Forbidden Values for Wiener Indices of Chain / Threshold Graphs

K ARATHI BHAT and SHAHISTHA HANIF*

Abstract—**Chain graphs and threshold graphs have received considerable attention of researchers in the field of spectral graph theory, due to extremity in the spectral radius among all the bipartite graphs (former one) and all the connected graphs (latter one). Wiener index of chain graphs have been studied in the literature and an algorithm returning a chain graph with the given Wiener index has been given. In this article, we give a list of integers which are forbidden values for Wiener indices of chain graphs, hence contributing further knowledge to the existing theory of inverse Wiener index problem. We further derive results on Wiener index of threshold graphs giving the bounds and carry out the similar study. We conclude the article with an algorithm for inverse Wiener index problem for threshold graphs.**

Index Terms—**Chain, Bipartite graph, Bi-star graph, Wiener index.**

I. Introduction

FROM the contemporary literature, one can conclude the importance of Wiener index in chemical graph theory. Wiener index is one of the oldest topological indices enabling the study of three basic structural features of molecules namely branching, cyclicity, centricity (or centrality) and their specific patterns. The wide majority of previous and ongoing studies related to Wiener index focus on inverse Wiener index problem. 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 term inverse Wiener index problem refers to the problem of constructing the graph of order n with the given Wiener index $W(G) = k$. It turned out that every positive integer, except for two and five, is the Wiener index of some connected graph. A great deal of knowledge on the Wiener index is accumulated in the literature ([13] and [14]).

Throughout the article, we denote a bipartite graph with bipartition $V(G) = V_1 \cup V_2$ by $G(V_1 \cup V_2, E)$ and a bi-star graph (a graph obtained by making the central vertices of two star graphs $K_{1,p-1}$ and $K_{1,q-1}$ adjacent) by $B(p, q)$. The adjacency and the non adjacency between two vertices v_i and v_j are symbolically represented respectively, by $v_i \sim v_j$ and $v_i \nsim v_j$.

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A chain graph is a bipartite graph with the property that neighborhood of vertices of each partite set form a chain with respect to set inclusion. Each of V_i $(i = 1, 2)$ in a chain graph $G(V_1 \cup V_2, E)$ can be partitioned into h non-empty cells $V_{1,1}, V_{1,2}, \ldots, V_{1,h}$ and $V_{2,1}, V_{2,2}, \ldots, V_{2,h}$ such that $N_G(u) = V_{2,1} \cup \ldots \cup V_{2,h-i+1}$, for any $u \in V_{1,i}$, $1 \le i \le h$. If $m_i = |V_{1,i}|$ and $n_i = |V_{2,i}|$, then we write $G = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$. Due to this nesting property, the chain graphs are also called Double Nested Graphs (DNGs). The interesting facts concerned with chain graphs are available in the literature [2], [4], [6], [8], [9], [15] and [16].

A split graph is a graph which admits a partition of its vertex set into two parts, say W_1 and W_2 such that W_1 induce a co-clique and W_2 induce a clique. All other cross edges, join a vertex of W_1 with a vertex of W_2 ([10]). A threshold graph is a split graph with the split partition $V(G) = \{W_1, W_2\}$ such that each of W_i $(i = 1, 2)$ can be further partitioned into h cells $W_1 = W_{1,1} \cup W_{1,2} \cup \cdots \cup W_{1,h}$ and $W_2 = W_{2,1} \cup W_{2,2} \cup \cdots \cup W_{2,h}$ satisfying the following nesting property: For each vertex $u \in W_{1,i}$, $1 \le i \le h$, $N_G(u) = W_{2,1} \cup \ldots \cup W_{2,h-i+1}$. If $|W_{1,i}| = m_i$ and $|W_{2,i}| = n_i$, then we write $G = NSG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$. The readers are referred to [1], [3], [5], [7], [11] and [12] for more results on threshold graphs.

The chain graphs and threshold graphs are often referred as extremal graphs due to the fact that, they have the largest spectral radius among all the bipartite graphs (former one) and all the connected graphs (latter one) with prescribed order and size. Further, any threshold graph can be obtained from a chain graph G by replacing one color class of G by a clique, keeping all other edges unchanged. The schematic representation of both DNGs, as well as NSGs, are given in Figure 1.

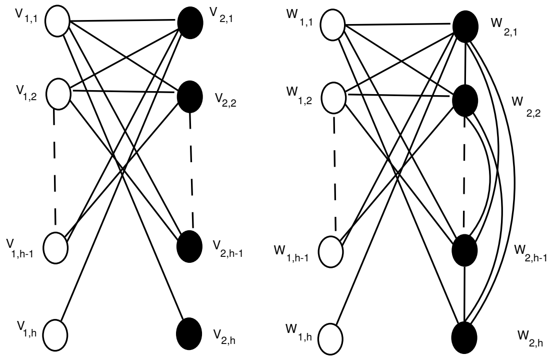

Fig. 1. Schematic diagram of chain and threshold graphs

Authors of [1] have derived bounds for Wiener index and other variants of chain graphs. The highlight of the article is a quadratic time algorithm for the inverse Wiener index problem. We extend the study further and give a set of integers except which every other integer is the Wiener index of some chain graph.

II. Wiener index of Chain graphs

We summarize the frame work to be used in this article, done by authors of [1], which are essential to derive our main results.

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

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

Theorem 2.2: 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

$$p^2+q^2+pq-p-q \leq W(G) \leq p^2+q^2+3\left(pq-p-q\right)+2.$$

The upper and the lower bound in the above theorem is attained by the complete bipartite graph $K_{p,q}$ and the bi-star graph $B(p,q)$, respectively. Further, the upper bound and the lower bound for $W(G)$ given by Theorem 2.2 are either both even or both odd.

Remark 2.1: 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.

That is, Wiener index of a chain graph being even or odd just depends on the cardinalities of the partite sets, irrespective of the structure and the number of edges. We also note that $W(G)$ is odd if and only if both p, q are odd and is even otherwise. The following theorem ([16]) gives the conditions for addition of edges to a chain graph G such that the resultant graph is also a chain graph.

Theorem 2.3: Let $G = DNG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ be a chain graph where $m_i = |U_i|$ and $n_i = |V_i|$ for $1 \leq i \leq h$. The graph $G + e$ obtained by adding an edge $e = (u, v)$ to G is a chain graph if and only if $u \in U_i$ and $v \in V_{h-i+2}$ for some $2 \leq i \leq h$.

From Theorem 2.1, we note that, Wiener index on addition (removal) of an edge to a chain graph decreases (increases) by two. We now proceed to our results.

Lemma 2.4: Let $a = p^2+q^2+pq-p-q$ and $b = p^2+q^2+3\left(pq-p-q\right)+2$ where $p, q \geq 1$. If either of p, q is even, then for every even integer $k \in [a, b]$, there exists at least one chain graph $G(V_1 \cup V_2, E)$ ($|V_1| = p$, $|V_2| = q$) with the Wiener index k. If not, for every odd integer $k \in [a, b]$, there exists at least one chain graph $G(V_1 \cup V_2, E)$ ($|V_1| = p$, $|V_2| = q$) with the Wiener index k.

Proof: We note that a and b, respectively, are the lower and upper bounds for Wiener index of a chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = p$ and $|V_2| = q$. Both the bounds a and b are odd if and only if both p, q are odd and even otherwise. Further, the proof follows directly from the fact that removal (addition) of an edge increases (decreases) the Wiener index by two. Starting from the bi-star graph $B(p, q)$, which has the Wiener index b, adding the edges sequentially decreases the Wiener index by two and attains the minimum value a when the graph is a complete bipartite graph $K_{p,q}$. ■

We observe that, for a chain graph on n vertices, the lower bound decreases and the upper bound increases as the difference $|p - q|$ decreases.

Theorem 2.5: Let $A = 3n^2 - 2n$ and $B = 5n^2 - 6n + 2$ where $n \geq 2$. Then for every integer $k \in [A, B]$, there exists at least one chain graph on $2n$ vertices with the Wiener index k.

Proof: We note that $A \leq W(G) \leq B$ for Wiener index $W(G)$ of a chain graph on $2n$ vertices i.e., for a chain graph $G(V_1 \cup V_2, E)$ on $2n$ vertices with $|V_1| = p$, $|V_2| = q$, the lower and the upper bounds are attained when $p = q = n$ (for the graphs $K_{n,n}$ and $B(n, n)$, respectively). We note that the bounds when $p = n-1$ and $q = n+1$ differ from the bounds when $p = q = n$ exactly by 1. Thus, suppose all the chain graphs on $2n$ vertices with $p = q = n$ have Wiener indices even, then all the chain graphs with $p = n - 1, q = n + 1$ have Wiener indices odd and vice versa. Suppose A, B are even and k is an even integer such that $k \in [A, B]$. Then by Lemma 2.4, there exists at least one chain graph on $2n$ vertices with $p = q = n$ having Wiener index k. Suppose k is an odd integer such that $k \in [A, B]$, then we know that the bounds for Wiener index when $p = n - 1$ and $q = n + 1$ is $[A + 1, B - 1]$ and $k \in [A + 1, B - 1]$. Again by Lemma 2.4, there exists at least one chain graph on $2n$ vertices with $p = n - 1$ and $q = n + 1$ having Wiener index k. Similarly, we can prove the same when both A, B are odd. ■

When k is odd, then there exists no chain graph G on odd number of vertices with $W(G) = k$. Similar to the above theorem about the existence of chain graphs of even order with the given Wiener index, we have the following theorem for odd order.

Theorem 2.6: Let $A^{'} = 3n^2 + n$ and $B^{'} = 5n^2 - n$ for some $n \geq 1$. Then for every even integer $k \in [A', B']$, there exists at least one chain graph G on $2n+1$ vertices with the Wiener index k.

For the sake of simplicity to address, we define realizability of a positive integer in the above said context. An integer $k \in Z^+$ is said to be realizable Wiener index for a chain graph if there exists at least one chain graph G with Wiener index k. If not, we say k is forbidden. Authors of [6] have given the bounds for Wiener index of chain graphs, but in this article, for every integer k within the respective bounds, we guarantee the existence of at least one chain graph with Wiener index k.

Theorem 2.7: An integer $k \in Z^+$ is realizable Wiener index for a chain graph if and only if at least one of the following conditions is true:

i. $k \in [3n^2 - 2, 5n^2 - 6n + 2]$ for some $n \in Z^+$.
ii. k is an even integer such that $k \in [3n^2 + n, 5n^2 - n]$ for some $n \in Z^+$.

The above theorem is a direct consequence of all the previous theorems and lemmas. We now investigate the set of integers satisfying the condition (1) in Theorem 2.7. In the interval $[3n^2 - 2, 5n^2 - 6n + 2]$, for all consecutive integers n and $n + 1$ whenever $n \geq 5$, it is true that the upper bound for n is less than the lower bound for $n + 1$. For an instance, when $n = 5, 6$, we get the bounds $[65, 75]$ and $[96, 146]$, respectively. Thus, all the integers $k \geq 65$ are realizable Wiener indices as they satisfy (1) of Theorem 2.7. Further, for $n = 1, 2, 3, 4$, the bounds in (1) turn out to be $[1, 1], [8, 10], [21, 29]$ and $[40, 58]$, respectively and all the integers in these intervals are realizable. Thus, all the integers except $2, 3, 4, 5, 6, 7, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 59, 60, 61, 62, 63, 64$ satisfy the condition (1) of Theorem 2.7.

Since we characterize the integers which are forbidden to be Wiener indices of any chain graph, we examine the above listed integers if they satisfy condition (2) of Theorem 2.7. One can easily note that the integers $4, 14, 16, 18, 30, 32, 34, 36, 38, 60, 62, 64 \in [3n^2 + n, 5n^2 - n]$. With all this theory and conclusions, we now propose the main theorem of the article.

Theorem 2.8: Every integer except $2, 3, 5, 6, 7, 11, 12, 13, 15, 17, 19, 20, 31, 33, 35, 37, 39, 59, 61, 63$ is the Wiener index of some chain graph G.

Thus, the above set of integers are forbidden to be the Wiener indices of any chain graph.

III. Wiener index of threshold graphs

Threshold graphs are another class of graphs playing similar role as that of chain graphs in the field of spectral graph theory. Recently, some of the articles have been published on comparative studies on chain and threshold graphs. We specify the split partition $V(G) = \{W_1, W_2\}$ of a threshold graph G where $\langle W_1 \rangle$ is a co-clique and $\langle W_2 \rangle$ is a clique by denoting it as $G(W_1 \cup W_2, E)$ (just like a bipartite graph where both the partite sets induce co-clique). Before moving into the Wiener index, we derive some preliminary results which are necessary in the further part of the article.

Remark 3.1: Suppose G is connected threshold graph on n vertices, then G has at least one vertex of degree $n-1$.

Remark 3.2: Let $G(W_1 \cup W_2, E)$ be a threshold graph with $|W_1| = p$, $|W_2| = q$ and $|E| = m$. Then

$$\binom{q}{2} + p + q - 1 \leq m \leq \binom{q}{2} + pq$$

The lower bound is attained by the graph $NSG(1, p-1; 1, q-1)$ and the upper bound is attained by $NSG(p; q)$. For all $m \in [\binom{q}{2} + p, \binom{q}{2} + pq]$, it is possible to construct threshold graphs with $|W_1| = p$, $|W_2| = q$ on $n = p + q$ vertices and m edges by successively adding edges to the graph $NSG(1, p-1; 1, q-1)$ until we get $NSG(p; q)$. But adding an edge e to a threshold graph G such that $G + e$ is also threshold graph is done not at random, but according to the condition given in the following theorem.

Theorem 3.1: Let $G = NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ be a threshold graph with $m_i = |W_{1,i}|$ and $n_i = |W_{2,i}|$ for $1 \leq i \leq h$. Then the graph $H = G + e$ obtained from G by adding an edge $e = (x, y)$ is also a threshold graph if and only if either both $x, y \in W_{1,1}$ or $y \in W_{2,h-i+2}$ whenever $x \in W_{1,i}$ for $2 \leq i \leq h$.

Proof: Let $H(W_1^{'} \cup W_2^{'}, E^{'})$ be a threshold graph obtained from G by adding an edge $e = (x, y)$ and $E^{'} = E \cup (x, y)$. Then either both $x, y \in W_1$ or $x \in W_1$ and $y \in W_2$ in G.

Let $x, y \in W_1$ in G. Since $\langle W_1^{'} \rangle$ is a co-clique, the vertices x, y belong to the different partite sets $W_1^{'}$ and $W_2^{'}$ of H. Thus, $W_1^{'} = W_1 \setminus \{y\}$ and $W_2^{'} = W_2 \cup \{y\}$. Further, since $\langle W_2^{'} \rangle$ is a clique, y is adjacent with every other vertex of W_2 in G, i.e $y \in W_{1,1}$ in G. Now, suppose $x \in W_{1,j}$ in G for $j > 1$, then there exists at least one vertex $z \in W_{1,1}^{'}$ in H such that $N_H(x) \nsubseteq N_H(z)$ as y is in $N_H(x)$, but not in $N_H(z)$. Thus, $j = 1$ and $x \in W_{1,1}$ in G.

Let $x \in W_1$ and $y \in W_2$ in G, in which case $W_1^{'} = W_1$ and $W_2^{'} = W_2$. Without loss of generality, let $x \in W_{1,i}$ and $y \in W_{2,j}$ for $2 \leq i, j \leq h$. Since $N_G(x) = W_{2,1} \cup W_{2,2} \cup \cdots \cup W_{2,h-i+1}$ and x is not adjacent to y in G, it is clear that $y \in W_{2,j}$ where $j > h - i + 1$, say $j = h - i + k$ for $k \geq 2$. For all the vertices $z \in W_{1,i-1}$, then $N_H(z) = W_{2,1} \cup W_{2,2} \cup \cdots \cup W_{2,h-i+1} \cup W_{2,h-i+2}$. But when $k > 2$, neither $N_H(x) \subseteq N_H(z)$ nor $N_H(z) \subseteq N_H(x)$. Thus $k = 2$.

Conversely, let H be a graph obtained by adding an edge $e = (x, y)$ to a threshold graph $G = NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$. If both $x, y \in W_{1,1}$ in G, then $H = NSG(1, m_1 - 2, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h, 1)$. If $x \in W_{1,i}$ and $y \in W_{2,h-i+2}$ for some $2 \leq i \leq h$, then $V(H) = W_1 \cup W_2$ such that $\langle W_1 \rangle, \langle W_2 \rangle$ are co-clique and clique, respectively. Further, $N_H(x) = W_{2,1} \cup W_{2,2} \cup \cdots \cup W_{2,h-i+1} \cup \{y\}$ where $y \in W_{2,h-i+2}$. Clearly, $N_H(W_{1,h}) \subseteq N_H(W_{1,h-1}) \subseteq \cdots \subseteq N_H(W_{1,i+1}) \subseteq N_H(x) \subseteq N_H(W_{1,i}) \subseteq \cdots \subseteq N_H(W_{1,2}) \subseteq N_H(W_{1,1})$. ∎

We now move into the main part, the Wiener index.

Theorem 3.2: Let G be a threshold graph of order n and size m. Let $W(G)$ be the Wiener index of G. Then

$$W(G) = n^2 - n - m.$$

Proof: Let $\{W_1, W_2\}$ be the split partition of $V(G)$ such that $\langle W_1 \rangle$ is a co-clique and $\langle W_2 \rangle$ is a clique. Further, let $|W_1| = p$ and $|W_2| = q$ and $v \in W_2$ be a dominating vertex (a vertex of degree $n-1$) in G. For any pair of vertices (u_i, v_j) such that $u_i \nsim v_j$, then either $u_i, v_j \in W_1$ or $u_i \in W_1$ and $v_j \in W_2$. In both the cases, $d(u_i, v_j) = 2$ as there is a path $u_i - v - v_j$ of length two in G. Thus

$$d(u_i, v_j) = \begin{cases} 1, & \text{if } u_i \sim v_j \\ 2, & \text{else} \end{cases}.$$

Also, the number of edges in any threshold graph is at most $pq + \binom{q}{2}$. Since G has m edges in it, there are $m - \binom{q}{2}$ edges having end vertices in different partite sets. Thus G has $\binom{p}{2} + pq - m + \binom{q}{2}$ pairs of vertices (u_i, v_j) such that $u_i \nsim v_j$. Thus the Wiener index is

$$W(G) = m + 2\left(\binom{p}{2} + pq - m + \binom{q}{2}\right) = n^2 - n - m$$

∎

We surprisingly note that the Wiener index of a threshold graph of order n is neither depending on cardinality of the partite sets nor on the structure. It just depends on the number of edges. For example, all the three threshold graphs having 7 vertices and 11 edges have the Wiener index 37 (Figure 2).

We know that every threshold graph $H = NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ can be obtained from the chain graph $G = DNG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ by making any one of the partite sets complete. In the next theorem, we give the relation between the

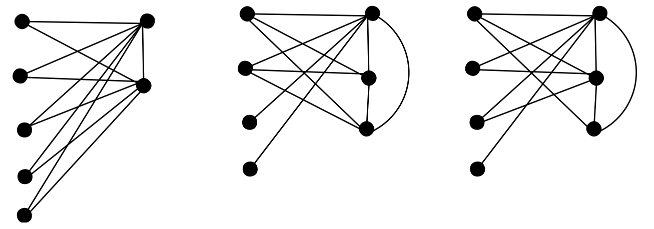

Fig. 2. Threshold graphs having Wiener index 37

Wiener index of a threshold graph and the corresponding chain graph from which it is obtained.

Theorem 3.3: Let $G = DNG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ be a chain graph, where $|U| = p = \sum_{i=1}^{h} m_i$ and $|V| = q = \sum_{i=1}^{h} n_i$ with m edges. Let $H = NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ be the threshold graph obtained from G by making V complete. Suppose $W(G), W(H)$ are the Wiener indices of the graphs G and H, respectively, then $W(H) = W(G) - \binom{q}{2} - pq + m$.

Proof: Proof follows from noting that, the $\binom{q}{2}$ pairs of vertices from V which are at distance two in G are at distance one in H and $(pq - m)$ pairs of vertices which are at distance three in G are at distance two in H. ■

For the graph $DNG(1,1,1;1,2,1)$ in Figure 3, $W(DNG(1,1,1;1,2,1)) = 38$. The Wiener index of corresponding threshold graph is given by $W(NSG(1,1,1;1,2,1)) = W(DNG(1,1,1;1,2,1)) - \binom{4}{2} - 12 + 8 = 28$.

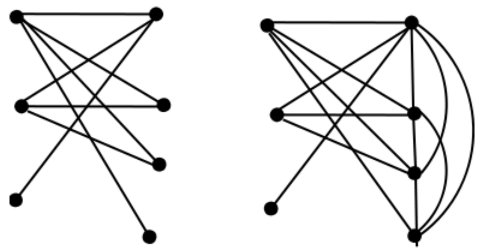

Fig. 3. DNG(1,1,1;1,2,1) and NSG(1,1,1;1,2,1)

In the next theorem, among all the threshold graphs with split partition $\{W_1, W_2\}$ such that $|W_1| = p$ and $|W_2| = q$, the graphs having extreme values of Wiener indices are given.

Theorem 3.4: Let G be a threshold graph with split partition $\{W_1, W_2\}$ such that $|W_1| = p$ and $|W_2| = q$. Let $W(G)$ be the Wiener index of G. Then

$$\frac{2n^2 - 2n - 2pq - q^2 + q}{2} \leq W(G) \leq \frac{2n^2 - 4n + 2 - q^2 + q}{2}$$

.

Proof: From Theorem 3.2, $W(G)$ is at the maximum when the total number of edges is at the minimum and vice versa. That is the graph $NSG(1, p-1; 1, q-1)$ with $n = p+q$ and $m = \binom{q}{2} + p + q - 1$ has the maximum Wiener index and is given by

$$\begin{aligned} W(NSG(1, p-1; 1, q-1)) &= n^2 - n - \binom{q}{2} - p - q + 1 \\ &= \frac{2n^2 - 4n + 2 - q^2 + q}{2} \end{aligned}$$

Similarly, the graph $NSG(p; q)$ with the total number of edges $m = \binom{q}{2} + pq$ has the minimum Wiener index given by

$$\begin{aligned} W(NSG(p; q)) &= n^2 - n - \binom{q}{2} - pq \\ &= \frac{2n^2 - 2n - 2pq - q^2 + q}{2} \end{aligned}$$

■

We also guarantee the existence of a threshold graph on n vertices and m edges for every m in the bounds given in Remark 3.2. We can further improvise the bounds for m in Remark 3.2 by taking appropriate values for p, q for which m takes extreme values. A threshold graph of order n has at least $n-1 (p = n-1, q = 1)$ edges and at most $\frac{n(n-1)}{2} (p = 1, q = n-1)$ edges.

Remark 3.3: Let n be an integer. For every $m \in [n-1, \frac{n(n-1)}{2}]$, there exists at least one threshold graph G on n vertices and m edges and is obtained from $NSG(n-1; 1)$ (having $n-1$ edges) by successively adding edges using Theorem 3.1 until we get $NSG(1; n-1)$ (having $\frac{n(n-1)}{2}$ edges).

From Theorem 3.2, the Wiener index of threshold graph is inversely proportional to the number of edges. Using the extreme values for m given in the above remark, we give the bounds for the Wiener index of a threshold graph G on n vertices:

$$\frac{n(n-1)}{2} \leq W(G) \leq (n-1)^2 \tag{1}$$

Since addition of an edge to a threshold graph increases the Wiener index by 1, Remark 3.3, which guarantees the existence of at least one threshold graph on n vertices and m edges for every $m \in [n-1, \frac{n(n-1)}{2}]$, in turn guarantees the existence of at least one threshold graph G on n vertices with the Wiener index $W(G) = k$ for every $k \in [\frac{n(n-1)}{2}, (n-1)^2]$.

Remark 3.4: Let $A = \frac{n(n-1)}{2}$ and $B = (n-1)^2$ for some $n \geq 1$. Then for every integer $k \in [A, B]$, there exists at least one threshold graph G on n vertices with the Wiener index k.

An integer k is a realizable Wiener index for a threshold graph, if there exists at least one threshold graph on n vertices and $n^2 - n - k$ edges for some $n \geq 2$.

Thus, an integer $k \in Z^+$ is realizable Wiener index for threshold graph if $k \in [\frac{n(n-1)}{2}, (n-1)^2]$ for some n. Also, on addition of an edge to a threshold graph increases the Wiener index by one. As in the case of chain graphs, in the interval $[A, B]$, for every consecutive integers $n, n+1$, it is true that the upper bound for n is less than the lower bound of Wiener index for $n+1$ whenever $n \geq 5$. For $n = 5, 6$, we have the bounds $[10, 16]$ and $[15, 25]$. Thus, we have the following lemma.

Lemma 3.5: All the integers $k \geq 10$ are realizable Wiener indices for threshold graph.

Further, for $n = 2, 3, 4$, the bounds $[A, B]$ turns out to be $[1, 1], [3, 4]$ and $[6, 9]$, respectively. With all the remarks and lemma, we now propose the main theorem characterizing the forbidden integers for Wiener indices of threshold graphs.

Theorem 3.6: Every integer except 2 and 5 is the Wiener index of some threshold graph G.

We now focus on the inverse Wiener index problem for threshold graphs. We generate a procedure, which takes the inputs n, k and presents a threshold graph G on n vertices with the Wiener index k.

IV. Inverse Wiener index problem for threshold graphs

The inputs for this algorithm are the number of vertices n and a positive integer k. The task is to check for the existence of a threshold graph on n vertices having k as its Wiener index. Once the existence of a threshold graph G on n vertices with $W(G) = k$ is guaranteed, the graph G is returned. The algorithm first checks if the given input integer $k \in [\frac{n(n-1)}{2}, n^2 - 2n + 1]$. If yes, we partition the vertex set such that $V = W_1 \cup W_2$ with $|W_1| = p, |W_2| = q$ and $p + q = n$ starting from $q = 2$. For given p, q, again the algorithm checks if $k \in [A, B]$, where $A = \frac{2n^2-2n-2pq-q^2+q}{2}, B = \frac{2n^2-4n+2-q^2+q}{2}$ are the lower and upper bounds for Wiener index of a threshold graph $G(W_1 \cup W_1, E)$ with $|W_1| = p, |W_2| = q$. If $k \in [A, B]$, then we start from a graph $G = NSG(1, p-1; 1, q-1)$ and evaluate the number of edges to be added to G, keeping in mind that an edge added to any threshold graph increases the Wiener index by one. We then add the edges according to one of the ways mentioned in Theorem 3.1.

The graph $G = NSG(1, p-1; 1, q-1)$ which we use in the algorithm has the split partition $V(G) = W_1 \cup W_2$ such that $|W_1| = p, |W_2| = q$ $(p + q = n)$ with $\langle W_1 \rangle$, $\langle W_2 \rangle$ as co-clique and clique respectively. The vertices of G are labeled as follows: $W_1 = \{0, 1, \ldots, p-1\}$ and $W_2 = \{0, 1, \ldots, q-1\}$.

Algorithm:

Algorithm 1 function Wiener (k, n)

Input: k, n
Output: A threshold graph G if exists with given Wiener index

1: **if** $k \notin [\frac{n(n-1)}{2}, n^2 - 2n + 1]$ **then**
2: **print** "There is no threshold graph G on n vertices with $W(G) = k$."
3: **else if** $k == \frac{n(n-1)}{2}$ **then**
4: $G = NSG(1; n-1)$
5: **return** G
6: **else if** $k == n^2 - 2n + 1$ **then**
7: $G = NSG(n-1; 1)$
8: **return** G
9: **else**
10: **for** $q = 2 : n-2$ **do**
11: $p = n - q$
12: $A = \dfrac{2n^2 - 2n - 2pq - q^2 + q}{2}$
13: $B = \dfrac{2n^2 - 4n + 2 - q^2 + q}{2}$
14: **if** $k \notin [A, B]$ **then**
15: **continue**
16: **else if** $k == A$ **then**
17: $G = NSG(p; q)$
18: **return** G
19: **else if** $k == B$ **then**
20: $G = NSG(1, p-1; 1, q-1)$
21: **return** G
22: **end if**
23: $c = B - k$
24: $G = NSG(1, p-1; 1, q-1)$
25: **for** $i = 1 : p-1$ **do**
26: **for** $j = 1 : q-1$ **do**
27: **if** $c \neq 0$ **then**
28: $E(G) = E(G) \cup (i, j)$
29: $c = c - 1$
30: **end if**
31: **end for**
32: **end for**
33: **end for**
34: **return** G
35: **end if**

The concept of Wiener index has noteworthy applications, not only in the field of molecular studies, but also in communication, cryptography and facility location. This article extends the study of Wiener index of structured graphs, namely chain and threshold graphs. For an integer k, there may be more than one threshold graphs on n vertices having Wiener index k. But the above algorithm do not generate all the threshold graphs with the given Wiener index k, but outputs any one graph.
The working procedure of the algorithm is illustrated with an example as follows.

Example 4.1: For the inputs $k = 36$ and $n = 8$, the algorithm intends to return a threshold graph G on 8 vertices with $W(G) = 36$.

— As $k \in [28, 49]$, there exist such a graph (*Step 1*).
— Since $k \neq 28$ (*Step 3*) and $k \neq 49$ (*Step 6*), directly go to *Step 10* and start the for loop: for $q = 2$ to 6.
  – When q= 2:
    $p = 6$ (*Step 11*), $A = 43$ (*Step 12*), $B = 48$ (*Step 13*). Further $k \notin [43, 48]$, go back to *Step 10* and $q = 2+1$ (*Step 14*).
  – When $q = 3$
    $p = 5$, $A = 38, B = 46$.
    Further$k \notin [38, 46]$, go back to step 10 and $q = 4$.
  – When $q = 4$.
    $p = 4, A = 34, B = 42$.
    Since $k \in [34, 42]$ (*Step 14*) and $k \neq 34$ (*Step 17*), $k \neq 42$ (*Step 19*), go to *Step 23*.
— $c = B - k = 42 - 36 = 6$ (*Step 23*).
— Take $G = NSG(1, 3; 1, 3)$ with $W_1 = 0, 1, 2, 3$ and $W_2 = 0, 1, 2, 3$ (step 24) and add 6 edges to G.
— The consecutive *Steps 25-29* add the edges (1,1),(1,2),(1,3),(2,1),(2,2),(2,3) sequentially to G until *c=0*.

The resultant output graph $G = NSG(3, 1; 1, 3)$ is shown in Figure 4.

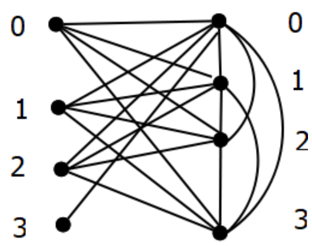

Fig. 4. DNG(3,1;1,3)

V. Conclusion

The highlight of the article is the list of integers which would never be the Wiener indices of any chain/threshold graphs. The strategies used to derive these main results are also proved in the article. Analogous to the algorithm for inverse Wiener index problem for chain graphs, we carry out a similar study and present an algorithm for threshold graphs.

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