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WIENER NUMBER SEQUENCE FOR SEQUENCE OF PLANAR GRAPHS

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ABSTRACT: The structure of a chemical compound usually represented by molecular graph where atoms are represented by vertices and the chemical bonds are represented by edges, It has been found that many properties of chemical compound are closely related to some topological indices, the Wiener index is the most important one. It is defined as the sum of shortest distance between every pair of vertices in G. In this paper we obtain Wiener polynomial for planar graph $P\ell_n$ with maximal number of edges and also discuss the inverse Wiener index problem for the same graph.

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1. Introduction

A topological representation of a molecule can be carried out through molecular graph. A molecular graph is collection of points representing the atoms in the molecule and a set of lines representing covalent bonds. The points are called vertices and lines are called edges. Quantities associated with a molecular graph to estimate various physical properties are called topological indices. The oldest topological index is Wiener index introduced by Harold Wiener in 1947. The Wiener index is a distance based graph invariant, used as one of the structure descriptors for predicting physicochemical properties of organic compounds. The Wiener index correlates physicochemical properties of organic compounds and the topological structure of their molecular graphs. This concept has been one of the most widely used descriptors in relating chemical compound's property to its molecular graph. Therefore, in order to construct a compound with a certain property, one may want to build some structure that has the corresponding Wiener index.

The biological community has been using the Wiener index to correlate a compound's molecular graph with experimentally gathered data regarding the compound's characteristics. In the drug design process, one wants to construct chemical compounds with certain properties. The basic idea is to construct chemical compounds from the most common molecules so that the resulting compound has the expected Wiener index. We first give the definitions of Wiener index and Wiener polynomial for connected graphs.

Definition 1.1: Wiener index is the half sum of shortest distance between every pair of vertices in the graph G.

$$W(G) = \frac{1}{2}\sum_i \sum_j d_{ij} \text{ Where } d_{ij} \text{ is the shortest distance between to } v_i \text{ and } v_j.$$

For any graph G we have $W(K_n) \le W(G) \le W(P_n)$.

Conjecture 1.1 (Wiener Index Conjecture [3, 4]): Except for some finite set, every positive integer is the Wiener index of some tree.

Problem 1.1 (Inverse Wiener Problem: Given an integer n, construct a tree whose Wiener index is n.

Problem 1.2 (Inverse Wiener Covering Problem: Given an integer n, for every $i \le n$ construct a tree with Wiener index i.

Definition 1.2: Wiener polynomial of a connected graph G is defined as

$$W(G; q) = \sum_{\{u, v\} \subset V(G)} q^{d_G(u, v)}$$

Where $d_G(u, v)$ denotes the distance between two vertices u and v in G and

$$W(G) = \sum_{\{u, v\} \subset V(G)} d_G(u, v) = \left.\frac{dW(G; q)}{dq}\right|_{q=1}$$

Definition 1.3: A graph is said to be complete if each vertex of it is connected to all other vertices by an edge. If $K_n = (V < E)$ is a complete graph with n vertices where $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{v_i v_j : i \ne j \text{ and } i < j \;\forall 1 \le i, j \le n\}$, then it has $n(n-1)/2$ edges and $W(K_n) = \frac{n(n-1)}{2}$.

Definition 1.4 [1]: The class $P\ell_n (n \ge 5)$ of planar graphs with maximal edges over n vertices is obtained by removing $(n-4)(n-3)/2$ edges from the complete graph K_n. Let $P\ell_n = (V, E), n \ge 5$ be tha planar graph with maximal edges where $V = \{v_1, v_2, \ldots, v_n\}$, $E = E(K_n) \backslash \{v_k v_i : 3 \le k \le n-2, k+2 \le i \le n\}$.

In general, for $P\ell_n$, $|V| = n$ and $|E| = 3(n-2)$ with $2(n-2)$ faces.

$\deg(v_1) = \deg(v_2) = (n-1)$, $\deg(v_3) = \deg(v_n) = 3$, $\deg(v_i) = 4$, $4 \le i \le n-1$

$P\ell_6$ is described in Figure 1. $W(P\ell_n)\; n^2 - 4n + 6$. [2]

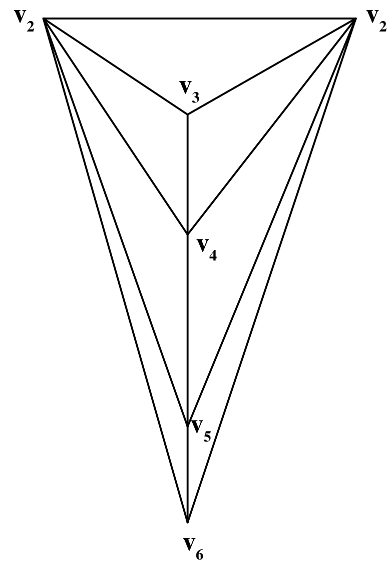

Figure 1: $P\ell_6$

Algorithm 1.1:

Input: Complete Graph K_n

Output: $P\ell_n$ and gradual decrease in Wiener index.

Step 1: Consider a complete graph K_n and label the vertices as $v_1, v_2, \ldots, v_n$.

Step 2: Edges $E(K_n) = \{(k, \ell) : 1 \leq k, \ell \leq n, k < \ell\}$

Step 3: Start removing edges

$(v_1, v_3), (v_1, v_4), (v_1, v_5), \ldots, (v_1, v_{n-1}),$

$(v_2, v_3), (v_2, v_4), (v_2, v_5), \ldots, (v_2, v_n)$, …which leads to increase in Wiener index sequence by one.

In this paper we investigate inverse Wiener covering problem for graphs. Given any integer n which is not equal to 2 and 5 we can obtain a graph with Wiener number n which is derived from the class of planar graph $P\ell_n$ with maximum edges. We obtain a sequence of such graphs for a sequence for a sequence of integers respectively.

2. Calculation of Wiener Index and Wiener Covering Polynomial of class $P\ell_N$

Theorem 2.1: The Wiener Index for the class of planar graph $P\ell_n$ ($n \geq 5$) with maximal edges is $n^2 - 4n + 6$.

Proof: From definition 1.4, the distance between any two vertices in $P\ell_n$ class of graphs is given as

$$\begin{aligned}
d(v_1, v_i) &= 1;\ 2 \le i \le n \\
d(v_2, v_i) &= 1;\ 3 \le i \le n \\
d(v_i, v_{i-1}) &= 1;\ 3 \le i \le n-1 \\
d(v_i, v_j) &= 2;\ i \ne j, j - i > 1, 3 \le i \le n-2 \text{ and } 5 \le n \text{ and let } G = P\ell_n. \\
W(G) &= \sum_{i<j} d(u_i, v_j) \\
&= (n-1) + (n-2) + [1 + 2(n-4)] + [1 + 2(n-5)] \\
&\quad + \dots + [1 + 2(n-(n-1)) + 1 \\
&= (n-1) + (n-2) + (n-3) + 2(1 + 2 + \dots + (n-4)) \\
W(G) &= n^2 - 4n + 6.
\end{aligned}$$

Theorem 2.2: Wiener polynomial for is $(3n-6)q + (n-4)(n-3)/2\ q^2$.

Proof: By definition 1.3 the two vertices v_1 and v_2 are of degree $(n-1)$, the distance between v_1 to all the other $(n-1)$ vertices is one and the distance between v_2 to all other $(n-2)$ vertices is one. Among the vertices $v_3, v_4, \dots, v_n$ there are $(n-3)$ vertices at distance one and $(n-4)$, $(n-5)$, $(n-6)$, …, 1 pair of vertices are at distance two. Hence

$$W[P\ell_n; q] = (n-1)q + (n-2)q + (n-3)q + \{(n-4) + (n-5) + \dots + 1\}q^2$$
$$W[P\ell_n; q] = (3n-6)q + (n-4)(n-3)/2\ q^2.$$

3. DISCUSSION ON INVERSE WIENER INDEX PROBLEM

Given a positive integer n, can we find a graph with Wiener index n?.

We solve this problem with the help of the class of planar graphs $P\ell_n$ with maximal number of edges. We do this by the following procedure. We take the complete graph K_n and remove the edges one by one until it becomes $P\ell_n$. We get a sequence of graphs for which the Wiener index is also sequence of consecutive positive integers in increasing order. This process is implemented in the proof of the following theorem.

Theorem 3.1: For every positive integer $n \ne 2$ & 5 there exist a planar graph with Wiener index n.

Proof: Consider a complete graph K_n with n vertices and $\frac{n(n-1)}{2}$ edges. The Wiener index of K_n is $n(n-1)/2$. To obtain $P\ell_n$, we need to remove $m = \frac{(n-4)(n-3)}{2}$ edges. We remove these m edges one by one and calculate Wiener index at each stage.

Step 1: Let $m = 1$, except the two vertices v_i, v_j which are incident with the removed edge, the remaining $(n-2)$ vertices are of degree $(n-1)$. The two vertices v_i and v_j are of degree $(n-1)$ distance between these two vertices is two, since the edge between v_i and v_j has been removed. Hence,

$$W(K_n - 1 \text{ edge}) = \frac{1}{2}\,[(n-2)(n-1) + 2(n-2+2)] = \frac{1}{2}\,[n^2 - n + 2].$$

Step 2: Let $m = 2$, since in K_n every vertex is connected to any other vertex by an edge, only three vertices say v_i, v_j and v_k are incident with the removed two edges. Except the three vertices v_i, v_j and v_k, the reaming $(n-3)$ vertices are of degree $(n-1)$. Among these three v_i, v_j and v_k, any one of the vertex say v_i will be of degree $(n-3)$ and the remaining two vertices are of degree $(n-2)$ and the distances between v_i & v_j and v_i & v_k are two. Hence,

$$W(K_n - 2 \text{ edges}) = \frac{1}{2}\,[(n-3)(n-1) + 2\{(n-2)+2\} + \{(n-3)+2+2\}]$$

$$= \frac{1}{2}\,[n^2 - n + 2].$$

Step 3: Let $m = 3$, Except the four vertices v_i, v_j, v_k and v_1, the reaming $(n-4)$ vertices are of degree $(n-1)$. Among these four v_i, v_j, v_k, and v_1 any one of the vertex say v_i will be of degree $(n-4)$ and the remaining three vertices are of degree $(n-2)$ and the distances between v_i & v_j, v_i & v_k and v_i & v_1 are two.

$$W(K_n - 3 \text{ edges}) = \frac{1}{2}\,[(n-4)(n-1) + 3\{(n-2)+2\} + \{(n-4)+3*2\}]$$

$$= \frac{1}{2}\,[n^2 - n + 6].$$

Step 4: The removal of (v_i, v_j), (v_i, v_k), (v_i, v_1) and (v_i, v_m) will give Wiener index

$$W(K_n - 4 \text{ edges}) = \frac{1}{2}\,[(n-5)(n-1) + 4\{(n-2)+2\} + \{(n-5)+4*2\}]$$

$$= \frac{1}{2}\,[n^2 - n + 8].$$

By induction on the removal of $m = \frac{(n-5)(n-2)}{2}$ edges, we get

$$W\left(K_n - \frac{(n-5)(n-2)}{2}\text{edges}\right) = \frac{1}{2}\left[\begin{array}{l}\left(n - \frac{(n-4)(n-3)}{2}\right)(n-1) + \frac{(n-5)(n-2)}{2}\{(n-2)+2\} \\ +\left\{\left(n - \frac{(n-4)(n-3)}{2}\right) + \frac{(n-5)(n-2)}{2} * 2\right\}\end{array}\right]$$

$$= \frac{1}{2}[n^2 - n + (n-5)(n-2)].$$

Now we have to prove the theorem for $\frac{(n-4)(n-3)}{2}$ edges.

When we remove one edge from $K_n - \frac{(n-5)(n-2)}{2}$, there will be $\left(n - \frac{(n-4)(n-3)}{2}\right)$ vertices are of degree $(n-1)$, only one vertex from where all the edges are removed is of degree $\left(n - \frac{n^2-7n+14}{2}\right)$ and $\frac{n^2-7n+12}{2}$ pairs of vertices are of distance two, the remaining $\frac{n^2-7n+12}{2}$ are of degree $(n-2)$ and distance between any two vertices among these vertices is two. Hence,

$$W\left(K_n - \frac{(n-4)(n-3)}{2}\text{edges}\right) = \frac{1}{2}\left[\begin{array}{l}\left(n - \frac{(n^2-7n+14)}{2}\right)(n-1) + \frac{(n-4)(n-3)}{2}\{(n-2)+2\} \\ +\left\{\left(n - \frac{(n^2-7n+14)}{2}\right) + \frac{(n-4)(n-3)}{2} * 2\right\}\end{array}\right]$$

$$= \frac{1}{2}\left[\begin{array}{l}n(n-1) - \frac{n}{2}(n^2 - 7n + 14 - n^2 + 7n - 12) \\ + n + (n-4)(n-3)\end{array}\right]$$

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

$$= n^2 4n + 6 = W(P\ell_n).$$

The following Table shows the Wiener index for different values of n and $\frac{(n-4)(n-3)}{2}$.

N	*m*	*WI of K_n*	*WI of K_n-1 edge*	*WI of K_n-2 edges*	*WI of K_n-3 edges*	*WI of K_n-4 edges*	*WI of K_n-5 edges*	*WI of K_n-6 edges*	*WI of K_n-7 edges*	*WI of K_n-8 edges*	*WI of K_n-9 edges*	*WI of K_n-10 edges*
5	1	10	**11**	12	13	14						
6	3	15	16	17	**18**	19	20					
7	6	21	22	23	24	25	26	**27**				
8	10	28	29	30	31	32	33	34	35	36	37	**38**
9	15	36	37	38	39	40	41	42	43	44	45	46…51
10	21	45	46	47	48…							

The inverse Wiener index argument follows from the above Table.

$W(K_n) = 10, 15, 21, 28, 36, 45, \ldots, n \geq 5$ and $W(P\ell_n) = 11, 18, 27, 38, 51, \ldots, n \geq 5$

Wiener index increases as the number of edges decreases. When we start removing the edges from complete graph K_n one by one gradually the Wiener index increases by one.

(ie) $W(K_n) = n(n-1)/2$

$W(K_n - 1 \text{ edge}) = W(K_n) + 1$

$W(K_n - 2 \text{ edge}) = W(K_n) + 2$

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$$W\left(K_n - \frac{(n-4)(n-3)}{2}\text{ edges}\right) = W(K_n) + \frac{(n-4)(n-3)}{2} = \mathrm{W}(\mathrm{K}_\mathrm{n}) +$$

We find that this sequence of Wiener index is in arithmetic progression with common difference one which implies that for any positive integer between $n(n-1)/2$ and $n^2 - 4n + 6$ has an equivalent graph G. Also from the table we see that further removal of edges from $P\ell_5$ leads to Wiener index 12, 13, 14. Similarly, removal of edges successively from $P\ell_6$ leads to graph with Wiener index 19, 20. From $P\ell_7$ onwards there is a superimposition of Wiener index consequently in $P\ell_8$ and so on.

Further investigation shows that $W(K_2) = 1$, $W(K_3) = 3$, $W(K_4) = 6$.

On removal of edges in K_4 we get graphs with Wiener index 6, 7, 8 and 10.

Also $W(P_3) = 4$, $W(K_{1,3}) = 9$.

Given any natural number n we can find a graph G with Wiener index $W(G) = n$ excluding $n = 2$ and 5.

4. CONCLUSION

Finally we conclude from our investigation that there does not exist graph with Wiener index 2 and 5. The following procedure gives the graph G with n vertices for a given integer N as the Wiener number.

(i) $n = \lfloor \sqrt{2N} \rfloor$,

(ii) Find Wiener number for K_n.

(iii) $m_1 = \mathrm{N} - W(K_n)$

(iv) $G = K_n - m_1$ number of edges

REFERENCE

[1] J. Baskar Babujee, (2003), "Planar Graphs with Maximum Edges-Antimagic Property", *Journal of The Mathematics Education*, **37**(4), 194-198.

[2] J. Baskar Babujee, D. Prathap, and A. Joshi, (2007), "Wiener Index for Cartesian Product Graphs", *Proceeding of National Conference on Mathematical and Computational Models*, Narosa Publishing House, 225-232.

[3] Goldman D., Istrail S., Lancia G., and Piccolboni A., (2000), "Algorithmic Strategies in Combinatorial Chemistry", In *Proc. 11th ACM-SIAM Sympos. Discrete Algorithms*, 275-284.

[4] Lepovi'c M., and Gutman I., (1998), "A Collective Property of Trees and Chemical Trees", *J. Chem. Inf. Comput. Sci*., **38**, 823-826.

[5] Stephan G. Wagner, Hua Wang, and Gang Yu, (2005), "Molecular Graphs and the Inverse Wiener Index Problem", *Preprint Submitted to Elsevier Science*, 25 Feb 2005.

[6] Wiener H., (1947), Structural Determination of Paraffin Boiling Points, *J. Am. Chem. Soc*., **69**, 17-20.

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