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HYPER-WIENER INDEX USING DEGREE SEQUENCE

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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.*

2000 Mathematics subject classification: *05C12, 92E10.*

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,

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

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_p, path graph-P_n, star graph-$K_{1,(n-1)}$ and cycle graph C_n is given by the expressions

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

And

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

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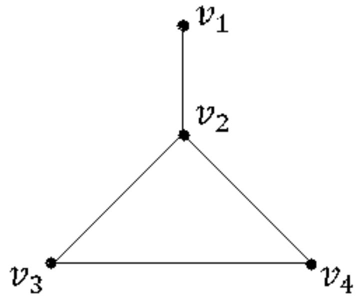
For example: Consider a graph G with vertices v_1, v_2, v_3 and v_4 as labeled in the figure below.



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 $WW(G) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$

$$= \frac{2\times 1}{2} + \frac{3\times 2}{2} + \frac{3\times 2}{2} + \frac{2\times 1}{2} + \frac{2\times 1}{2} + \frac{2\times 1}{2}$$
$$= 1 + 3 + 3 + 1 + 1 + 1$$
$$= 10$$

2. EXISTING RESULTS

Theorem 2.1: [4,6] If $G(p, q)$ is a is a graph, with $\Delta(G) = p - 1$ then $W(G) = p2 - p - q$.

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: Len n_i be any vertex of G. Then,

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

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

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.

$$WW(G) = \frac{1}{2}\sum_{i=1}^{n} d(u_i|G)^2$$
$$\geq \frac{1}{2}\sum_{i=1}^{n}\{3n - 3 - 2\deg(v_i)\}$$
$$= \frac{1}{2}\sum_{i=1}^{n}(3n-3) - \sum_{i=1}^{n} 2\deg(v_i)$$

$$= \frac{n(3n-3)}{2} - \frac{4m}{2} \quad \sum_{i=1}^{n} \deg(v_i) = 2m$$
$$= \frac{n(3n-3)-4m}{2}$$

$$WW(G) \geq \frac{3n^2-3n-4m}{2}$$

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 $\Delta(G) = n-1$ then WW(G) = $\frac{3n^2-3n-4m}{2}$.

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

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

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

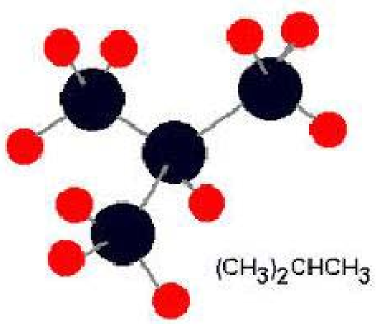
Let $V = v_1, v_2, \ldots, v_n$ and $\deg(v_n) = n-1$. For any arbitrary pair of vertices (v_i, v_j). If $d(v_i, v_j) > 2$ then we take shortest path $(v_i, v_j), (v_n, v_j)$ so that $d(v_i, v_j) = 2$ i.e. $d(v_i, v_j) \leq 2$ always. The meaning of $\deg(v_i)$ is the cardinality of $NBH(v_i)$. Number of vertices lie at distance 1 from v_i. Therefore $(n-1) - \deg(v_i)$ is the number of vertices v_j. Which is not in the neighborhood of v_i. i.e. $(n-1) - \deg(v_i)$ vertices has the distance 2 from v_i.

$$WW(G) = n^2 - n - m + \frac{1}{2}[\sum_{j=1}^{n}\{d(v_1,v_j)^2 + d(v_2,v_j)^2 + \cdots + d(v_n,v_j)^2\}]$$

$$WW(G) = n^2 - n - m + \frac{1}{2}\{\sum_{j=1}^{n} d(v_1,v_j)^2 + \sum_{j=1}^{n} d(v_2,v_j)^2 + \cdots + \sum_{j=1}^{n} d(v_n,v_j)^2$$
$$= n^2 - n - m + \tfrac{1}{2}[(n-1) - \deg(v_1) + (n-1) - \deg(v_2) + \cdots + (n-1) - \deg(v_i)]$$
$$= n^2 - n - m + \frac{1}{2}\{\sum_{i=1}^{n}(n-1) - \sum_{i=1}^{n}\deg(v_i)\}$$
$$= n^2 - n - m + \frac{1}{2}\{n(n-1) - 2m\}$$
$$= n^2 - n - m + \frac{n(n-1)}{2} - m$$
$$= \frac{3n(n-1)}{2} - m$$

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

Illustration: Following is the example for $diam \leq 2$ of graph,



$n = 4, m = 3$ 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 $\frac{3n^2-n-4m}{2}$

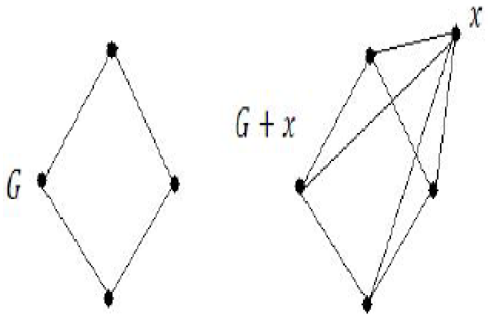
Proof: Let G be a graph with n vertices $(v_1, v_2, v_3, \dots, v_n)$. The graph $G+x$ is obtained from G by adding 'n' new edges by joining all the vertices of G to the vertex x. Let vertex set of the graph $G+x$ be $(v_1, v_2, v_3, \dots, v_n, x)$ and the edge set be $(e_1, e_2, \dots, e_m, e_{m+1}, \dots, e_{n+m})$. 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,

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

$$= \frac{\boldsymbol{3(n^2+1+2n) - 3(n+1) - 4n - 4m}}{\boldsymbol{2}}$$

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

Illustration: Following is the example for join of two graphs



$n=4, m=4$ 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.

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

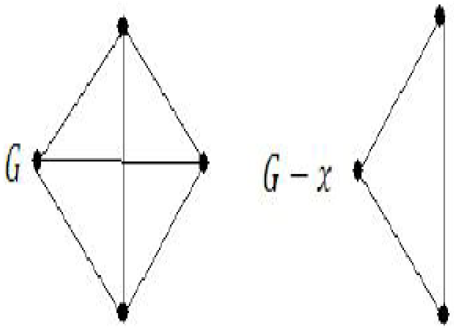
$$WW(G-x) = \frac{3(n-1)^2 - 3(n-1) - 4(m-n+1)}{2}$$

$$= \frac{3(n^2+1-2n) - 3n + 3 - 4m + 4n - 4}{2}$$

$$= \frac{3n^2 + 3 - 6n - 3n + 3 - 4m + 4n - 4}{2}$$

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

Illustration: Example for connected $G-x$ of graph



$n=4, m=6$ 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 $(d_1, d_2, d_3, \dots, d_{n_1})$. The graph G_2 has n_2 vertices with degree sequence $(g_1, g_2, g_3, \dots, g_{n_2})$. In $G_1 + G_2$ graph all the vertices of n_1 and n_2 are at distance one. In graph G_1, $(n_1 - 1) - \deg(v_{i_{n_1}})$ vertices are at distance two and similarly graph G_2, $(n_2 - 1) - \deg(v_{i_{n_2}})$ vertices are at distance two.

Then,

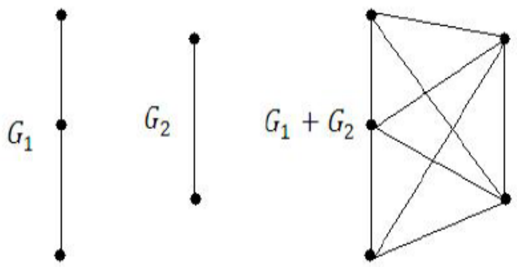
$$WW(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2 + \frac{1}{2}\sum_{1}^{n}\{(n_1 - 1) - \deg(v_{n_1}) + (n_1 - 1) - \deg(v_{i_{n_1}})\}$$

$$WW(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2 + \frac{1}{2}\{\sum_{1}^{n}(n_1 - 1) - \sum_{1}^{n}\deg(v_{n_1}) + \sum_{1}^{n}(n_1 - 1) - \sum_{1}^{n}\deg(v_{i_{n_1}})\}$$

$$WW(G_1 + G_2) = n_1(n_1 - 1) + n_2(n_2 - 1) + n_1n_2 - m_1 - m_2 + \frac{1}{2}\{n_1(n_1 - 1) - 2m_1 + n_2(n_2 - 1) - 2m_2\}$$

$$WW(G_1 + G_2) = \frac{3n_1(n_1 - 1)}{2} + \frac{3n_2(n_2 - 1)}{2} + n_1n_2 - 2m_1 - 2m_2$$

Illustration: Example for $G_1 + G_2$ of two graphs



$n_1 = 3, n_2 = 2, m_1 = 2, m_2 = 1$ 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 to the new l vertices of $(x_1, x_2, x_3, \dots, x_l)$, the vertex set of G^1 be $V(G^1) = \{v_1, v_2, \dots v_n, x_1, x_2, x_3, \dots, x_l\}$ and the edge set be $E(G^1) = E(G) \sqcup \{v_ix_j : 1 < i < n, 1 < j < l\}$.

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,

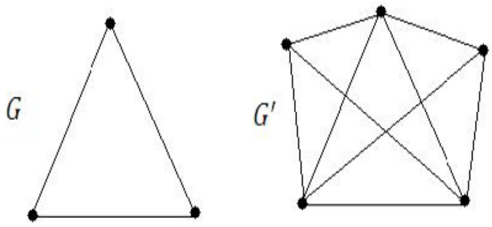
$$WW(G^1) = l(l-1) + n(n-1) + ln - m + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2$$

$$WW(G^1) = l(l-1) + n(n-1) + ln - m + \frac{1}{2}\{\sum_{i=1}^{n}(n-1) - \sum_{i=1}^{n} degv_i + \underbrace{1+1+\cdots+1}_{l(l-1)}\}$$

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

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

Illustration: Example for $G^1$of graphs



$l = 2, n = 3, m = 3$ and $WW(G^1) = 12$

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