HYPER-WIENER INDEX USING DEGREE SEQUENCE

SHIGEHALLI V. S.¹, SHANMUKH KUCHABAL*²

¹Professor, Department of Mathematics, Rani Channamma University, Vidya Sangama, Belagavi- 591 156, India.
²Research Scholar, Department of Mathematics, Rani Channamma University, Vidya Sangama, Belagavi- 591 156, India.

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ABSTRACT

Let G be the connected graph. The Wiener index \( W(G) \) is the sum of all distances between vertices of G, whereas the hyper-Wiener index \( WW(G) \) is defined as \( WW(G) = W(G) + \frac{1}{2} \sum_{[u,v] \subseteq V(G)} d(u,v)^2 \). In this paper we prove some general results on the hyper-Wiener index of graphs using degree sequence.

Keywords: molecular graphs and hyper-Wiener index.


1. INTRODUCTION

In mathematical terms a graph is represented as \( G = (V,E) \) where \( V \) is the set of vertices and \( E \) is the set of edges. Let \( G \) be an undirected connected graph without loops or multiple edges with \( n \) vertices, denoted by \( 1,2,\ldots,n \). The topological distance between the vertices \( u \) and \( v \) of \( V(G) \) is denoted by \( d(u,v) \) or \( d_{uv} \) and it is defined as the number of edges in a minimal path connecting the vertices \( u \) and \( v \).

The Wiener index \( W(G) \) of a connected graph \( G \) is defined as the sum the distances between all unordered pairs of vertices of \( G \). It was put forward by Harold Wiener [5]. The Wiener index is a graph invariant intensively studied both in mathematics and chemical literature, see for details [5 – 10].

The hyper-Wiener index was proposed by Randic [6] for a tree and extended by Klein et al. [1] to a connected graph. It is used to predict physicochemical properties of organic compounds. The hyper-Wiener index defined as,

\[
WW(G) = \sum_{[u,v] \subseteq V(G)} (d_{uv} + 1) = W(G) + \frac{1}{2} \sum_{[u,v] \subseteq V(G)} d(u,v)^2
\]

The hyper-Wiener index is studied both from a theoretical point of view and applications. We encourage the reader to consult [4, 5, 10 and 12 – 15] for further readings. The hyper-Wiener index of complete graph \( K_n \), path graph \( P_n \), star graph \( K_{1,(n-1)} \) and cycle graph \( C_n \) is given by the expressions

\[
WW(K_n) = \frac{n(n-1)}{2}, \quad WW(P_n) = \frac{n^4 + 2n^3 - n^2 - 2n}{24}, \quad WW(K_{1,(n-1)}) = \frac{1}{2} (n-1)(3n-4)
\]

And

\[
WW(C_n) = \begin{cases} \frac{n^2(n+1)(n+2)}{48}, & \text{if } n \text{ is even} \\ \frac{n(n^2-1)(n+3)}{48}, & \text{if } n \text{ is odd} \end{cases}
\]

Corresponding Author: Shanmukh Kuchabal*²
²Research Scholar, Department of Mathematics, Rani Channamma University, Vidya Sangama, Belagavi- 591 156, India.
For example: Consider a graph G with vertices $v_1, v_2, v_3$ and $v_4$ as labeled in the figure below.

Here $d(v_1, v_2) = 1$, $d(v_1, v_3) = 2$, $d(v_1, v_4) = 2$, $d(v_2, v_3) = 1$, $d(v_2, v_4) = 1$, $d(v_3, v_4) = 1$.

Therefore $WW(G) = \sum_{\{u,v\} \subseteq V(G)} (d_{uv} + 1) = 2 \times \frac{1}{2} + 3 \times \frac{2}{2} + 3 \times \frac{2}{2} + 2 \times \frac{1}{2} + 2 \times \frac{1}{2} + 2 \times \frac{1}{2} = 1 + 3 + 3 + 1 + 1 + 1 = 10$.

2. EXISTING RESULTS

Theorem 2.1: [4,6] If $G(p, q)$ is a is a graph, with $\Delta(G) = p - 1$ then $W(G) = p^2 - p - q$.

Theorem 2.2: [6] If $G(p, q)$ is a connected graph then the Wiener Index of $G + x$ is $p^2 - p$.

Theorem 2.3: [6] If $G(p, q)$ be a graph and $x$ is any vertex in $G$ of degree $p - 1$ such that the graph $G - x$ is connected then Wiener index of $G - x$ is $(p - 1)^2 - q$.

Theorem 2.4: [6] If $G_1(p_1, q_1)$ and $G_2(p_2, q_2)$ are two connected graphs then the Wiener index of $G_1 + G_2$ is $W(G_1 + G_2) = p_1(p_1 - 1) + p_2(p_2 - 1) + p_1p_2 - q_1q_2$.

Theorem 2.5: [6] The Wiener index of $W(G^{-1}) = m(m - 1) + p(p - 1) + mp - q$.

3. MAIN RESULTS

3.1 Bounds for the hyper-Wiener index in terms of Order, Size and Maximum Degree:

Lemma 3.1.1: Let G be the graph with n vertices m edges, then $WW(G) \geq \frac{3n^2 - 3n - 4m}{2}$.

Proof: Let $n_i$ be any vertex of G. Then,

$$d(n_i|G) \geq \deg(v_i) + 2[n - 1 - \deg(v_i)] = 2n - 2 - \deg(v_i)$$

$$d(n_i|G)^2 \geq \frac{d(n_i|G) + 1}{2} \times d(n_i|G) = 2n - 2 - \deg(v_i) + n - 1 - \deg(v_i) = 3n - 3 - 2\deg(v_i)$$

Since $\deg(v_i)$ number of vertices are adjacent to $u_i$ and the remaining vertices are at distance greater than or equal to two from $u_i$.

$$WW(G) = \frac{1}{2} \sum_{i=1}^{n} d(n_i|G)^2 \geq \frac{1}{2} \sum_{i=1}^{n} (3n - 3 - 2\deg(v_i)) = \frac{1}{2} \sum_{i=1}^{n} (3n - 3) - \sum_{i=1}^{n} 2\deg(v_i)$$
The bounds in the above lemma is sharp, for any graph G of diameter two, which we will see in the following theorem, Theorem 3.1.2: If G(n,m) is a graph with Δ(G) = n − 1 then WW(G) = \( \frac{3n^2 - 3n - 4m}{2} \).

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

By taking W(G) = \( n^2 - n - m \) in the theorem 2.1

We get \( WW(G) = n^2 - n - m + \frac{1}{2} \sum_{(u,v) \in V(G)} d(u,v)^2 \)

Let V = v₁, v₂, ..., vₙ and deg(vₙ) = n − 1. For any arbitrary pair of vertices (vᵢ, vⱼ). If \( d(vᵢ, vⱼ) > 2 \) then we take shortest path (vᵢ, vⱼ), (vⱼ, vⱼ) so that \( d(vᵢ, vⱼ) = 2 \) i.e. \( d(vᵢ, vⱼ) \leq 2 \) always. The meaning of deg(vᵢ) is the cardinality of NBH(vᵢ). Number of vertices lie at distance 1 from vᵢ. Therefore \( (n - 1) - \text{deg}(vᵢ) \) is the number of vertices vⱼ. Which is not in the neighborhood of vᵢ, i.e. \( (n - 1) - \text{deg}(vᵢ) \) vertices has the distance 2 from vᵢ.

\[ WW(G) = n^2 - n - m + \frac{1}{2} \left( \sum_{j=1}^{n} d(v₁, vⱼ)^2 + d(v₂, vⱼ)^2 + \ldots + d(vₙ, vⱼ)^2 \right) \]

\[ WW(G) = n^2 - n - m + \frac{1}{2} \sum_{j=1}^{n} d(v₁, vⱼ)^2 + \sum_{j=1}^{n} d(v₂, vⱼ)^2 + \ldots + \sum_{j=1}^{n} d(vₙ, vⱼ)^2 \]

\[ = n^2 - n - m + \frac{1}{2} \left( (n - 1) - \text{deg}(v₁) + (n - 1) - \text{deg}(v₂) + \ldots + (n - 1) - \text{deg}(vᵢ) \right) \]

\[ = n^2 - n - m + \frac{1}{2} \left( \sum_{i=1}^{n} (n - 1) - \sum_{i=1}^{n} \text{deg}(vᵢ) \right) \]

\[ = n^2 - n - m + \frac{1}{2} \left( (n(n - 1) - 2m) \right) \]

\[ = n^2 - n - m + \frac{1}{2} \frac{n(n - 1) - 2m}{2} - m \]

\[ = \frac{3n(n - 1) - 2m}{2} \]

\[ WW(G) = \frac{3n^2 - 3n - 4m}{2} \]

Illustration: Following is the example for \( \text{diam} \leq 2 \) of graph,

\[ n = 4, \ m = 3 \text{ and } WW(G) = 12 \]
Corollary 3.1.3 If \( G(n, m) \) is a connected graph then the hyper-Wiener index of \( G + x \) is \( \frac{3n^2 - n - 4m}{2} \)

Proof: Let \( G \) be a graph with \( n \) vertices \((v_1, v_2, v_3, ..., v_n)\). The graph \( G + x \) is obtained from \( G \) by adding \('n'\) new edges by joining all the vertices of \( G \) to the vertex \( x \). Let vertex set of the graph \( G + x \) be \((v_1, v_2, v_3, ..., v_n, x)\) and the edge set be \((e_1, e_2, ..., e_m, e_{m+1}, ..., e_{n+m})\). The graph \( G + x \) has \( n + 1 \) vertices and \( n + m \) edges. Hence substituting number of vertices as \( p = n + 1 \) and number of edges as \( q = n + m \) in the previous Theorem,

\[
WW(G + x) = \frac{3(n+1)^2 - 3(n+1) - 4(n + m)}{2} = \frac{3(n^2 + 2n + 1) - 3(n+1) - 4n - 4m}{2}
\]

\[
WW(G + x) = \frac{3n^2 - n - 4m}{2}
\]

Illustration: Following is the example for join of two graphs

\[
n = 4, m = 4 \text{ and } WW(G) = 14
\]

Corollary 3.1.4: If \( G(n, m) \) be a graph and \( x \) is any vertex in \( G \) of degree \( n - 1 \) such that the graph \( G - x \) is connected then hyper-Wiener index of \( G - x \) is \( \frac{3n^2 - 5n - 4m + 2}{2} \)

Proof: Let \( G \) be a graph without pendent vertices. If there exists at least one vertex \( v \) such that \( \deg(v) = n - 1 \). The vertex \( v \) is named as \( x \), we remove the vertex \( x \) from \( G \) is \( G - x \). The vertex of \( G - x \) is \( n - 1 \) and the edges be \( m - n + 1 \) then by the theorem 3.1.2.

\[
WW(G) = \frac{3n^2 - 3n - 4m}{2}
\]

\[
WW(G - x) = \frac{3(n - 1)^2 - 3(n - 1) - 4(m - n + 1)}{2} = \frac{3(n^2 + 2n - 1) - 3n + 3 - 4m + 4n - 4}{2} = \frac{3n^2 + 6n - 3n + 3 - 4m + 4n - 4}{2}
\]

\[
WW(G - x) = \frac{3n^2 - 5n - 4m + 2}{2}
\]

Illustration: Example for connected \( G - x \) of graph

\[
n = 4, m = 6 \text{ and } WW(G) = 3
\]
Theorem 3.1.5: If \( G_1(n_1, m_1) \) and \( G_2(n_2, m_2) \) are two connected graphs then the hyper-Wiener index of \( G_1 + G_2 \) is
\[
WW(G_1 + G_2) = \frac{3n_1(n_1 - 1)}{2} + \frac{3n_2(n_2 - 1)}{2} + n_1n_2 - 2m_1 - 2m_2.
\]

Proof: By definition,
\[
WW = W(G) + \frac{1}{2} \sum_{[u,v] \subseteq V(G)} d(u, v)^2
\]
From theorem 2.4
\[
W(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2
\]
Therefore,
\[
WW(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2 + \frac{1}{2} \sum_{[u,v] \subseteq V(G)} d(u, v)^2
\]
The graph \( G_1 \) has \( n_1 \) vertices with degree sequence \( (d_1, d_2, d_3, \ldots, d_{n_1}) \). The graph \( G_2 \) has \( n_2 \) vertices with degree sequence \( (g_1, g_2, g_3, \ldots, g_{n_2}) \). In \( G_1 + G_2 \) graph all the vertices of \( G_1 \) and \( G_2 \) are at distance one. In graph \( G_1 \) \((n_1 - 1) - \deg(v_{i_1}) \) vertices are at distance two and similarly graph \( G_2 \), \((n_2 - 1) - \deg(v_{i_2}) \) vertices are at distance two.

Then,
\[
WW(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2 + \frac{1}{2} \sum_{i=1}^{n} (n_1 - 1) - \deg(v_{i_1}) + (n_2 - 1) - \deg(v_{i_2})
\]
\[
WW(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2 + \frac{1}{2} \sum_{i=1}^{n} \deg(v_{i_1}) + \sum_{i=1}^{n} (n_1 - 1) - \sum_{i=1}^{n} \deg(v_{i_1})
\]
\[
WW(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2 + \frac{1}{2} (n_1(n_1 - 1) - 2m_1 + n_2(n_2 - 1) - 2m_2)
\]
\[
WW(G_1 + G_2) = \frac{3n_1(n_1 - 1)}{2} + \frac{3n_2(n_2 - 1)}{2} + n_1n_2 - 2m_1 - 2m_2
\]

Illustration: Example for \( G_1 + G_2 \) of two graphs

\[
n_1 = 3, n_2 = 2, m_1 = 2, m_2 = 1 \text{ and } WW(G) = 12.
\]

Theorem 3.6: The hyper-Wiener index of \( WW(G^1) = \frac{3l(l - 1)}{2} + \frac{3n(n - 1)}{2} + nl - 2m \). Where \( G^1 = G + lK_1 \)

Proof: Let \( G(n, m) \) be a connected graph. The graph \( G^1 = G + lK_1 \) is obtained from graph \( G \) by joining all the vertices of graph \( G \) to the new \( l \) vertices of graph \( G^1 \). The vertex set of \( G^1 \) be \( V(G^1) = \{v_1, v_2, \ldots, v_n, x_1, x_2, x_3, \ldots, x_l\} \) and the edge set be \( E(G^1) = E(G) \cup \{v_i x_j: 1 < i < n, 1 < j < l\} \).

By definition,
\[
WW(G^1) = W(G^1) + \frac{1}{2} \sum_{[u,v] \subseteq V(G)} d(u, v)^2
\]
From theorem 2.5
\[
WW(G^1) = l(l - 1) + n(n - 1) + ln - m
\]
Therefore,
\[ WW(G^1) = l(l - 1) + n(n - 1) + ln - m + \frac{1}{2} \sum_{(u,v) \in V(G)} d(u,v)^2 \]

\[ WW(G^1) = l(l - 1) + n(n - 1) + ln - m + \frac{1}{2} \left\{ \sum_{i=1}^{n} (n - 1) - \sum_{i=1}^{n} deg_v + 1 + 1 + \cdots + 1 \right\} \]

\[ WW(G^1) = l(l - 1) + n(n - 1) + ln - m + \frac{1}{2} (n(n - 1) - 2m + l(l - 1)) \]

\[ WW(G^1) = \frac{3l(l - 1)}{2} + \frac{3n(n - 1)}{2} + nl - 2m \]

Illustration: Example for \( G^1 \) of graphs

\[ l = 2, n = 3, m = 3 \text{ and } WW(G^1) = 12 \]

REFERENCES


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