - d(x, v_s)) (d(x, u_{m-1}) + d(x, v_s) + 2) < 0$.

In [16], it is shown that $W(G_{s,m}^*) < W(G_{s+1,m-1}^*)$. Together with $S(G_{s,m}^*) < S(G_{s+1,m-1}^*)$ we get $WW(G_{s,m}^*) < WW(G_{s+1,m-1}^*)$. ■

By Lemma 2.3, we immediately have

Lemma 2.4 For $3 \leq k \leq n - 1$, we have $WW(BS_{n,k-1}) > WW(BS_{n,k})$.

By Lemma 2.2 and Lemma 2.3, it follows

Theorem 2.5 Let G_0 be a connected graph and $u \in V(G_0)$. Assume that G_1 is the graph obtained from G_0 by attaching a tree T ($T \not\cong P_k$ and $T \not\cong S_k$) of order k to u ; G_2 is the graph obtained from G_0 by attaching a path P_k with its endvertex at u ; G_3 is the graph obtained from G_0 by attaching a star S_k with its center at u . Then $WW(G_3) < WW(G_1) < WW(G_2)$.

Let $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ be two integer arrays of length n . We say that x majorize y and write $x \succ y$ if elements of these arrays satisfy following conditions:

- (i) $x_1 \geq x_2 \geq \dots \geq x_n$ and $y_1 \geq y_2 \geq \dots \geq y_n$,
- (ii) $x_1 + x_2 + \dots + x_k \geq y_1 + y_2 + \dots + y_k$, for every $1 \leq k < n$,
- (iii) $x_1 + x_2 + \dots + x_n = y_1 + y_2 + \dots + y_n$.

Theorem 2.6 Let $p = (p_1, p_2, \dots, p_k)$ and $q = (q_1, q_2, \dots, q_k)$ be two arrays of length $k \geq 2$, such that $p \prec q$ and $n = \sum_{i=1}^k p_i = \sum_{i=1}^k q_i$. Then

$$WW(S_{p_1, p_2, \dots, p_k}) \leq WW(S_{q_1, q_1, \dots, q_k}), \tag{3}$$

with equality holding if and only if $p_i = q_i, (i = 1, 2, \dots, k)$.

Proof. For the array (p_1, p_2, \dots, p_k) , let s be the largest index such that $q_1 = q_2 = \dots = q_s$ and r be the smallest index such that $q_r = q_{r+1} = \dots = q_k$. We apply the transformation from Lemma 2.2 on tree S_{q_1, q_2, \dots, q_k} and get the new tree $S_{q_1, q_2, \dots, q_{s-1}, q_s-1, q_{s+1}, \dots, q_{r-1}, q_r+1, q_{r+1}, \dots, q_k}$. The condition $p \prec q$ is preserved. So we can continue the above process until the array q transforms into p , while at every step we decrease the hyper-Wiener index. ■

Corollary 2.7 *Let $T = S_{n_1, n_2, \dots, n_k}$ be a starlike tree on n vertices with k pendent paths. Then*

$$WW(BS_{n,k}) \leq WW(T) \leq WW(B_{n,k}).$$

The left equality holds if and only if $T \cong BS_{n,k}$, and the right equality holds if and only if $T \cong B_{n,k}$.

3 Main results

Lemma 3.1 *If $T \in \mathfrak{T}_{n,k}$ ($3 \leq k \leq n - 2$) has the minimal hyper-Wiener index, then there is only one vertex of degree greater than 2 in T , or equivalently, T is a starlike tree.*

Proof. Suppose $T \in \mathfrak{T}_{n,k}$ ($3 \leq k \leq n - 2$) has the minimal hyper-Wiener index. Let $S_T = \{v \in V(T) : \deg(v) \geq 3\}$. If $|S_T| = 1$, then by Corollary 2.7, it follows that $BS_{n,k}$ is the unique tree that has minimal Hyper-Wiener index. If $|S_T| \geq 2$, then there must exist at least two vertices of degree at least 3 and there are only pendent paths attached to them. We can consider T as the tree rooted at the center vertex and choose a vertex $v \in S_T$ furthest from the center vertex. After applying δ -transformation to T by Lemma 2.2, we decrease the hyper-Wiener index while keeping the number of pendent vertices fixed. This is a contradiction. ■

Theorem 3.2 *Among all the trees on n vertices with k ($3 \leq k \leq n - 2$) pendent vertices, $BS_{n,k}$ is the unique tree with the minimal hyper-Wiener index.*

Proof. By Lemma 3.1, we have that if $T \in \mathfrak{T}_{n,k}$ has the minimal hyper-Wiener index, then T is a starlike tree. By Lemma 2.3, we get the result. ■

Lemma 3.3 *The hyper-Wiener index of $A_{n,m}$ is*

$$WW(A_{n,m}) = \frac{1}{2}(10n^2 + m^2 - 8mn + 21m - 34n + 24).$$

Proof. There are four types of vertices in $A_{n,m}$.

- For each pendent vertex attached to the center vertex: $D(v) = 3n - m - 4$; $DD(v) = 9n - 5m - 12$;
- For the center vertex: $D(v) = 2n - m - 2$; $DD(v) = 4n - 3m - 4$;
- For each vertex of degree 2, different from the center vertex: $D(v) = 3n - m - 6$; $DD(v) = 9n - 5m - 20$;

- For each pendent vertex not attached to the center vertex: $D(v) = 4n - m - 8$; $DD(v) = 16n - 7m - 36$.

By the definition of the hyper-Wiener index, we get

$$\begin{aligned}
 WW(A_{n,m}) &= \frac{1}{4} \sum_{u \in V(A_{n,m})} D_{A_{n,m}}(u) + \frac{1}{4} \sum_{u \in V(A_{n,m})} DD_{A_{n,m}}(u) \\
 &= \frac{1}{4} \left[((2m+1-n)(3n-m-4) + (2n-m-2) \right. \\
 &\quad \left. + (n-m-1)(3n-m-6) + (n-m-1)(4n-m-8)) \right. \\
 &\quad \left. + ((2m+1-n)(9n-5m-12) + (4n-3m-4) \right. \\
 &\quad \left. + (n-m-1)(9n-5m-20) \right. \\
 &\quad \left. + (n-m-1)(16n-7m-36) \right] \\
 &= \frac{1}{2} (10n^2 + m^2 - 8mn + 21m - 34n + 24).
 \end{aligned}$$

This proves the result. ■

Theorem 3.4 *Let T be a tree on n vertices with matching number β . Then*

$$WW(T) \geq \frac{1}{2} (3n^2 + 6n\beta - 13n + \beta^2 - 21\beta + 24),$$

with equality holding if and only if $T \cong A_{n,n-\beta}$.

Proof. Suppose T has k pendent vertices. Then we have $k \leq \beta + n - 2\beta = n - \beta$. By Lemma 2.4 and Theorem 3.2, we have $WW(T) \geq WW(BS_{n,k})$ and $WW(BS_{n,k}) \geq WW(BS_{n,n-\beta}) = WW(A_{n,n-\beta})$ since $n - \beta \geq \frac{n}{2}$. So $WW(T) \geq WW(A_{n,n-\beta})$, with equality holding if and only if $T \cong A_{n,n-\beta}$. By Lemma 3.3 for $m = n - \beta$, we get the result. ■

Corollary 3.5 *Let T be a tree on n vertices with independence number α . Then*

$$WW(T) \geq \frac{1}{2} (10n^2 + \alpha^2 - 8n\alpha + 21\alpha - 34n + 24),$$

with equality holding if and only if $T \cong A_{n,\alpha}$.

Proof. Since for a bipartite graph G , the sum of the independence number and matching number equals to the number of vertices [4], from Theorem 3.4 we get the result. ■

Corollary 3.6 *Let T be a tree on n vertices with domination number γ . Then*

$$WW(T) \geq \frac{1}{2} (3n^2 + 6\gamma n - 13n + \gamma^2 - 21\gamma + 24),$$

with equality holding if and only if $T \cong A_{n,n-\gamma}$.

Proof. Note that the complement of the maximum independent set is just the minimum dominating set, from Corollary 3.5, we get the result. ■

Theorem 3.7 *Of all the trees on n vertices with diameter d , $C_{n,d,\lceil \frac{n}{2} \rceil}$ is the unique tree with the minimal hyper-Wiener index.*

Proof. Let T be the tree having the minimal hyper-Wiener index and diameter d . Let $P_{d+1} = v_0v_1 \dots v_{d-1}v_d$ be a path of length d . We show the following facts. $T \cong C_{n,d}(p_1, \dots, p_{d-1})$. By Theorem 2.5, all the trees attached to the path P_{d+1} must be stars, which implies the result. By Lemma 2.2 for $C_{n,d}(p_1, \dots, p_{d-1})$, we can get $T \cong T_{n,d,i}$. For the tree $C_{n,d,i}$, by Lemma 2.3, we have $i = \lceil \frac{n}{2} \rceil$. ■

According to the Equation (1), we have $2r(T) = d(T)$ or $2r(T) - 1 = d(T)$. Applying Lemma 2.3 to the center vertex of T , it follows that $WW(C_{n,2r,\lceil \frac{n}{2} \rceil}) > WW(C_{n,2r-1,\lceil \frac{n}{2} \rceil})$.

Corollary 3.8 *Let T be an arbitrary tree on n vertices with radius r . Then*

$$WW(T) \geq WW(C_{n,2r-1,\lceil \frac{n}{2} \rceil}),$$

with equality if and only if $T \cong C_{n,2r-1,\lceil \frac{n}{2} \rceil}$.

If $d > 2$, we can apply the transformation from Lemma 2.3 at the central vertex in $C_{n,d,\lceil \frac{n}{2} \rceil}$ and obtain $C_{n,d-1,\lceil \frac{n}{2} \rceil}$. Thus, we have $WW(P_n) = WW(C_{n,n-1,\lceil \frac{n}{2} \rceil}) > WW(C_{n,n-2,\lceil \frac{n}{2} \rceil}) > \dots > WW(C_{n,3,\lceil \frac{n}{2} \rceil}) > WW(C_{n,2,\lceil \frac{n}{2} \rceil}) = WW(S_n)$.

Also, it follows that $WW(C_{n,3,\lceil \frac{n}{2} \rceil})$ has the second minimal hyper-Wiener index among trees on n vertices.

By Lemma 2.3, we can get the following known result

Theorem 3.9 *Among all trees on n vertices with maximum degree Δ , $B_{n,\Delta}$ is the unique tree with the maximal hyper-Wiener index.*

Proof. Let T be a tree and $u \in V(T)$ such that $deg(u) = \Delta$. Suppose further $N(u) = \{u_1, u_2, \dots, u_\Delta\}$. By Theorem 2.5, if T has the maximal hyper-Wiener index, then all subtrees attached to u_i are paths for $1 \leq i \leq \Delta$. By Lemma 2.3, we get the result. ■

If $\Delta > 2$, we can apply the transformation from Lemma 2.3 at the vertex of degree Δ in $B_{n,\Delta}$ and obtain $B_{n,\Delta-1}$. Thus, $WW(S_n) = WW(B_{n,n-1}) < WW(B_{n,n-2}) < \dots < WW(B_{n,3}) < WW(B_{n,2}) = WW(P_n)$.

Also, it follows that $B_{n,3}$ has the second maximal hyper-Wiener index among trees on n vertices.

For the sake of completeness, we state the minimum case obtained in [18]. The complete Δ -ary tree is defined as follows. Start with the root

having Δ children. Every vertex different from the root, which is not in one of the last two levels, has exactly $\Delta - 1$ children. In the last level, while not all vertices have to exist, the vertices that do exist fill the level consecutively. Thus, at most one vertex on the level second to last has its degree different from Δ and 1.

Theorem 3.10 [18] *Among all trees on n vertices with maximum degree Δ , the complete Δ -ary tree is the unique tree with the mainimal hyper-Wiener index.*

Fischermann et al. in [9] proved that complete Δ -ary tree minimizes the Wiener index in the same class of trees.

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