Wiener Index of Chain Graphs

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Abstract—**A bipartite graph is called a chain graph if the neighborhoods of the vertices in each partite set form a chain with respect to set inclusion. Chain graphs are discovered and re-discovered by various researchers in various contexts. Also, they were named differently according to the applications in which they arise. In the field of Spectral Graph Theory, chain graphs play a remarkable role. They are characterized as graphs with the largest spectral radius among all the connected bipartite graphs with prescribed number of edges and vertices. Even though chain graphs are significant in the field of Spectral Graph Theory, the area of graph parameters remains untouched. Wiener index is one of the oldest and most studied topological indices, both from theoretical point of view and applications. The Wiener index of a graph is defined as the sum of distances between every pair of vertices in it. In this article, we give bounds for Wiener index and hence for average distance of chain graphs. We also present a quadratic time algorithm that returns a realising chain graph G (if exists) whose Wiener index is the given integer w. The algorithm presented in this article contributes to the existing knowledge in the theory of inverse Wiener index problem. We conclude this article by exploring some more graph parameters called edge Wiener index, hyper Wiener index and Zagreb indices of chain graphs.**

Index Terms—**Bipartite graphs, Bi-star graph, Edge Wiener index, Average distance, Zagreb index, Hyper Wiener index.**

I. Introduction

A BIGRAPH or a bipartite graph is a graph G whose vertex set $V(G)$ can be partitioned into two subsets V_1 and V_2 such that every edge of G joins a vertex of V_1 with a vertex of V_2. We denote a bipartite graph with the bipartition $V(G) = V_1 \cup V_2$ by $G(V_1 \cup V_2, E)$. If G contains every edge joining the vertices of V_1 and V_2, then it is a complete bipartite graph. A complete bipartite graph with $|V_1| = m, |V_2| = n$ is denoted by $K_{m,n}$. A star graph is a complete bipartite graph where at least one of $|V_i| = 1 (i = 1, 2)$. A bi-star graph $B(p, q)$ is the graph obtained by joining the central (apex) vertices of two star graphs $K_{1,p-1}$ and $K_{1,q-1}$ by an edge. We write $u \sim v$ or $u \sim_G v$ if the vertices u and v are adjacent in G, $u \nsim v$ or $u \nsim_G v$ if they are not. The neighborhood of a vertex $u \in V(G)$ is the set $N_G(u)$ consisting of all the vertices v such that $v \sim u$ in G. For a bipartite graph, the adjacency matrix can be written as $\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$, where B is called the biadjacency matrix. A vertex $v \in V_i$ $(i = 1, 2)$ in a bipartite graph $G(V_1 \cup V_2, E)$ is said to be dominating vertex if $N_G(v) = V_j$ where $j \neq i$. In other words, v is of full degree with respect to the other partite set. We refer [1] for further concepts and notations.

The distance $d(u, v)$ between a pair of vertices u, v in G is the length of the shortest path between u and v if exists, else $d(u, v) = \infty$. The Wiener index is a graph invariant which belongs to the molecular structure descriptors known as topological indices, which are used for the designing the molecules with required properties according to the practical convinience. The Wiener index $w(G)$ of a graph G is the sum of all distances between all pairs of vertices in G.

$$w(G) = \sum_{\{u,v\} \in V(G)} d(u, v).$$

The line graph $L(G)$ of a graph G is a graph whose vertices are the edges of G, with two vertices of $L(G)$ are adjacent whenever the corresponding edges in G share a vertex in common. The edge Wiener index, $w_e(G)$ is defined as the sum of distances between all pairs of edges of the underlying (connected) graph. In other words, the edge Wiener index is defined as the sum of distances of their corresponding vertices in the line graph $L(G)$ [2]. That is,

$$w_e(G) = w(L(G)).$$

Due to the significance of Wiener index in the area of molecular chemistry, the inverse Wiener index problem is posed and some classes have been investigated in [3] and [4]. Peterson graph is one of the significant cubic graph which serves as the example/counter example for most of various problems in graph theory. Wiener index and other chemical indices of generalized Peterson's graph has been investigated in detail by the authors of [5]. The average path length $Av(G)$ of a graph G is another distance related graph parameter which is defined as follows:

$$Av(G) = \frac{\sum_{\{u,v\} \in V(G)} d(u, v)}{\binom{n}{2}}.$$

This parameter is one of the quantitative performance measure to describe and compare two or more graphs when it is considered as a network. The Zagreb indices are another set of parameters, that can be viewed as structure descriptors of the underlying graph of the molecule. In 1972, the Zagreb indices have been introduced to explain mathematically, the properties of compounds at the molecular level. The first Zagreb index and the second Zagreb index are denoted by $M_1(G)$ and $M_2(G)$ respectively. That is

$$M_1(G) = \sum_{v \in V(G)} deg(v)^2 = \sum_{(u,v) \in E(G)} [deg(u) + deg(v)]$$

and

$$M_2(G) = \sum_{(u,v) \in E(G)} deg(u) deg(v).$$

These indices reflect the extent of branching of the molecular carbon atom skeleton [6], [7].

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A. Chain graphs

A class of sets $S = \{S_1, S_2, ..., S_n\}$ is called a chain with respect to the operation of set inclusion if for every $S_i, S_j \in S$, either $S_i \subseteq S_j$ or $S_j \subseteq S_i$. Chain graphs are the special case of bipartite graphs, which is defined as follows.

Definition 1.1: A graph is called a chain graph if it is bipartite and the neighborhoods of the vertices in each partite set form a chain with respect to set inclusion.

In other words, for every two vertices u and v in the same partite set and their neighborhoods $N_G(u)$ and $N_G(v)$, either $N_G(u) \subseteq N_G(v)$ or $N_G(v) \subseteq N_G(u)$. Chain graphs are often called Optimal graphs, Double Nested graphs (DNG) or Difference graphs [8], [9], [10]. The color classes of a chain graph $G(V_1 \cup V_2, E)$ can be partitioned into h non-empty cells given by

$$V_1 = V_{11} \cup V_{12} \cup ... \cup V_{1h}$$

and

$$V_2 = V_{21} \cup V_{22} \cup ... \cup V_{2h}$$

such that $N_G(u) = V_{21} \cup V_{22} \cup ... \cup V_{2(h-i+1)}$, for any vertex $u \in V_{1i}$, $1 \leq i \leq h$. If $m_i = |V_{1i}|$ and $n_i = |V_{2i}|$, then we write

$$G = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h).$$

If $m_i = n_i = 1$ for all $1 \leq i \leq h$, then the graph is called half graph [8]. We note that, every partite set in a chain graph has at least one dominating vertex, that is, a vertex adjacent to all the vertices of the other partite set. Chain graphs are also known as Difference graphs due to the property that every vertex of v_i of G can be assigned a real number a_i for which there exists a positive real number R such that $|a_i| < R$ for all i and two vertices v_i, v_j are adjacent if and only if $|a_i - a_j| \geq R$ [8].

The following example illustrates the definition.

Example 1.1: Consider the graph $G(V_1 \cup V_2, E)$ (as shown in Figure 1) where $V_1 = \{v_1, v_2, v_3, v_4, v_5\}$ and $V_2 = \{v_6, v_7, v_8, v_9, v_{10}\}$.

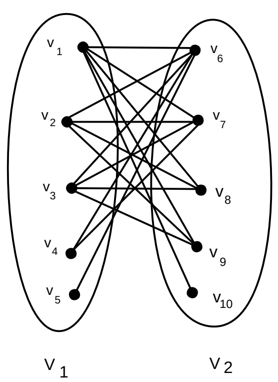

Fig. 1. A chain graph $G = DNG(1, 2, 1, 1; 1, 1, 2, 1)$

The neighborhoods of vertices of G are given by, $N_G(v_1) = \{v_6, v_7, v_8, v_9, v_{10}\}, N_G(v_2) = N_G(v_3) = \{v_6, v_7, v_8, v_9\}, N_G(v_4) = \{v_6, v_7\}, N_G(v_5) = \{v_6\}, N_G(v_6) = \{v_1, v_2, v_3, v_4, v_5\}, N_G(v_7) = \{v_1, v_2, v_3, v_4\}, N_G(v_8) = N_G(v_9) = \{v_1, v_2, v_3\}$ and $N_G(v_{10}) = \{v_1\}$. We observe that
$N_G(v_5) \subseteq N_G(v_4) \subseteq N_G(v_3) \subseteq N_G(v_2) \subseteq N_G(v_1)$ and $N_G(v_{10}) \subseteq N_G(v_9) \subseteq N_G(v_8) \subseteq N_G(v_7) \subseteq N_G(v_6)$. The vertices v_1 and v_6 are dominating in the above example.
Chain graphs are the maximizers for the largest eigenvalue of the graphs among bipartite graphs (connected) of fixed size and order. It is interesting to note that chain graphs have no eigenvalues in the interval $(0, \frac{1}{2})$ and all their non-zero eigenvalues are simple [8]. It was conjectured that no chain graph shares a non-zero eigenvalue with its vertex deleted subgraphs. But later it was disproved and a weaker version of the conjecture came out to be true. That is, the conjecture is true only for the subgraphs obtained by deleting vertices of maximum degrees (dominating vertices) in either of the color classes [8]. For the other important and interesting results concerned with the chain graphs, the readers are referred to [9], [10], [11], [12], [13], [14], [15], [16] and [17].

The outline of the remainder of this paper is as follows: In section 2, after the introduction, we give bounds as well as some characterizations for Wiener index of chain graphs. In the third section, for a given pair of integers (w, n), we present an algorithm which returns the chain graph of order n and Wiener index w if exists. Section 4 deals with 'edge version' of Wiener index of chain graphs. We conclude this article by giving bounds for Zagreb indices of chain graphs.

II. Wiener index

In this section, we give an expression as well as bounds for Wiener index of chain graphs.

Theorem 2.1: Let $G(V_1 \cup V_2, E)$ be a chain graph of size m where $|V_1| = p, |V_2| = q$. Then the Wiener index $w(G)$ of G is given by

$$w(G) = p^2 + q^2 + 3pq - p - q - 2m.$$

Proof: Since each of the partite set has at least one dominating vertex, without loss of generality, let $u_1 \in V_1, v_1 \in V_2$ be the dominating vertices. We note that any two vertices that are in the same partite set are at a distance two due to the existence of dominating vertex in the other partite set. For any non dominating vertex $v_i \in V_1$, all the vertices $u_j \in V_2$ which are not adjacent to v_i are at a distance three due to the shortest path $(v_i - u_1 - v_1 - u_j)$. Thus for any two vertices $u_i, v_j \in V(G)$,

$$d(u_i, v_j) = \begin{cases} 1, & if\ u_i, v_j\ belong\ to\ the\ different \\ & partite\ sets\ and\ u_i \sim v_j \\ 2, & if\ u_i, v_j\ belong\ to\ the\ same\ partite \\ & sets \\ 3, & if\ u_i, v_j\ belong\ to\ the\ different \\ & partite\ sets\ and\ u_i \nsim v_j \end{cases}$$

The graph G has $\binom{p}{2} + \binom{q}{2}$ pairs of vertices having distance two between them. Since there are m edges, there are m pairs of vertices having distance one between them and the rest of the pairs have distance three between them. We know that, a bipartite graph $G(V_1 \cup V_2, E)$ has at most pq edges, p and q being the cardinalities of the partite sets V_1 and V_2, respectively. Thus there are $(pq-m)$ pairs of vertices (u_i, v_j) such that $u_i \in V_1, v_j \in V_2$ and $u_i \nsim v_j$. Hence the number of pairs of vertices having distance three between them is $(pq-m)$. The Wiener index is given by,

$$\begin{aligned} w(G) &= 2\binom{p}{2} + 2\binom{q}{2} + m + 3(pq-m) \\ &= p^2 + q^2 + 3pq - p - q - 2m. \end{aligned}$$

■

A chain graph having no pairs of duplicate vertices are the half graphs. In a half graph, both the partite sets are of equal cardinalities. The number of edges in a half graph of order $2n$ is given by $\frac{n(n+1)}{2}$. We obtain the expression for Wiener index of half graphs in the next Corollary.

Corollary 2.2: Let G be a half graph of order $2n$. Then the Wiener index $w(G)$ of G is given by

$$w(G) = n(4n-3).$$

Proof: The proof follows from the Theorem 2.1 on substituting $p = q = n$ and $m = \dfrac{n(n+1)}{2}$. ■

The following theorems give upper and lower bounds for Wiener index of chain graphs.

Theorem 2.3: Let $G(V_1 \cup V_2, E)$ be a chain graph with $|V_1| = p$ and $|V_2| = q$ $(p, q > 1)$. Let $w(G)$ be the Wiener index of G. Then

$$p^2+q^2+pq-p-q \le w(G) \le p^2+q^2+3\,(pq-p-q)+2.$$

Proof: We note that, for any two vertices $u_i, v_j \in V(G)$, $d(u_i, v_j) \in \{1,2,3\}$. For any chain graph G, there are $\binom{p}{2}+\binom{q}{2}$ pairs of vertices having distance two between them. In order to have a minimum Wiener index, the number of pairs of vertices having distance three (distance one) between them is as minimum (maximum) as possible. In other words, the number of pairs of vertices $(u_i, v_j), u_i \in V_1, v_j \in V_2$ which are adjacent (non adjacent) to each other is as maximum (minimum) as possible. Thus, G has the minimum Wiener index when every vertex of V_1 is adjacent to every vertex of V_2 (which results in zero pairs of vertices having distance three between them) and the resulting graph is $K_{p,q}$. It is noted that $w(K_{p,q}) = 2\binom{p}{2} + 2\binom{q}{2} + pq$. Thus $p^2+q^2+pq-p-q \le w(G)$.

In order to have a maximum Wiener index, in addition to $\binom{p}{2} + \binom{q}{2}$ pairs of vertices having distance two between them, we must have maximum (minimum) number of pairs of vertices at distance three (distance one) between them. In other words, the number of pairs of vertices (u_i, v_j), $u_i \in V_1, v_j \in V_2$ and $u_i \nsim v_j$ is as maximum as possible. But in any chain graph, there is at least one dominating vertex in each of the partite sets (say $u_1 \in V_1, v_1 \in V_2$). Apart from this, in order that $w(G)$ is maximum, all the vertices u_j, v_j $(i, j \neq 1)$ are adjacent to minimum number of vertices (say one). The graph G where $N_G(u_1) = V_2, N_G(u_j) = v_k$ for all vertices $u_j \in V_1 (j \neq 1)$ and for some $v_k \in V_2$ is the graph with maximum number of pairs of vertices having distance three. The graph G has $q + (p-1)$ pairs of vertices at distance one and $(p-1)(q-1)$ vertices at distance three between them. Hence

$$\begin{aligned} w(G) &= 2\binom{p}{2} + 2\binom{q}{2} + q + (p-1) + 3(p-1)(q-1) \\ &= p^2 + q^2 + 3\,(pq-p-q) + 2. \end{aligned}$$

Thus, for any chain graph G,
$w(G) \le p^2 + q^2 + 3\,(pq-p-q) + 2.$ ■

The graph G where $N_G(u_1) = V_2, N_G(u_j) = v_k$ for all vertices $u_j \in V_1 (j \neq 1)$ and for some $v_k \in V_2$ (which attains the upper bound of the above theorem) is $B(p,q)$. This is the minimal structure that any chain graph has. In other words, the graph $B(p,q)$ is a spanning tree for every chain graph $G(V_1 \cup V_2, E)$ where $|V_1| = p, |V_2| = q$. In the next theorem, we fix the total number of vertices $N (N = 2n$ when N is even and $N = 2n+1$ when N is odd) and find the cardinalities of the partite sets p and q, which optimizes the Wiener index.

Theorem 2.4: Let $G(V_1 \cup V_2, E)$ be a chain graph on $2n$ vertices. Let $w(G)$ be the Wiener index of G. Then

$$3n^2 - 2n \le w(G) \le 5n^2 - 6n + 2.$$

Proof: Let $|V_1| = p, |V_2| = q$ such that $p + q = 2n$. The only chain graph when $p = 1$ is the star graph $K_{1,2n-1}$ and $w(K_{1,2n-1}) = (2n-1)^2$, which satisfies the bounds given. For all other $p, q \ge 2$, the bounds for $w(G)$ is given in the Theorem 2.3. Since $q = 2n - p$, we write the lower and upper bounds as $f(p) = 4n^2 - 2np + p^2 - 2n$ and $g(p) = 4n^2 - p^2 + 2np - 6n + 2$. For a given $2n$, we evaluate the minima of the lower bound $f(p)$ as well as the maxima of the upper bound $g(p)$. The function $f(p)$ has the critical point $p = n$. Since $\dfrac{d^2 f}{dp^2} > 0$, $f(p)$ attains the minima when $p = n$ and the minimum value is $f = 3n^2 - 2n$. Similarly, $p = n$ is the critical point of the function $g(p)$ and $\dfrac{d^2 g}{dp^2} < 0$. Thus $g(p)$ has the maxima when $p = n$ and the maximum value is $g = 5n^2 - 6n + 2$.

■

Theorem 2.5: Let G be a chain graph on $2n+1$ vertices. Let $w(G)$ be the Wiener index of G. Then

$$3n^2 + n \le w(G) \le 5n^2 - n.$$

Proof: The proof is similar to the proof of Theorem 2.4. The extreme values for both upper and lower bounds are attained at $p = n+1$ and $q = n$. ■

In network topology, average path length is a concept which enumerates the average number of steps through the shortest paths for every pair of nodes. It measures the efficiency of mass transport on a network. We give the bounds for the average path length of chain graphs.

Corollary 2.6: Consider a chain a graph G with the average distance $Av(G)$.

- If G has $2n$ vertices, then
$$\frac{6n-4}{n-1} \le Av(G) \le \frac{10n^2 - 12n + 4}{n^2 - n}.$$
- If G has $2n+1$ vertices, then
$$\frac{6n+2}{n-1} \le Av(G) \le \frac{10n-2}{n-1}.$$

Lemma 2.7: For a chain graph $G(V_1 \cup V_2, E)$, the upper bound and the lower bound for $w(G)$ given by the Theorem 2.3 are either both even or both odd.

Proof: Every chain graph $G(V_1 \cup V_2, E)$ where $|V_1| = p, |V_2| = q$ is a spanning subgraph of the complete bipartite graph $K_{p,q}$. So, the graph G can be obtained from the complete bipartite graph $K_{p,q}$ by removing one or more edges. Equivalently, any chain graph can be obtained by adding one or more edges to the minimal structure of the chain graph $B(p,q)$. Also, removal of an edge from $K_{p,q}$ increases the Wiener index $w(G)$ by two as exactly one pair of vertices with distance one is replaced by distance three. Similarly, the addition of one edge to the graph $B(p,q)$ decreases $w(G)$ by two. In general, removal of k edges from $K_{p,q}$ increases $w(G)$ by $2k$. Equivalently, addition of k edges to $B(p,q)$ decreases $w(G)$ by $2k$.

Let G be a chain graph obtained by adding k_1 edges to $B(p,q)$ or by deleting k_2 edges from $K_{p,q}$. If exactly one of the bound is even and the other is odd, say the upper bound is even and the lower bound is odd, then

$w(G) = lower\ bound + 2k_1$,(an odd number)

$= upper\ bound - 2k_2$,(an even number), a contradiction. Thus the upper and lower bounds are either both even or both odd. ■

In the following lemma, we show that the parity of the Wiener index depends only on the size of the partite sets.

Lemma 2.8: Let $G(U \cup U', E)$ and $H(V \cup V', F)$ be any two chain graphs such that $|U| = |V| = p$ and $|U'| = |V'| = q$. Then the Wiener indices $w(G)$ and $w(H)$ are either both even or both odd.

Proof: Proof follows from the fact that any chain graph $G(V_1 \cup V_2, E)$ can be obtained by removing (adding) one or more edges of the complete bipartite graph $K_{p,q}$ (to graph $B(p,q)$). By Lemma 2.7, we know that the upper and lower bounds for $w(G)$ are either both even or both odd. For given p, q, if the bounds are even (odd), all the chain graphs having bipartition with the cardinalities p, q are even (odd). ■

We note the following remark which is a consequence of the above lemmas.

Remark 2.1: All the chain graphs with the bipartition having cardinalities p and q have Wiener index either all even or all odd depending upon the bounds given in the Theorem 2.3 .

By Lemmas 2.7, 2.8 and the Remark 2.1, the next theorem follows.

Theorem 2.9: Let $G(V_1 \cup V_2, E)$ be any chain graph such that $|V_1| = p, |V_2| = q$. Then the Wiener index

$$w(G) = \begin{cases} odd, & when\ both\ p, q\ are\ odd \\ even, & else \end{cases}.$$

In the above series of theorems, we have given the bounds for Wiener index of chain graphs. Now, naturally the question arises that, for a given integer w which is not beyond the given bounds, what is the guarantee that there exists a chain graph on n vertices with the Wiener index w. If yes, how do we get that graph. We now give an algorithm which checks if there exists a chain graph G whose Wiener index is the given integer w.

III. Algorithm

From the close relationship between the Wiener index and the chemical properties of a molecule, the importance of inverse Wiener index problem arises which states as follows: given a Wiener index, find a graph (if possible) from a prescribed class that attains this value. In this section, we present an algorithm that returns the chain graph G with the given Wiener index. The inputs for this algorithm are the number of vertices n and an integer w which has to be examined such that the chain graph with Wiener index w exists or not.

Algorithm 1

Input:	The integer w and the number of vertices n
Output	Returns yes/no if there exists a chain graph on n vertices with the given Wiener index w. If yes, specifies how to obtain the corresponding graph G.

Algorithm 1 function Wiener(w, n)

Input: w, n

Output: A chain graph G if exists

if $n \equiv 0(mod\ 2)$ **then**
    $s = \frac{n}{2}$
else
    $s = \frac{n+1}{2}$
end if
for $p = 2 : s$ **do**
    $q = n - p$
    $LB = pq + p^2 + q^2 - p - q$
    $UB = p^2 + q^2 + 3pq - p - q$
    if $w < LB$ **or** $w > UB$ **then**
        continue
    else
        $k_1 = \frac{w-LB}{2}$
        $k_2 = \frac{UB-w}{2}$
        if $2k_1 \equiv 1(mod\ 2)$ **then**
            continue
        else if $k_1 == 0$ **then**
            $G = B(p,q)$
            return G
        else if $k_2 == 0$ **then**
            $G = K_{p,q}$
            return G
        else
            if $k_1 \le k_2$ **then**
                $G = B(p,q)$
                $G = add\_edge(G, p, q, k_1)$
                return G
            else
                $G = K_{p,q}$
                $G = remove\_edge(G, p, q, k_2)$
                return G
            end if
        end if
    end if
end for
Print 'There is no chain graph G on n vertices with Wiener index w.'

If a chain graph G with the given Wiener index w exists, algorithm 1 redirects to algorithm 2 or algorithm 3 depending upon certain conditions. If no such graph G exists, then it displays the message. The input graph G in the following algorithms have the bipartition $V(G) = V_1 \cup V_2$ such that $|V_1| = p, |V_2| = q$ $(p + q = n)$ and the vertices labelled as follows:

$$V_1 = \{0, 1, \ldots, p-1\}\ and\ V_2 = \{0, 1, \ldots q-1\}.$$

Further, algorithm 2 and 3 starts with the input graph G, which is specifically $G = K_{p,q}$ and $G = B(p, q)$ respectively.

Algorithm 2

To obtain the required chain graph G from complete bipartite graph $K_{p,q}(q \geq p)$, we remove a total of k_2 edges from $K_{p,q}$ in the manner given in algorithm 2.

Input:	The graph $G = K_{p,q}, p, q, k_2$
Output	The chain graph G whose Wiener index is w.

Algorithm 2 function remove_edge(G, p, q, k_2)

```
1:  if q − 1 ≥ k2 then
2:      for j = 1 : k2 do
3:          E(G) = E(G) \ (p − 1, j)
4:      end for
5:      return G
6:  else
7:      for j = 1 : q − 1 do
8:          E(G) = E(G) \ (p − 1, j)
9:      end for
10:     p = p − 1
11:     k2 = k2 − (q − 1)
12:     remove_edge(G, p, q, k2)
13: end if
```

Algorithm 3

Similarly, to obtain the required chain graph G from the bi-star graph $B(p, q)(q \geq p)$, we add a total of k_1 edges to $B(p, q)$ in the manner given in algorithm 3.

Input:	The graph $G = B(p, q), p, q, k_1$
Output	The chain graph G whose Wiener index is w.

Algorithm 3 function add_edge(G, p, q, k_1)

```
if q − 1 ≥ k1 then
    for j = 1 : k1 do
        E(G) = E(G) ∪ (p − 1, j)
    end for
    return G
else
    for j = 1 : q − 1 do
        E(G) = E(G) ∪ (p − 1, j)
    end for
    p = p − 1
    k1 = k1 − (q − 1)
    add_edge(G, p, q, k1)
end if
```

Time complexity

The **for** loop given in line 6 has $(s - 1)$ iterations. In each iteration, the algorithm may do nothing or execute either of algorithm 2 and algorithm 3. But in the latter two cases, the computation terminates after the execution of the respective algorithm. The algorithm 2 contains a **for** loop (line 7) with $(q - 1)$ iterations, which is executed in each call as long as $k_2 \leq (q - 1)$. It takes $\lceil \frac{k_2}{q-1} - 1 \rceil$ number of steps for k_2 to become less than or equal to $(q - 1)$. Thus the total number of steps required until this point is $(q - 1)\lceil \frac{k_2}{q-1} - 1 \rceil \leq k_2 + q - 2$. Then the **for** loop in line 2 of algorithm 2 is executed k_2 number of times where k_2 is now less than or equal to $(q - 1)$. Thus the total time taken by algorithm 2 is at most $k_2 + 2q - 3 = \frac{p^2+q^2+3pq-p-q-w}{2} + 2q - 3 = \frac{p^2+q^2+3pq-p+3q-w-6}{2}$ (from lines 9 and 14 of algorithm 1). Similarly, total time taken by algorithm 3 is at most $k_1 + 2q - 3 = \frac{w-p^2-q^2-pq+p+q}{2} + 2q - 3 = \frac{w-p^2-q^2-pq+p+5q-6}{2}$. The **if** statement given in the line 24-31 of algorithm 1 guarantees that algorithm 2 or algorithm 3 is called depending on which one will take less time. Thus the time taken by the algorithm 1 is $(s-1)min\{\frac{p^2+q^2+3pq-p+3q-w-6}{2}, \frac{w-p^2-q^2-pq+p+5q-6}{2}\}$. Since $s = \lceil \frac{n}{2} \rceil, p + q = n$ and w is bounded above by quadratic polynomials in n (Theorem 2.4 and Theorem 2.5), it follows that the complexity of algorithm 1 is $O(n^2)$. This proves the following result.

Theorem 3.1: The time complexity of algorithm 1 is $O(n^2)$ where n is the number of vertices in the required graph.

As reviewed, the chemical and mathematical applications of Wiener index are well documented by various researchers. Meanwhile, a slight invariant of the Wiener index introduced later has attracted much attention of theoretical chemists. This is named as hyper Wiener index, traditionally denoted by $ww(G)$ and defined as follows.

$$ww(G) = \frac{1}{2}\left(\sum_{\{u,v\}\in V(G)} d(u,v) + \sum_{\{u,v\}\in V(G)} d(u,v)^2\right).$$
$$= \frac{1}{2}\left(w(G) + \sum_{\{u,v\}\in V(G)} d(u,v)^2\right).$$

The hyper Wiener index is another graph based molecular structure descriptor used by chemists to predict the properties of organic compounds ([18], [19]). We give the expression for hyper Wiener index of chain graphs.

Corollary 3.2: Let $G(V_1 \cup V_2, E)$ be a chain graph of size m where $|V_1| = p, |V_2| = q$. Then the hyper Wiener index $ww(G)$ of G is given by

$$ww(G) = \frac{3}{2}\left(p^2 + q^2 - p - q\right) + 6pq - 5m.$$

Proof: For a chain graph G, $d(u, v) \in \{1, 2, 3\}$ for all $u, v \in V(G)$. On enumerating the distances as in the proof of Theorem 2.1, we get the hyper Wiener index. ■

When G is a half graph on $2n$ vertices, then

$$ww(G) = \frac{1}{2}\left(13n^2 - 11n\right).$$

IV. Edge Wiener index

We prove some results on line graph of a chain graphs, which are necessary for deriving the edge Wiener index.

Theorem 4.1: Let $G(V_1 \cup V_2, E)$ be a chain graph on n vertices where $G \neq K_{1,n-1}$. Let $L(G)$ be the line graph of G. Then $diam(L(G)) = 2$.

Proof: Let $G(V_1 \cup V_2, E)$ be a chain graph where $V_1 = \{u_1, u_2, ..., u_p\}$ and $V_2 = \{v_1, v_2, ..., v_q\}$ such that $p + q = n$. Without loss of generality, for all $(1 \leq i, k \leq p)$, let $N_G(u_i) \subseteq N_G(u_k)$ if $i > k$ and $N_G(u_k) \subseteq N_G(u_i)$

otherwise. Since G has at least two dominating vertices, let $u_1 \in V_1$ and $v_1 \in V_2$ be two dominating vertices of G. Let $L(G)$ be the line graph of G. We note that a vertex $(u_i, v_j) \in V(L(G))$ if and only if $u_i \sim_G v_j$. It follows that, $(u_1, v_j), (u_i, v_1) \in V(L(G))$ for all $v_j \in V_2$ and for all $u_i \in V_1$. Let $u_i \sim_G v_j$ and consider the vertex $(u_i, v_j) \in V(L(G))$. Then we have the following cases:

1) At least one of u_i, v_j is dominating.
2) None of u_i, v_j is dominating.

We first note that, since $G \neq K_{1,n-1}$, each of $|V_i| > 1$ ($i = 1, 2$) and there exists at least two vertices $u_k \in V_1$ ($k \neq i$) and $v_l \in V_2$ ($l \neq j$).
Case 1: When at least one of them, say $u_i \in V_1$ is dominating, then all the vertices (u_i, v_l) for all $v_l \in V_2$ ($l \neq j$) and (u_k, v_j) for all $u_k \in V_1$ ($k \neq i$) and $u_k \sim_G v_j$ are at distance one from (u_i, v_j), i.e. $d\big[(u_i, v_j), (u_i, v_l)\big] = d\big[(u_i, v_j), (u_k, v_j)\big] = 1$. All the other vertices (u_k, v_l) where $u_k \in V_1$ ($k \neq i$), $v_l \in V_2$ ($l \neq j$) and $u_k \sim v_l$ are at distance 2 from (u_i, v_j) with the shortest path given by $(u_i, v_j) - (u_k, v_j) - (u_k, v_l)$. Thus $d\big[(u_i, v_j), (u_k, v_l)\big] = 2$.
Case 2: When none of them are dominating, then all the vertices (u_i, v_l) for all $v_l \in V_2$ ($l \neq j$), $v_l \sim_G u_i$ and (u_k, v_j) for all $u_k \in V_2$ ($k \neq i$), $u_k \sim_G v_j$ are at distance 1 from (u_i, v_j), i.e. $d\big[(u_i, v_j), (u_i, v_l)\big] = d\big[(u_i, v_j), (u_k, v_j)\big] = 1$. Now consider rest of the vertices, let $u_k \sim_G v_l$ and $k \neq i, j \neq l$. Suppose $k > i$, then $N_G(u_k) \subseteq N_G(u_i)$. Thus $v_l \in N_G(u_k) \subseteq N_G(u_i)$. This means that $(u_i, v_l) \in V(L(G))$. We get a path in $L(G)$ given by $(u_i, v_j) - (u_i, v_l) - (u_k, v_l)$. Thus $d\big[(u_i, v_j), (u_k, v_l)\big] = 2$. Suppose $k < i$, then $N_G(u_i) \subseteq N_G(u_k)$. Thus $v_j \in N_G(u_i) \subseteq N_G(u_k)$. This means that $(u_k, v_j) \in V(L(G))$. We get a path in $L(G)$ given by $(u_i, v_j) - (u_k, v_j) - (u_k, v_l)$, that is $d\big[(u_i, v_j), (u_k, v_l)\big] = 2$. Thus $diam(L(G)) = 2$. ■

Corollary 4.2: Let $G(V_1 \cup V_2, E)$ be a chain graph on n vertices here $G \neq K_{1,n-1}$. Let $L(G)$ be the line graph of G. Then $rad(L(G)) = 2$.

Proof: We know that $rad(L(G)) \leq diam(L(G))$. Since G is a chain graph, there exists at least two dominating vertices $u_1 \in V_1, v_1 \in V_2$. For any vertex $(u_i, v_j) \in V(L(G))$ ($i, j \neq 1$), there exists at least one vertex $(u_1, v_1) \in V(L(G))$ such that $d\big[(u_i, v_j), (u_1, v_1)\big] = 2$. Also, for every vertex $(u_1, v_j) \in V(L(G))$, there exists at least one vertex $(u_k, v_l) \in V(L(G))$ ($k \neq 1, l \neq j$) such that $d\big[(u_1, v_j), (u_k, v_1)\big] = 2$. Similarly, for every vertex $(u_i, v_1) \in V(L(G))$, there exists at least one vertex $(u_k, v_l) \in V(L(G))$ ($l \neq 1, k \neq j$) such that $d\big[(u_i, v_l), (u_k, v_l)\big] = 2$. Thus eccentricity of every vertex is two and radius is 2. ■

We note that $L(K_{1,n}) = K_{n-1}$, diameter and radius of which is one. From the above theorems, it is clear that the distance between any two edges in a chain graph is either one or two. The edge Wiener index of a chain graph is sum of terms in which each term is either one or two. We note that, for a graph G on prescribed number of vertices, $w_e(G)$ increases as the number of vertices in the corresponding line graph (the number of edges in G) increases. The following theorems give upper and lower bounds for edge Wiener index of chain graphs.

Theorem 4.3: Let $G(V_1 \cup V_2, E)$ be a chain graph on $2n$ vertices. Let $w_e(G)$ be the edge Wiener index of G. Then

$$(2n-1)(n-1) \leq w_e(G) \leq n^3(n-1).$$

Proof: Let $|V_1| = p, |V_2| = q$ such that $p + q = 2n$. The edge Wiener index $w_e(G)$ is minimum (maximum) when the number of edges in G is minimum (maximum). The chain graph G has a minimum number of edges when G is a tree. That is, G has a minimum of $(2n-1)$ edges when G is either a star graph or a bi-star graph. Since the distance between any two vertices in the line graph of a chain graph is either one or two, $w_e(G)$ is minimum when the number of pairs of vertices of $L(G)$ having distance one (two) between them is maximum (minimum). We know that, line graph of a star graph $G = K_{1,2n-1}$ is given by $L(K_{1,2n-1}) = K_{2n-1}$, a complete graph in which every pairs of vertices are at distance one. Thus G has minimum edge Wiener index when $G = K_{1,2n-1}$. And the minimum value of $w_e(G)$ is given by,

$$\begin{aligned} w_e(K_{1,2n-1}) &= w(L(K_{1,2n-1})) = w(K_{2n-1}) = \tbinom{2n-1}{2} \\ &= (n-1)(2n-1). \end{aligned}$$

Thus $w_e(G) \geq (n-1)(2n-1)$.
A chain graph G has maximum number of edges when $G = K_{p,q}$ and the number of edges is equal to pq. Further, the product pq takes the maximum value when $p = q = n$. Thus, a chain graph G on $2n$ vertices has maximum number of edges when $G = K_{n,n}$. Consider the graph $G = K_{n,n}$ and let $V_1 = \{u_1, u_2, ..., u_n\}$ and $V_2 = \{v_1, v_2, ..., v_n\}$. The line graph $L(G)$ has $V(L(G)) = \{(u_i, v_j) \mid u_i \in V_1, v_j \in V_2\}$ and $|V(L(G))| = n^2$. Further, for all $1 \leq i, j, k, l \leq n$, the distance between any pair of vertices is given by,

$$d\big[(u_i, v_j), (u_k, v_l)\big] = \begin{cases} 1, & if\ either\ u_i = u_k \\ & or\ v_j = v_l \\ 2, & else \end{cases}.$$

We note that, for each $1 \leq i \leq n$, the set of vertices $\{(u_i, v_1), (u_i, v_2), ..., (u_i, v_n)\},\ i = 1, 2, ..., n$ as well as $\{(u_1, v_j), (u_2, v_j), ..., (u_n, v_j)\},\ j = 1, 2, ..., n$ induces complete graph K_n. Thus, each of the set of vertices given above has $n \times \binom{n}{2}$ pairs of vertices having distance 1 between them. Totally, the graph $L(G)$ has $2n \times \binom{n}{2} = n^3 - n^2$ pairs of vertices at distance one between them. The rest of the pairs are at distance two with each other. The number of pairs of vertices of $L(G)$ having distance two between them is given by $\binom{|V(L(G))|}{2} - n^3 + n^2$. Thus

$$\begin{aligned} w_e(G) &= w(L(G)) = n^3 - n^2 + 2\big[\tbinom{n^2}{2} - n^3 + n^2\big] \\ &= n^3(n-1). \end{aligned}$$

Hence $w_e(G) \leq n^3(n-1)$. ■

Theorem 4.4: Let $G(V_1 \cup V_2, E)$ be a chain graph on $2n+1$ vertices. Let $w_e(G)$ be the edge Wiener index of G. Then

$$n(2n-1) \leq w_e(G) \leq \frac{n(n+1)(2n^2-1)}{2}.$$

Proof: Let $|V_1| = p, |V_2| = q$ such that $p + q = 2n + 1$. As in the case of Theorem 4.3, the chain graph G has minimum edge Wiener index when $G = K_{1,2n}$. Hence the minimum value of $w_e(G)$ is given by,

$$w_e(K_{1,2n}) = w(L(K_{1,2n})) = w(K_{2n}) = \tbinom{2n}{2} = n(2n-1).$$

Thus $w_e(G) \geq n(2n-1)$.
A chain graph G has maximum number of edges when $G = K_{n,n+1}$. Let $V_1 = \{u_1, u_2, ..., u_n\}$ and $V_2 = \{v_1, v_2, ..., v_n, v_{n+1}\}$. The line graph $L(G)$

has $V(L(G)) = \{(u_i, v_j) \mid u_i \in V_1, v_j \in V_2\}$ and $|V(L(G))| = n(n+1)$. Further, for all $1 \le i, k \le n$ and $1 \le j, l \le n+1$, the distance between any pair of vertices given by

$$d\big[(u_i, v_j), (u_k, v_l)\big] = \begin{cases} 1, & if\ and\ only\ if\ either\ u_i = u_k \\ & or\ v_j = v_l \\ 2, & else \end{cases}.$$

We note that, for each $1 \le i \le n$, the set of vertices $\{(u_i, v_1), (u_i, v_2), ..., (u_i, v_{n+1})\}$, $i = 1, 2, ..., n$ induce the complete graph K_{n+1}. And, for each $1 \le j \le n+1$, the set of vertices $\{(u_1, v_j), (u_2, v_j), ..., (u_n, v_j)\}$, $j = 1, 2, ..., n+1$ induces complete graph K_n. Thus, there are $n \times \binom{n+1}{2} + (n+1) \times \binom{n}{2}$ pairs of vertices having distance 1 between them. On simplification, we get the number of pairs of vertices in $L(G)$ having distance one between them is, $n \times \binom{n+1}{2} + (n+1) \times \binom{n}{2} = \frac{n(n+1)(2n-1)}{2}$. The rest of the pairs are at distance two with each other. The number of pairs of vertices of $L(G)$ having distance two between them is given by $\binom{|V(L(G))|}{2} - \frac{n(n+1)(2n-1)}{2}$. Thus $w_e(G) = w(L(G))$

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

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

Hence $w_e(G) \le \frac{n(n+1)(2n^2-1)}{2}$. ■

Theorem 4.5: Let $G(V_1 \cup V_2, E)$ be a chain graph on n vertices and m edges. Let $d : (d_1, d_2, d_3, \ldots, d_n)$ be the degree sequence of G. Then the edge Wiener index $w_e(G)$ is given by

$$w_e(G) = m(m-1) - \sum_{\substack{i=1 \\ d_i \ge 2}}^{n} \binom{d_i}{2}.$$

Proof: Let G be a chain graph where $V_1 = \{u_1, u_2, \ldots, u_k\}$ and $V_2 = \{v_{k+1}, v_{k+2}, \ldots, v_n\}$. Without loss of generality, let the integers in the degree sequence be arranged in the following manner. Let $deg(u_i) = d_i\ (1 \le i \le k),\ n-k = d_1 \ge d_2 \ge d_3 \cdots \ge d_k$ and $deg(v_i) = d_i\ (k+1 \le i \le n),\ k = d_{k+1} \ge d_{k+2} \ge d_{k+3} \cdots \ge d_n$. Accordingly, let the neighborhood of vertices of G is given by : $N_G(u_i) = \{v_{k+1}, v_{k+2}, \ldots, v_{k+d_i}\}, (k+1 \le d_i \le n)$. Let $L(G)$ be the line graph of G where $V(L(G)) = \{(u_i, v_{k+j}) | u_i \in V_1, v_{k+j} \in V_2\ and\ u_i \sim_G v_{k+j}\}$. In the line graph $L(G)$, the set of vertices $\{(u_1, v_{k+1}), (u_1, v_{k+2}), ..., (u_1, v_{k+d_1})\}$, $\{(u_2, v_{k+1}), (u_2, v_{k+2}), ..., (u_2, v_{k+d_2})\}$, $\ldots$, $\{(u_k, v_{k+1}), (u_k, v_{k+2}), ..., (u_k, v_{k+d_k})\}$ induce complete graphs of orders $d_1, d_2, \ldots, d_k$ respectively. This contributes $\sum_{i=1}^{k} \binom{d_i}{2}$ pairs of vertices having distance one between them. Similarly, the set of vertices given by $\{(u_1, v_{k+1}), (u_2, v_{k+1}), ..., (u_{d_{k+1}}, v_{k+1})\}$, $\{(u_1, v_{k+2}), (u_2, v_{k+2}), ..., (u_{d_{k+2}}, v_{k+2})\}$, $\ldots$, $\{(u_1, v_n), (u_2, v_n), ..., (u_{d_n}, v_n)\}$ induce the complete graphs of orders $d_{k+1}, d_{k+2}, \ldots, d_n$ respectively, which results in $\sum\limits_{i=k+1}^{n} \binom{d_i}{2}$ pairs of vertices which are adjacent. Thus, out of total of $\binom{m}{2}$, there are $\sum\limits_{i=1}^{n} \binom{d_i}{2}$ pairs of vertices in $L(G)$ having distance one between them. And the rest of the pairs of vertices are having distance two between them. Hence

$w_e(G) = w(L(G)) = \sum\limits_{i=1}^{n} \binom{d_i}{2} + 2\Big[\binom{m}{2} - \sum\limits_{i=1}^{n} \binom{d_i}{2}\Big]$. i.e $w_e(G) = 2\binom{m}{2} - \sum\limits_{i=1}^{n} \binom{d_i}{2}$.

■

The edge Wiener index of half graphs is given by the following corollary.

Corollary 4.6: Let G be a half graph of order $2n$. Then the edge Wiener index $w_e(G)$ of G is given by

$$w_e(G) = \frac{n(n^2-1)(3n+2)}{12}.$$

Proof: The proof follows from the Theorem 4.5 on substituting the number of edges $m = \frac{n(n+1)}{2}$ and the degree sequence $d : \{1, 1, 2, 2, \ldots, n-1, n-1, n, n\}$ ■

As discussed in the above sections, for a chain graph $G(V_1 \cup V_2, E)$ on prescribed number of vertices, the Wiener index decreases (increases) by two on addition (removal) of an edge $e = (u, v)$ such that $u \in V_1, v \in V_2$. That is, for a given chain graph G of order n, the graph $w(G)$ versus m is uniformly decreasing. In the following remark, we note that unlike Wiener index, the number of edges and the edge Wiener index $w_e(G)$ are in inverse proportion which is not uniform.

Remark 4.1: Let $G(V_1 \cup V_2, E)$ be a chain graph on n vertices. Then addition (removal) of an edge $e = (u, v)$ to (from) the graph G such that $u \in V_1, v \in V_2$ increases (decreases) the edge Wiener index by $(2m - deg(u) - deg(v))$ where m is the number of edges and $deg(u), deg(v)$ are the degrees of u, v respectively.

Thus the rate of change of edge Wiener index on addition (removal) of an edge is not uniform and it depends on the degrees of end vertices of the edge added (removed).

V. Zagreb Indices

This section deals with Zagreb indices of chain graphs.

Theorem 5.1: Let $G(V_1 \cup V_2, E)$ be a chain graph with $|V_1| = p$ and $|V_2| = q$. Let $M_1(G)$ and $M_2(G)$ be the first and second Zagreb indices of G respectively. Then,

$$p^2 + q^2 + p + q - 2 \le M_1(G) \le qp^2 + pq^2$$

and

$$p^2 + q^2 + pq - p - q \le M_2(G) \le p^2q^2.$$

Proof: By the definition of first Zagreb index, it is minimum when every vertex of the chain graph has minimum possible degree. Since every partite set of G has at least one full degree vertex, every vertex of G has minimum degree when $G = B(p, q)$. But, $M_1(B(p, q)) = p^2 + q^2 + p + q - 2$ as $B(p, q)$ has one vertex of degree p, one of degree q and the rest are of degree one. Similarly $M_1(G)$ is maximum when every vertex of G is of full degree, that is $G = K_{p,q}$. Since $M_1(K_{p,q}) = qp^2 + pq^2$ as it has p vertices of degree q and q vertices of degree p. Thus

$$p^2 + q^2 + p + q - 2 \le M_1(G) \le qp^2 + pq^2.$$

In the similar way, the second Zagreb index $M_2(G)$ attains maximum and minimum value when $G = K_{p,q}$ and $G = B(p, q)$ respectively. It can be evaluated that $M_2(K_{p,q}) = p^2q^2$ and $M_2(B(p, q)) = p^2 + q^2 + pq - p - q$.

Thus $p^2 + q^2 + pq - p - q \le M_2(G) \le p^2q^2$. ■

Theorem 5.2: Let G be a chain graph on $2n$ vertices. Let $M_1(G)$ and $M_2(G)$ be the first and second Zagreb indices of G respectively. Then,

$$2n^2 + 2n - 2 \leq M_1(G) \leq 2n^3$$

and

$$3n^2 - 2n \leq M_2(G) \leq n^4.$$

Proof: Let $q = 2n - p$. Then the bounds given in the Theorem 5.1 are
$4n^2 + 2p^2 + 2n - 4np - 2 \leq M_1(G) \leq 2np(2n - p)$ and

$p^2 + 4n^2 - 2np - 2n \leq M_2(G) \leq p^2(2n - p)^2$.
We minimize (maximize) the lower (upper) bound. Let $f_1(p) = 4n^2 + 2p^2 + 2n - 4np - 2$. As $\dfrac{d^2 f_1}{dp^2} = 4 > 0$, the function $f_1(p)$ has minima at the critical point $p = n$ and the minimum value is $f_1(p) = 2n^2 + 2n - 2$. Thus $2n^2 + 2n - 2 \leq M_1(G)$.
On maximization of the upper bound for $M_1(G)$, $f_2(p) = 2np(2n - p)$, we get $f_2(p)$ has maxima at $p = n$ and the maximum value is $f_2(p) = 2n^3$. Thus $M_1(G) \leq 2n^3$.
Similarly, the minimum value of the lower bound and the maximum value of the upper bound for $M_2(G)$ is obtained at the critical point $p = n$. Thus $3n^2 - 2n \leq M_2(G) \leq n^4$. ■

Theorem 5.3: Let G be a chain graph on $2n + 1$ vertices. Let $M_1(G)$ and $M_2(G)$ be the first and second Zagreb indices of G respectively. Then

$$2n^2 + 4n \leq M_1(G) \leq 2n^3 + 3n^2 + n$$

and

$$3n^2 + n \leq M_2(G) \leq n^2(n + 1)^2.$$

Proof: The proof is similar to the proof of Theorem 5.2. And the optimum values are obtained at the critical point $p = n + 1$ and $q = n$. ■

VI. Concluding remarks

Wiener index $w(G)$ of a graph is a concept of primary significance in the field of chemical graph theory due to the correlation between $w(G)$ and physico-chemical properties of paraffins i.e., hydrocarbons, where G is taken to be the molecular graph of the corresponding chemical compound. Chain graphs are one of the significant classes of graphs in the field of spectral graph theory whose chemical indices were untouched. We give bounds for Wiener index and hence for average distance of chain graphs. We have presented an algorithm that returns a chain graph on n vertices (if exists) for a given Wiener index w. We have also given the expression for 'edge-version' of Wiener index and hyper Wiener index of chain graphs.

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