Some Properties and Topological Indices of k-nested Graphs

SHASHWATH S SHETTY and K ARATHI BHAT*

Abstract—**A double nested graph is a bipartite graph with the property that the neighborhood of vertices of each partite set form a chain with respect to set inclusion. Motivated by this structure, we generalize and define a new class of graphs and name it as k-nested graphs and study its properties. Characterization of a k-nested 2-self centered graph which is edge maximal is discussed and also we show that none of the k-nested 2-self centered graph is edge minimal. We extend the study and gave the bounds for Wiener index and some Szeged indices of k-nested graphs. We conclude this article by exploring some more degree based topological indices of k-nested graphs.**

Index Terms—**k-partite graphs, chain graphs, 2-self centered graphs, distance and degree based topological index.**

I. Introduction

By a graph $G = (V, E)$ we mean a finite, undirected and connected graph without loops and multiple edges. A k-partite graph G is a graph whose vertex set $V(G)$ can be partitioned into k subsets $V_1, V_2, \ldots, V_k$ such that every edge of G joins a vertex of V_i with a vertex of V_j, $i \neq j$. We denote k-partite graph with the k-partition $V(G) = V_1 \cup V_2 \cup \ldots \cup V_k$ by $G(\bigcup_{i=1}^{k} V_i, E)$. If G contains every edge joining the vertices of V_i and $V_j, i \neq j$, then it is complete k-partite graph. A complete k-partite graph with $|V_i| = p_i, 1 \leqslant i \leqslant k$ is denoted by $K_{p_1,p_2,\ldots,p_k}$. We write $u \sim v$ if the vertices u and v are adjacent in G and $u \nsim v$ if they are not adjacent in G. The neighborhood of the vertex $u \in V(G)$ is the set $N_G(u)$ consisting of all the vertices v such that $v \sim u$ in G. A vertex $v \in V_i (1 \leqslant i \leqslant k)$ in a k-partite graph $G(\bigcup_{i=1}^{k} V_i, E)$ is a dominating vertex if $N_G(v) = \bigcup_{j=1}^{k} V_j,\ j \neq i$. In other words v is of full degree with respect to other partite set. 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. Readers are referred to [1] for all the elementary notations and definitions not described but used in this paper.

A class of sets $S = \{S_1, S_2, \ldots, S_n\}$ is called chain with respect to set inclusion, if for every $S_i,\ S_j \in S$ either $S_i \subseteq S_j$ or $S_j \subseteq S_i$.

Definition 1.1: A chain graph is a bipartite graph such that the neighborhoods of the vertices in each partite set form a chain with respect to set inclusion.

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Shashwath S Shetty is a research scholar in the Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India-576104 (email: shashwathsshetty01334@gmail.com).

*Corresponding author: K Arathi Bhat is an Assistant Professor - Selection Grade in the Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India-576104 (Phone: 9964282648; email: arathi.bhat@manipal.edu).

For more results related to chain graphs (2-nested graphs), reader is referred to [2]–[4].

We extend the concept of this nesting property to a k-partite graph and define a k-nested graph as follows.

Definition 1.2: A graph is called a k-nested graph, if it is k-partite and neighborhood of the vertices in each partite set form a chain with respect to set inclusion and each partite set have at least one dominating vertex.
In other words for every two vertices u and v in the same partite set and for their neighborhoods $N_G(u)$ and $N_G(v)$, either $N_G(u) \subseteq N_G(v)$ or $N_G(v) \subseteq N_G(u)$. Due to the existence of at least one dominating vertex in each partite set, a k-nested graph is always connected.

A chain graph is a 2-nested graph which is also known as double nested graph (DNG in short). Figure 1 represents a 4-nested graph G with $V_1 = \{v_{11}, v_{12}, v_{13}, v_{14}\}$, $V_2 = \{v_{21}, v_{22}\}, V_3 = \{v_{31}, v_{32}, v_{33}\}$ and $V_4 = \{v_{41}\}$.

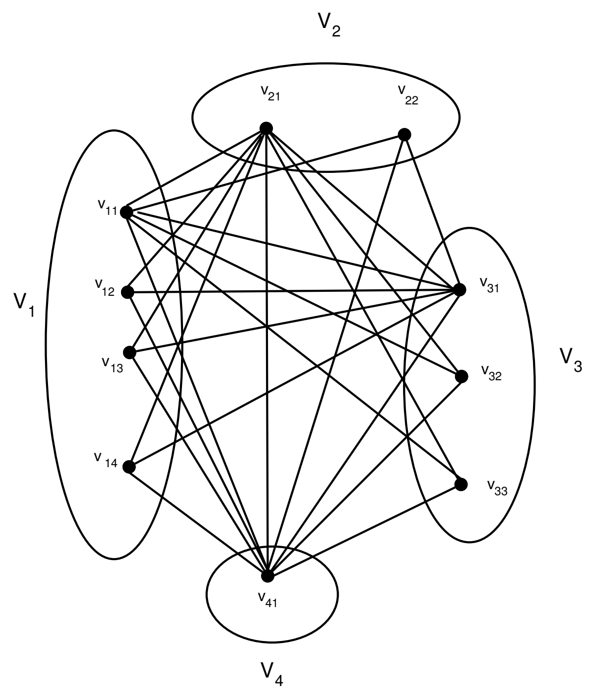


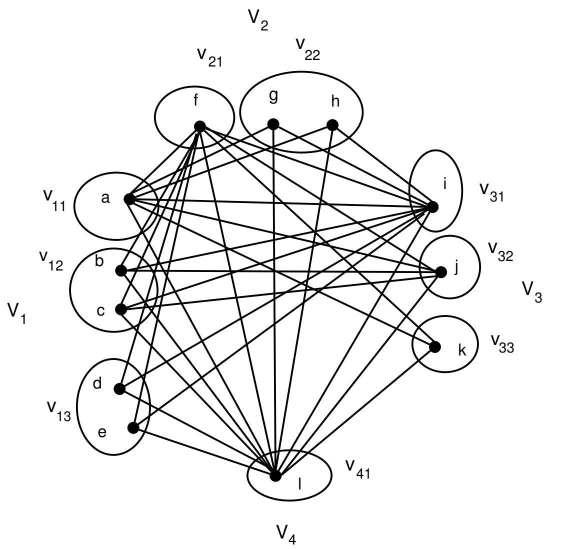
Fig. 1. 4-nested Graph G

The vertices v_{11}, v_{21}, v_{31} and v_{41} are the dominating vertex of the sets V_1, V_2, V_3 and V_4 respectively. Also, $N_G(v_{14}) \subseteq N_G(v_{13}) \subseteq N_G(v_{12}) \subseteq N_G(v_{11})$.

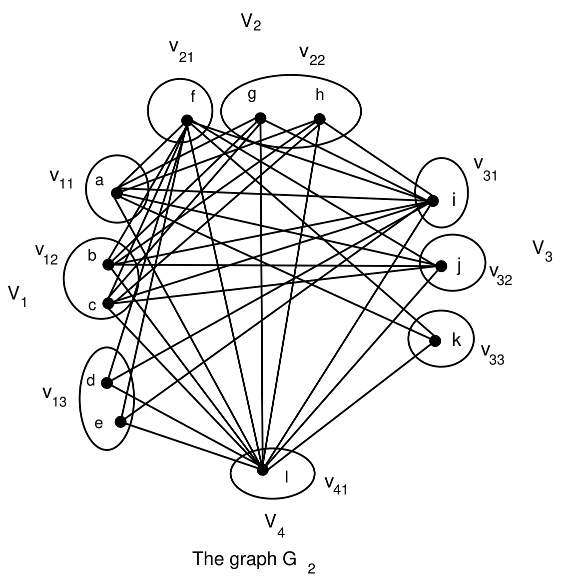
Given a chain graph $G(V_1 \cup V_2, E)$, each of $V_i\ (i = 1, 2)$ can be partitioned into h non-empty cells $V_{11}, V_{12}, \ldots, V_{1h}$ and $V_{21}, V_{22}, \ldots, V_{2h}$ such that $N_G(u) = V_{21} \cup \ldots \cup V_{2\ h-i+1}$, for any $u \in V_{1i}$, $1 \leq i \leq h$. If $m_i = |V_{1i}|$ and $n_i = |V_{2i}|$, then we write $G = DNG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$. Similarly, we can partition each partite set $V_i,\ 1 \leqslant i \leqslant k$ as

$V_{i1}, V_{i2}, \ldots, V_{ih_i}$ of a k-nested graph with the property that for any two vertices say u, v in $V_{ij}, 1 \leqslant j \leqslant h_i$, $N_G(u) = N_G(v)$. Suppose $|V_{ij}| = m_{ij}$, then we can write $G = KNG(m_{11}, ..., m_{1h_1}; m_{21}, \ldots, m_{2h_2}; ...; m_{k1}, ..., m_{kh_k})$. The graph in Figure 1 represents $KNG(1, 3; 1, 1; 1, 2; 1)$.
Also, $G = KNG(m_{11}, \ldots, m_{1h_1}; \ldots; m_{k1}, \ldots, m_{kh_k})$ does not represent a single graph, but a family of graphs G_f with nesting as said above. Thus, we write
$G_f = KNG(m_{11}, \ldots, m_{1h_1}; \ldots; m_{k1}, \ldots, m_{kh_k})$ (instead of just G).

Example 1.1: The graphs G_1 and G_2 (Figure 2) are the 4-nested graphs with 12 vertices in the family $G_f = KNG(1, 2, 2; 1, 2; 1, 1, 1; 1)$.



The graph G_1



The graph G_2

Fig. 2. The graph $G_1, G_2 \in G_f = KNG(1, 2, 2; 1, 2; 1, 1, 1; 1)$

The graph G_1 has 32 edges where as the graph G_2 has 36 edges. The vertices $a \in V_1, f \in V_2, i \in V_3, l \in V_4$ are the 4 dominating vertices of the graphs G_1 and G_2. The vertices $a, b, c, d, e \in V_1$. Since $N_G(b) = N_G(c)$, we have $b, c \in V_{12}$. Similarly $d, e \in V_{13}$ as $N_G(d) = N_G(e)$. Hence, $V_1 = V_{11} \cup V_{12} \cup V_{13}$. Similarly, $V_2 = V_{21} \cup V_{22}$, $V_3 = V_{31} \cup V_{32} \cup V_{33}$ and $V_4 = V_{41}$. So, $|V_{11}| = 1, |V_{12}| = |V_{13}| = 2$.
A complete graph K_n is an n-nested graph. We note that P_2, P_3 and P_4 are the only path graphs which are k-nested graphs with $k = 2$. Also, $C_3 = K_3$ is a 3-nested graph and C_4 is a 2-nested graph. Bi stars are the only trees which are k-nested graphs with $k = 2$.

II. Properties

In this section, we study some of the properties of k-nested graphs. First we note the following.

Note 2.1: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph with $3 \leqslant k \leqslant n-1$. Then $k - 1 \leqslant deg(v) \leqslant n - 1$.

Let G be a k-nested graph with $|V_i| = p_i, 1 \leqslant i \leqslant k$. The *maximal k-nested graph G* on n vertices is a k-nested graph with the property that addition of any edge to G results in a non k-nested graph. We note that $G = K_{p_1, p_2, \ldots, p_k}$ is the maximal k-nested graph.
Let G be a k-nested graph with $|V_i| = p_i, 1 \leqslant i \leqslant k$. The *minimal k-nested graph G* on n vertices is a k-nested graph with the property that removal of any edge from G results in a non k-nested graph.
The bi star $B(p, q)$ on n vertices with $|V_1| = p$ and $|V_2| = q$ is the minimal 2-nested graph ([3]) and has $n - 1$ edges. We obtain the structure and number of edges in the minimal k-nested graph.

Theorem 2.1: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph with $|V_i| = p_i, 1 \leqslant i \leqslant k$. If G is minimal k-nested graph then, $G = KNG(1, p_1 - 1; 1, p_2 - 1; \ldots; 1, p_k - 1)$.

Proof: Let $v_{ij} \in V_i, 1 \leq i \leq k, 1 \leq j \leq p_i$ be the vertices of G. The k-nested graph G' in which $N_G(v_{i1}) = \bigcup_{j \neq i} V_j$, and $N_G(v_{il}) = \{v_{j1} | 1 \leq j \leq k; 2 \leq l \leq p_i, j \neq i\}$, is the minimal k-nested graph. Then $v_{i1} \in V_i, 1 \leq i \leq k$, is the dominating vertex of the partite sets $V_1, V_2, \ldots, V_k$ respectively. Hence, the result follows. ■

Lemma 2.2: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a minimal k-nested graph on n vertices and m edges with $|V_i| = p_i, 1 \leq i \leq k$. Then, $m = n(k-1) - \binom{k}{2}$.

Proof: The proof follows by noting that the dominating vertices $v_{i1}, 1 \leq i \leq k$, have degree $n - p_i$ and degree of all other vertices are equal to $k - 1$. ■

Theorem 2.3: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on n vertices with $3 \leq k \leq n-1$. Then G is r-regular if and only if $G = K_{p,p,\ldots,p}$ and $r = (k-1)p$.

Proof: Let G be a k-nested r-regular graph on n vertices. For any two vertices on the same partite set say V_1 there are r vertices in the remaining $k - 1$ partite sets, i.e. $|V_2| + |V_3| + \ldots + |V_k| = r$. Similarly, we have $|V_1| + |V_3| + \ldots + |V_k| = r$ and so on. Adding all these we get $(k-1)n = kr$ or $r = \frac{(k-1)n}{k}$. Hence n is a multiple of k. Let $n = pk$. Then $r = p(k-1)$. Hence, we get $|V_i| = |V_j| = p$, i.e., $G = K_{p,p,\ldots,p}$. Converse is trivial. ■

Lemma 2.4: Let $G(\bigcup_{i=1}^{k} V_i, E_1)$ be a minimal k-nested graph on n vertices and m_1 edges and $H(\bigcup_{i=1}^{r} V_i, E_2)$ be a minimal r-nested graph on n vertices and m_2 edges with $3 \leq k < r \leq n-1$. Then $m_1 < m_2$.

Proof: From Lemma 2.2, $m_1 = n(k-1) - \binom{k}{2}$ and $m_2 = n(r-1) - \binom{r}{2}$. $m_2 - m_1 = \frac{(r-k)(2n+1-k-r)}{2}$. As $n > \frac{k+r-1}{2}$ and $r > k$, we get $m_2 - m_1 > 0$. ■

Theorem 2.5: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on n vertices and m edges with $3 \leq k \leq n-1$. Then, $2n-3 \leq m \leq \binom{n}{2} - 1$.

Proof: From Lemma 2.2, the number of edges m in the minimal k-nested graph is $n(k-1) - \binom{k}{2}$. From Lemma 2.4, we know that as k increases, m increases. Therefore, G has minimum number of edges when $k = 3$ and $m = 2n-3$. Similarly, G has maximum number of edges when $k = n-1$ and $m = \binom{n}{2} - 1$. ■

Note 2.2: In a k-nested graph $(3 \leq k \leq n-1)$, if there exists at least one partite set $V_i, 1 \leq i \leq k$ such that $|V_i| = 1$, then $diam(G) = 2$ and $radius(G) = 1$. If $|V_i| \geq 2$, for every $1 \leq i \leq k$, then $diam(G) = radius(G) = 2$, which means the eccentricity of every vertex is equal to $2(i.e.e(v) = 2$. Hence G is 2-self centered graph.

Theorem 2.6: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested 2-self-centered graph on n vertices and m edges with $3 \leq k \leq n-1$. Then,

$$2n-3 \leq m \leq \begin{cases} \dfrac{n(n-2)}{2}; & \text{n even} \\ \dfrac{(n-3)(n+1)}{2}; & \text{otherwise.} \end{cases}$$

Proof: From Theorem 2.5, G has minimum number of edges when $k = 3$ and $m = 2n-3$. From Note 2.2, we have $|V_i| \geq 2$. Hence, G will have maximum number of edges when k is as large as possible. When n is even, $k = \frac{n}{2}$. Therefore, $G = K_{2,2,\ldots,2}$ and $m = \frac{n(n-2)}{2}$. When n is odd, $k = \frac{n-1}{2}$. Hence, $G = K_{2,2,\ldots,2,3}$ and $m = \dfrac{(n-3)(n+1)}{2}$. ■

A 2-self-centered graph G is said to be *edge-maximal* if there are no non adjacent pairs of vertices $u, v \in V(G)$ such that $G + uv$ is 2-self-centered. The following theorem is a characterization for edge-maximal 2-self-centered graphs.

Theorem 2.7: [5] Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a 2-self-centered graph. Then G is edge-maximal if and only if G is disconnected and each connected component of G is a star with at least two vertices.

Now, we give a characterization for an edge maximal 2-self centered graph below.

Theorem 2.8: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested 2-self centered graph on n vertices and m edges with $3 \leq k \leq n-1$. Then G is edge maximal, if and only if $G = K_{2,2,\ldots,2}$.

Proof: From Theorem 2.7, we know that if G is edge maximal, then $\overline{G}$ is disconnected and each connected component of G is a star with at least two vertices. Suppose, there exist a partite set with 3 or more vertices in G, then in $\overline{G}$ there exist a component which is complete graph on 3 or more vertices. Hence from Theorem 2.7, $G = K_{2,2,\ldots,2}$. Suppose n is odd, then from Theorem 2.6, G has maximum number of edges when $G = K_{2,2,\ldots,2,3}$. Then in $\overline{G}$, there exist a component which is K_3. Hence G is not edge maximal. ■

Note 2.3: Let $G = K_{2,2,\ldots,2,3}$ and if we add an edge between the vertices u, v where $u, v \in V_i$, where $|V_i| = 3$, we can observe that $\overline{G}$ is disconnected with each component, a star on 2 or more vertices. Hence G is edge maximal 2-self centered graph with $m = \frac{n^2-2n-1}{2}$.

A 2-self-centered graph G is said to be *edge-minimal* if for each $e \in E(G)$, $G \setminus e$ is not a 2-self-centered graph.

Theorem 2.9: Let G be k-nested 2-self-centered graph on n vertices and m edges with $3 \leq k \leq n-1$. Then G is not edge minimal.

Proof: From Theorem 2.6, G will have minimum number of edges when $k = 3$ and $m = 2n-3$. If we remove any one edge between two dominating vertices, still G is 2-self-centered. Hence G is not 2-self-centered edge minimal graph. ■

Note 2.4: Let G be a 3-nested 2-self centered graph with n vertices and $2n-3$ edges. If we remove any one edge between any two of the dominating vertices, we get a 2-self centered graph with $2n-4$ edges. All the non dominating vertices are of degree 2. From the 3 dominating vertices remove one more edge. Let the dominating vertex from which both the edges to other 2 dominating vertices removed be v. Now $d(v, x) = 3$, when v and x belongs to same partite set. Hence G is edge minimal 2-self-centered graph, if we remove only one edge between any two of the 3 dominating vertices of a 3-nested graph.

Remark 2.1: From Note 2.4, we can show the existence of a 2-self centered edge minimal graph on $2n-4$ edges. It is possible to construct a 2-self centered edge minimal graph on m edges, where m is an even number with $m \geq 8$ and $n = \frac{m+4}{2}$. Consider a 3-nested graph on n vertices with $|V_i| \geq 2$. Then remove one edge between any two of the dominating vertices. The resulting graph is 2-self centered edge minimal graph with $2n-4$ edges.

Remark 2.2: Given an even number $m \geq 8$, there exists a 2-self-centered edge minimal graph on m edges and $n = \frac{m+4}{2}$ vertices. From a 3-nested 2-self centered graph on 8 vertices we can construct a 2-self centered edge minimal graph on 12 edges (Figure 3(a)). But for $n = 8$, there exists a 2-self centered edge minimal graph on 11 edges also as shown in Figure 3(b).

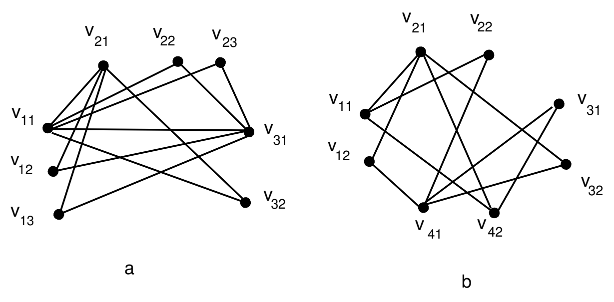


Fig. 3. 2-self-centered edge minimal graphs

III. Distance Based Topological Indices

The nature of inter-molecular interactions depends on the degree and distance parameters, moreover a number of physico-chemical properties of compounds [6] have been shown to correlate with topological properties as good starting points. Wiener index [7], which is a distance-based topological descriptor has been studied over the years since it is readily computed and it appears to correlate with many physico-chemical properties of organic compounds and has found to have applications in other fields also. For the other important and interesting results concerned with the Wiener index and other distance based topological indices, the readers are referred to [7]–[11]. In this section we obtain bounds and expressions for some distance based topological indices.

A. Wiener index

The Wiener index $W(G)$ of a graph G is the sum of all distances between all pairs of vertices in G.

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

Authors of the article [12] have given the expressions for Wiener and other indices of a chain graph. In this section, we give an expression as well as bounds for Wiener index of k-nested graphs.

Theorem 3.1: Let $G(\bigcup\limits_{i=1}^{k} V_i, E)$ be a k-nested graph ($k \geqslant 3$) on n vertices and m edges, where $|V_i| = p_i$. Then

$$W(G) = 2\left(\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i,j=1,\ i<j}^{k} p_i p_j\right) - m.$$

Proof: Since each of the partite set have at least one dominating vertices, without loss of generality, let $v_{i1} \in V_i$, $1 \leqslant i \leqslant k$, be the dominating vertices.
We note that any two vertices which are in the same partite set are at a distance two, due to the existence of the dominating vertices in other partite sets. For the vertex $v_{il} \in V_i$, all the vertices $v_{jm} \in V_j$ which are not adjacent to v_{il} are also at distance two, due to the shortest path $(v_{il} \sim v_{z1} \sim v_{jm})$, $1 \leqslant l \leqslant p_i$, $1 \leqslant m \leqslant p_j$, $1 \leqslant i, j, z \leqslant k$, $i \neq j \neq z$.
Thus for any two vertices $v_{il}, v_{jm} \in V(G)$,
$d(v_{il}, v_{jm}) =$

$$\begin{cases} 1, & \text{if } v_{il}, v_{jm} \text{ belong to the different partite set and} \\ & v_{il} \sim v_{jm} \\ 2, & \text{if } v_{il}, v_{jm} \text{ belong to the same partite set and when} \\ & v_{il}, v_{jm} \text{ belong to the different partite sets and} \\ & v_{il} \nsim v_{jm}. \end{cases}$$

Since there are m edges, there are m pairs of vertices having distance one between them. We know that, a k-partite graph $G(\bigcup\limits_{i=1}^{k} V_i, E)$ has at most $\sum_{i<j} p_i p_j$ edges where ($p_i = |V_i|$ and $p_j = |V_j|$). Thus there are $\sum_{i<j}(p_i p_j) - m$ pairs of vertices (v_{il}, v_{jm}), such that $v_{il} \in V_i, v_{jm} \in V_j, i \neq j$ and $v_{il} \nsim v_{jm}$. Hence the number of pairs of vertices which are at a distance two between them is

$$\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i=1,i<j}^{k} p_i p_j - m.$$

Therefore the Wiener index of G is given by,

$$\begin{aligned} W(G) &= 2\left[\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i,j=1,i<j}^{k} p_i p_j - m\right] + m \\ &= 2\left(\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i,j=1,i<j}^{k} p_i p_j\right) - m. \end{aligned}$$

■

Analogous to half graph we define k-half graph as follows.

Definition 3.1: A k-half graph on kn vertices is defined as $KNG(\underbrace{1,1,\ldots,1}_{\text{n times}};\underbrace{1,1,\ldots,1}_{\text{n times}};\ldots;\underbrace{1,1,\ldots,1}_{\text{n times}})$.

A half graph of order $2n$ has $\dfrac{n(n+1)}{2}$ edges [3]. The number of edges in a k-half graph of order kn is given by $\binom{k}{2}\left(\dfrac{n(n+1)}{2}\right)$. Figure 4 represents a 4-half graph with 12 vertices and 36 edges.

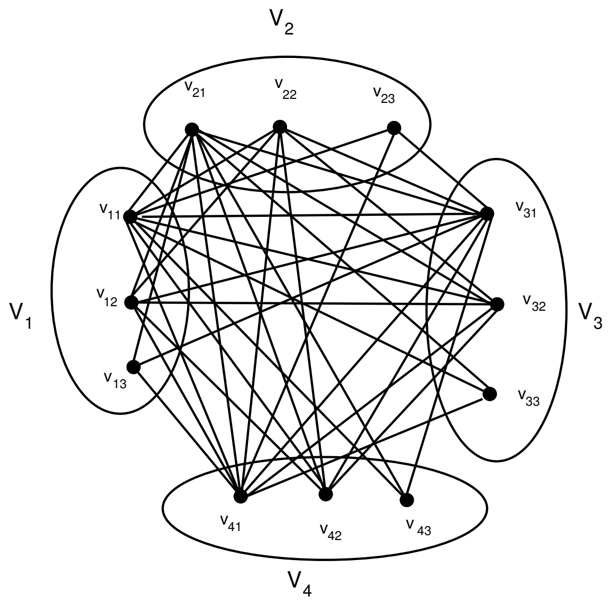


Fig. 4. 4-Half Graph on 12 vertices

Theorem 3.2: Let $G(\bigcup\limits_{i=1}^{k} V_i, E)$ be a k-half graph of order kn. Then,

$$W(G) = \frac{kn}{4}\left(3kn - k + n - 3\right).$$

Proof: By Theorem 3.1 we have, $W(G) = 2\sum_{i=1}^{k}\binom{p_i}{2} + 2\sum_{i<j} p_i p_j - m$. We know that in a k-half graph, all the partite sets have equal cardinalities $i.e$, $p_i = n, \forall\ 1 \leqslant i \leqslant k$ and the size of k-half graph is, $\binom{k}{2}\left(\dfrac{n(n+1)}{2}\right)$. Then

$$\begin{aligned} W(G) &= 2\sum_{i=1}^{k}\binom{n}{2} + 2\sum_{i<j} n.n - \binom{k}{2}\left(\frac{n(n+1)}{2}\right) \\ &= \frac{kn}{4}[3kn - k + n - 3]. \end{aligned}$$

■

Theorem 3.3: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on n vertices with $|V_i| = p_i, 1 \leqslant i \leqslant k$. Then,

$$2\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i,j=1,i<j}^{k} p_ip_j \leqslant W(G) \leqslant 2\sum_{i=1}^{k}\binom{p_i}{2} +2\sum_{i,j=1,i<j}^{k}(p_i-1)(p_j-1)+\frac{(k-1)(2n-k)}{2}.$$

Proof: Let $v_{ij} \in V_i,\ 1 \leqslant i \leqslant k,\ 1 \leqslant j \leqslant p_i$ be the vertices of G. We note that for any two vertices $v_{il}, v_{jm} \in V(G)$, $d(v_{il}, v_{jm}) \in \{1,2\}$. For a k-nested graph G, there is at least $\sum_{i=1}^{k}\binom{p_i}{2}$ pairs of vertices having distance two between them. In order to have a minimum Wiener index, the number of pairs of vertices, having distance two between them is as minimum as possible. In other words number of pairs of vertices (v_{il}, v_{jm}), where $v_{il} \in V_i, v_{jm} \in V_j, i \neq j$, which are adjacent to each other is as maximum as possible. Thus G has a minimum Wiener index, when every vertex of V_i is adjacent to every vertex of $V_j, (i \neq j)$, (which results in zero pairs of vertices having distance two between the partite sets) and the resulting graph is $K_{p_1,p_2\ldots,p_k}$. It is noted that

$$W(K_{p_1,p_2,\ldots,p_k}) = 2\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i<j} p_ip_j.$$

This implies $W(G) \geqslant 2\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i,j=1,i<j}^{k} p_ip_j$, $1 \leqslant i,j \leqslant k$.
In order to have maximum Wiener index, in addition to $\sum_{i=1}^{k}\binom{p_i}{2}$ pairs of vertices having distance two between them, we must have maximum pairs of vertices between the partite sets having distance two between them. In other words the number of pairs of vertices (v_{il}, v_{jm}) with $v_{il} \in V_i, v_{jm} \in V_j$ and $v_{il} \nsim v_{jm}$ is as maximum as possible. But in any k-nested graph, there is at least one dominating vertex in each of the partite sets, say $v_{i1} \in V_i, \forall 1 \leqslant i \leqslant k$.
Apart from this in order that $W(G)$ is maximum, if all the vertices $v_{il}, v_{jm} (l,m \neq 1)$ are adjacent to minimum number of vertices. The graph G' where $N_G(v_{i1}) = \bigcup_{j\neq i} V_j$, $N_G(v_{il}) = \{v_{j1} | 1 \leqslant j \leqslant k; j \neq i\}$, for all vertices $v_{il} \in V_i, (l \neq 1)$ is the graph with maximum number of pairs of vertices having distance two between the partite sets. The graph G' has $\frac{(k-1)}{2}\left[2\sum_{i=1}^{k} p_i - k\right] = \frac{(k-1)(2n-k)}{2}$ pairs of vertices at a distance one and $\sum_{i,j=1,i<j}^{k}(p_i-1)(p_j-1)$ pairs of vertices which are at a distance two between the partite sets.

$W(G') = 2\left[\sum_{i=1}^{k}\binom{p_i}{2} + \sum_{i,j=1,i<j}^{k}(p_i-1)(p_j-1)\right] + \frac{(k-1)(2n-k)}{2}$.

This implies,

$W(G) \leqslant 2\sum_{i=1}^{k}\binom{p_i}{2} + 2\sum_{i,j=1,i<j}^{k}[(p_i-1)(p_j-1)] + \frac{(k-1)(2n-k)}{2}$. ■

Theorem 3.4: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on kn vertices. Let $v_{i1} \in V_i$, $1 \leqslant i \leqslant k$, be the dominating vertices. Then,

$$\frac{kn}{2}(kn+n-2) \leqslant W(G) \leqslant (kn-k+1)(kn-1)+\binom{k-1}{2}.$$

Proof: Let $|V_i| = p_i, 1 \leqslant i \leqslant k$, such that $\sum_{i=1}^{k} p_i = kn$. The only k-nested graph when $p_j = kn-k+1$ and $p_i = 1, \forall i \neq j$, (say $j=1$) is the graph $G = K_{kn-k+1,1,\ldots,1}$, Therefore,

$$\begin{aligned} W(G) &= 2\binom{p_1}{2} + \left(p_1(k-1) + \binom{k-1}{2}\right) \\ &= p_1(p_1+k-2) + \binom{k-1}{2} \\ &= (kn-k+1)(kn-1) + \binom{k-1}{2}. \end{aligned}$$

By Lemma 2.2, the Wiener index of G is same as that of the Wiener index of minimal k-nested graph on kn vertices and this is the upper bound for the Wiener index of k-nested graph on kn vertices.
The complete k-partite graph on kn vertices with $|V_i| = p_i = n,\ 1 \leqslant i \leqslant k$, is a k-nested graph on kn vertices with maximum number of edges. Hence the Wiener index of the above graph is given by,

$$W(K_{n,n,\ldots,n}) = 2\left[k\binom{n}{2}\right] + \binom{k}{2}n^2$$

and hence

$$W(G) \geqslant \frac{kn}{2}(kn+n-2).$$

■

Theorem 3.5: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on $kn+b$ vertices, $1 \leqslant b \leqslant k-1$. Then,

$$bn(k+1) + \tfrac{kn}{2}(kn+n-2) + \tbinom{b}{2} \leqslant W(G) \leqslant (kn+b-k+1)(kn+b-1) + \tbinom{k-1}{2}.$$

Proof: Let $|V_i| = p_i,\ 1 \leqslant i \leqslant k$, such that $\sum_{i=1}^{k} p_i = kn+b$. The only k-nested graph when $p_j = kn+b-k+1, p_i = 1, \forall i \neq j$ (say j=1), is the graph $G = K_{kn+b-k+1,1,1,\ldots,1}$.
Then,

$$\begin{aligned} W(G) &= 2\binom{p_1}{2} + \left[p_1(k-1) + \binom{k-1}{2}\right] \\ &= p_1(p_1+k-2) + \binom{k-1}{2} \\ &= (kn+b-k+1)(kn+b-1) + \binom{k-1}{2}. \end{aligned}$$

The Wiener index of G is same as that of the Wiener index of a minimal k-nested graph on $kn+b$ vertices. This will be the upper bound for the Wiener index of the k-nested graph on $kn+b$ vertices.
The complete graph on $kn+b$ vertices with $|V_i| = p_i = n+1, 1 \leqslant i \leqslant b$ and $|V_j| = p_j = n, b < j \leqslant k$ is a k-nested graph on $kn+b$ vertices with maximum number of edges. Hence the Wiener index of $G = K_{\underbrace{n+1,\ldots,n+1}_{b \text{ times}},\underbrace{n,\ldots,n}_{k-b \text{ times}}}$ is given by,

$W(G) = 2\left[b\binom{n+1}{2} + (k-b)\binom{n}{2}\right] +$

$\left[\binom{k}{2}n^2 + \binom{b}{2} + b(k-1)n\right]$
$W(G) = bn(k+1) + \binom{kn}{2}(kn+n-2) + \binom{b}{2}$.
This implies

$$W(G) \geqslant bn(k+1) + \binom{kn}{2}(kn+n-2) + \binom{b}{2}.$$

■

The average path length is the sum of path lengths $d(u,v)$ between all pair of nodes (assuming that length is zero if u is not reachable from v), normalized by $n(n-1)$, where n is number of nodes in G.

The average path length, $A_v(G) = \dfrac{\sum\limits_{\{u,v\}\in V(G)} d(u,v)}{\binom{n}{2}}$.

The bound for average path length of k-nested graphs which is given in the following corollary follows from the Theorems 3.4 and 3.5.

Corollary 3.6: Consider a k-nested graph $G(\bigcup\limits_{i=1}^{k} V_i, E)$, with average path length $A_v(G)$. If G has kn vertices, then $\frac{kn+n-2}{kn-1} \leqslant A_v(G) \leqslant 2\left[\frac{(kn-k+1)(kn-1)}{kn(kn-1)}\right] + \frac{(k-1)(k-2)}{kn(kn-1)}$.

If G has $kn+b$ vertices, then
$\frac{2bn(k+1)+kn(kn+n-2)+(b-1)(b-2)}{(kn+b)(kn+b-1)} \leqslant A_v(G) \leqslant \left[\frac{2(kn+b-k+1)(kn+b-1)+(k-1)(k-2)}{(kn+b)(kn+b-1)}\right]$.

B. Szeged Indices

In this section we give expressions for various Szeged indices of G, when G is either a minimal or a maximal k-nested graph.

1) Vertex-Szeged: The vertex-Szeged index (or simply Szeged index) of the graph G is given by

$$S_{Z_v}(G) = \sum_{e=uv\in E(G)} n_u(e|G).n_v(e|G),$$

where $n_u(e|G)$ is the number of vertices which are closer to the vertex u than v in the graph G and $n_v(e|G)$ is the number of vertices which are closer to the vertex v than u in G.

Theorem 3.7: Let $G(\bigcup\limits_{i=1}^{k} V_i, E)$ be a minimal k-nested graph on n vertices with $|V_i| = p_i$. Then the vertex-Szeged index of G is given by,

$$S_{Z_v}(G) = \sum_{i\leq j} p_i p_j + \sum_{i=1}^{k}(n-p_i-k+1)(n-p_i-k+2)$$

Proof: The edges of a minimal k-nested graph can be considered as follows.
Case 1: Let $e = uv$ be an edge between the dominating vertex u of V_i and dominating vertex v of V_j.

Then $n_u(e|G) = p_j$ (i.e., the vertex u and $p_j - 1$ vertices of V_j other than v), and $n_v(e|G) = p_i$. Therefore, $n_v(e|G).n_u(e|G) = p_i p_j$.

Case 2: Let $e = uv$ be an edge between the dominating vertex u of V_i and a non-dominating vertex v of V_j.

We note that there are $p_i - 1$ vertices of V_i which are at distance two from both u and v and $k-2$ vertices which are at distance one from both u and v. Hence, $n_u(e|G) = n-(p_i-1)-(k-2)-1 = n-p_i-k+2$ and $n_v(e|G) = 1$ (i.e., only vertex v is closer to v than u in the graph G). Therefore, $n_v(e|G).n_u(e|G) = n-p_i-k+2$ and there are exactly $n-p_i-k+1$ edges of this type which are connected to the vertex u in the graph G. Hence, the result follows. ■

Theorem 3.8: Let $G(\bigcup\limits_{i=1}^{k} V_i, E)$ be a maximal k-nested graph on n vertices with $|V_i| = p_i$. Then the vertex-Szeged index is given by,

$$S_{Z_v}(G) = \sum_{i\leq j}(p_i p_j)^2.$$

Proof: In a maximal k-nested graph all the vertices of the graph can be considered as a dominating vertex with respect to other partite sets. Let $e = uv$ be an edge between a vertex u of V_i and a vertex v of V_j. Then $n_u(e|G) = p_j$, and $n_v(e|G) = p_i$ and hence $n_v(e|G).n_u(e|G) = p_i p_j$. There are $p_i p_j$ number of edges between V_i and V_j (all the edges are of same type). Hence the result follows. ■

2) Edge-Szeged : The edge-Szeged index of the graph G is given by,

$$S_{Z_e}(G) = \sum_{e=uv\in E(G)} m_u(e|G).m_v(e|G).$$

The term $m_u(e|G)$ for the edge $e = uv$ of G gives the number of edges which are closer to the vertex u than v. The distance between an edge $e = uv$ and a vertex x of G is given by the $min\{d(u,x), d(v,x)\}$.

Theorem 3.9: Let $G(\bigcup\limits_{i=1}^{k} V_i, E)$ be a minimal k-nested graph on n vertices with $|V_i| = p_i$. Then the edge-Szeged index of G is given by,

$$S_{Z_e}(G) = \sum_{i\leq j}(n-p_i-1)(n-p_j-1) + \sum_{i=1}^{k}(n-p_i-k+1)[(2n-2p_i-k-1)(k-2)].$$

Proof: The edges of a minimal k-nested graph can be considered as follows.

Case 1: Let $e = uv$ be an edge between the dominating vertex u of V_i and dominating vertex v of V_j.

Then, $deg(u) = n-p_i$ and all of these edges excluding an edge connecting to the vertex v are closer to the vertex u than v. Hence, $m_u(e|G) = n-p_i-1$ and similarly, $m_v(e|G) = n-p_j-1$. Therefore, $m_u(e|G)m_v(e|G) = (n-p_i-1)(n-p_j-1)$.

Case 2: Let $e = uv$ be an edge between the dominating vertex u of V_i and a non-dominating vertex v of V_j.

We know $deg(u) = n-p_i$ and all of these edges excluding an edge connecting to the vertex v are closer to the vertex u than v (i.e. $n-p_i-1$). The edges that are incident to the dominating vertex w of V_j excluding the edges that are connecting the dominating vertices in the other partite set are at a distance one from u and two from v. This is equal to $(n-p_i-1)-(k-1) = n-p_i-k$. Hence, $m_u(e|G) = n-p_i-1+n-p_i-k = 2n-2p_i-k-1$. Since the degree of the vertex v is $k-1$, all these edges except $e = uv$ are at a distance zero from v and one from u. Hence, $m_v(e|G) = k-2$. Therefore, $m_u(e|G)m_v(e|G) = (2n-2p_i-k-1)(k-2)$ and there are $(n-p_i-k+1)$ edges of this type which are connected to the vertex u in the graph G. Hence the result follows. ■

Theorem 3.10: Let $G(\bigcup\limits_{i=1}^{k} V_i, E)$ be a maximal k-nested graph on n vertices with $|V_i| = p_i$. Then edge-Szeged index of G is given by,

$$S_{Z_e}(G) = \sum_{i \leq j} (p_i p_j)(n - p_i - 1)(n - p_j - 1).$$

Proof: Let $e = uv$ be an edge between a vertex u of V_i and a vertex v of V_j. Then the number of edges which are closer to the vertex u than v is $deg(u) - 1 = n - p_i - 1$. Similarly, the number of edges which are closer to the vertex v than u is $deg(v) - 1 = n - p_j - 1$. Hence, $m_u(e|G)m_v(e|G) = (n - p_i - 1)(n - p_j - 1)$. In total there are $p_i p_j$ number of edges between V_i and V_j. Hence we get the expression for $S_{Z_e}(G)$. ■

3) Edge-Vertex-Szeged: The edge-vertex-Szeged index of the graph G is given by, $S_{Z_{ev}}(G) = \frac{1}{2} \sum_{e=uv \in E(G)} [n_u(e|G).m_v(e|G) + n_v(e|G).m_u(e|G)]$.

Theorem 3.11: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a minimal k-nested graph on n vertices with $|V_i| = p_i$. Then the edge-vertex-Szeged index of G is given by,

$$S_{Z_{ev}}(G) = \frac{1}{2}\left[\sum_{i<j} [p_j(n - p_i - 1) + p_j(n - p_i - 1)]\right] + \frac{1}{2}\sum_{i=1}^{k}(n-p_i-k+1)[(n-p_i-k+2)(k-2)+(2n-2p_i-k-1)].$$

Theorem 3.12: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a maximal k-nested graph on n vertices, with $|V_i| = p_i$. Then the edge-vertex-Szeged index of the graph G is given by,

$$S_{Z_{ev}}(G) = \frac{1}{2}\left[\sum_{i<j} p_i p_j [p_j(n - p_i - 1) + p_i(n - p_j - 1)]\right].$$

4) Total-Szeged: The total-Szeged index of the graph G is given by,

$$S_{zt}(G) = S_{Z_v}(G) + S_{Z_e}(G) + 2S_{Z_{ev}}(G).$$

Theorem 3.13: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a minimal k-nested graph on n vertices with $|V_i| = p_i$. Then the total-Szeged index of G is given by,

$$S_{zt}(G) = \sum_{i<j}[p_i p_j + (n-p_i-1)(n-p_j-1)+p_j(n-p_i-1)+p_i(n-p_j-1)]+\sum_{i=1}^{k}(n-p_i-k+1)[(n-p_i-k+2)+(2n-2p_i-k-1)(k-2)+(n-p_i-k+2)(k-2)+(2n-2p_i-k-1)].$$

Theorem 3.14: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a maximal k-nested graph on n vertices with $|V_i| = p_i$. Then,
$S_{zt}(G) = \sum_{i<j} p_i p_j [p_i p_j + (n-p_i-1)(n-p_j-1)+p_j(n-p_i-1) + p_i(n - p_j - 1)]$.

IV. Degree based Topological Indices

In this section we give bounds for various degree based topological indices of a k-nested graph.

1) The first and second Zagreb index: The first and second Zagreb index is defined as

$$M_1(G) = \sum_{u \sim v} [deg(u)]^2$$

and

$$M_2(G) = \sum_{u \sim v} deg(u)deg(v)$$

respectively.

Theorem 4.1: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on n vertices with $|V_i| = p_i, 1 \leqslant i \leqslant k$. Then

$$\left[\sum_{i=1}(n - p_i)^2 + (n - k)(k - 1)^2\right] \leqslant M_1(G) \leqslant \left[\sum_{i=1}^{k} p_i(n - p_i)^2\right]$$

and

$$\sum_{i,j=1,i<j}^{k} (n - p_i)(n - p_j + \sum_{i,j=1,i<j}^{k} (n - p_i)(p_j - 1)(k - 1) \leqslant M_2(G) \leqslant \sum_{i,j=1,i<j}^{k} [p_i(n - p_i)][p_j(n - p_j)].$$

Proof: By the definition of the Zagreb index, it is minimum when every vertex of k-nested graph has minimum possible degree. Let G_1 denote the minimal k-nested graph. Since every partite set of G has at least one full degree vertex, every vertex of G has minimum degree when $G = G_1$.

$$M_1(G_1) = \sum_{i=1}^{k}(n - p_i)^2 + (k - 1)^2(n - k).$$

This implies

$$M_1(G) \geqslant \sum_{i=1}^{k}(n - p_i)^2 + (n - k)(k - 1)^2.$$

Similarly $M_1(G)$ is maximum when every vertex of G is of full degree i.e., $M_1(G)$ has maximum value when G is complete k-partite graph, $K_{p_1,p_2,...p_k}$, (call G_2). Then,

$$M_1(G_2) = \sum_{i=1}^{k} p_i(n - p_i)^2.$$

Therefore,

$$M_1(G) \leqslant \sum_{i=1}^{k} p_i(n - p_i)^2.$$

Hence we have the first part of the theorem.
In the similar way, the second Zagreb index $M_2(G)$ attains maximum when $G = K_{p_1,p_2,...,p_k}$ and minimum when $G = G_1$ is the minimal k-nested graph. It can be evaluated as,

$$M_2(K_{p_1,p_2,...,p_k}) = \sum_{i=1}^{k-1} \sum_{j=2,i<j}^{k} (n - p_i)(n - p_j)(p_i p_j).$$

This implies

$$M_2(G) \leqslant \sum_{i,j=1,i<j}^{k} [p_i(n - p_i)][p_j(n - p_j)].$$

Also,
$M_2(G_1) = \sum_{i,j=1,i<j}^{k}(n-p_i)(n-p_j)+\sum_{i,j=1,i<j}^{k}(n-p_i)(p_j-1)(k - 1)$.

This implies,
$M_2(G) \geqslant \sum_{i,j=1,i<j}^{k} (n-p_i)(n-p_j) + \sum_{i,j=1,i<j}^{k} (n-p_i)(p_j-1)(k-1)$. ■

2) Multiplicative Zagreb Indices: The first and second multiplicative Zagreb indices are given by

$$\Pi_1(G) = \prod_{u \in V(G)} [deg(u)]^2,$$

and

$$\Pi_2(G) = \prod_{u \sim v} deg(u)deg(v).$$

The lower bound and upper bound for the multiplicative Zagreb indices of a k-nested graph is attained by a minimal k-nested graph and a maximal k-nested graph respectively which is given in the following theorems.

Theorem 4.2: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on n vertices and $|V_i| = p_i, 1 \leqslant i \leqslant k$. Then
$(k-1)^{2(n-k)} \left(\prod_{i=1}^{k} (n-p_i)^2 \right) \leqslant \Pi_1(G) \leqslant \prod_{i=1}^{k} (n-p_i)^{2p_i}$,
and

$$\left[\prod_{i,j=1,i<j}^{k} (n-p_i)(n-p_j) \right] \left[\prod_{i=1}^{k} [(n-p_i)(k-1)]^{n-p_i-k+1} \right] \leqslant \Pi_2(G) \leqslant \prod_{i,j=1,i<j}^{k} [(n-p_i)(n-p_j)]^{p_i p_j}.$$

3) Generalized Multiplicative Zagreb Indices: The first and second generalized multiplicative Zagreb indices are given [13] by

$$MZ_1^a(G) = \prod_{u \sim v} [deg(u) + deg(v)]^a$$

and

$$MZ_2^a(G) = \prod_{u \sim v} [deg(u)deg(v)]^a.$$

Theorem 4.3: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on n verices with $|V_i| = p_i, 1 \leqslant i \leqslant k$. Then,

$$\left[\prod_{i<j} [(n-p_i)+(n-p_j)]^a \left[\prod_{i=1}^{k} (n-p_i+k-1)^{ap_i} \right] \right. \leqslant MZ_1^a(G)) \leqslant \prod_{i=1}^{k} (n-p_i+n-p_j)^{ap_i p_j}$$

and

$$\left[\prod_{i<j} [(n-p_i)(n-p_j)]^a \left[\prod_{i=1}^{k} [(n-P_i)(k-1)]^{ap_i} \right] \right. \leqslant MZ_2^a(G) \leqslant \prod_{i<j} [(n-p_i)(n-p_j)]^{ap_i p_j}.$$

Note 4.1: Substituting $a = 2$ in $MZ_1^a(G)$ and $MZ_2^a(G)$ we get the first and second Hyper-Zagreb indices $HM_1(G) = \prod_{u \sim v} [deg(u) + deg(v)]^2$ and $HM_2(G) = \prod_{u \sim v} [deg(u)deg(v)]^2$ defined in [14].

Note 4.2: Substituting $a = 1$ in $MZ_1^a(G)$ we get multiplicative version of Zagreb index which is also denoted by $\Pi_1^*(G)$ and defined by M. Eliasi et. al. [15]

4) Augmented Zagreb Index: The augmented Zagreb index of the graph G is given [16] by

$$AZI(G) = \sum_{u \sim v} \left[\frac{d_u d_v}{d_u + d_v - 2} \right]^3.$$

Here we give an expression for augmented Zagreb index of minimal and maximal k-nested graph.

Theorem 4.4: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a minimal k-nested graph on n vertices with $|V_i| = p_i$. Then,
$AZI(G) = \sum_{i<j} \left[\frac{(n-p_i)(n-p_j)}{(2n-p_i-p_j-2)} \right]^3 + \sum_{i=1}^{k} (n-p_i-k+1) \left[\frac{(n-p_i)(k-1)}{(n-p_i+k-3)} \right]^3$.

Theorem 4.5: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a maximal k-nested graph on n vertices with $|V_i| = p_i$. Then,
$AZI(G) = \sum_{i<j} p_i p_j \left[\frac{(n-p_i)(n-p_j)}{(n-p_i)+(n-p_j)-2} \right]^3 = \sum_{i<j} p_i p_j \left[\frac{(n-p_i)(n-p_j)}{(2n-p_i-p_j-2)} \right]^3$.

5) Sombor index: The Sombor index for the graph G is given by, $S(G) = \sum_{u \sim v} \sqrt{[deg(u)]^2 + [deg(v)]^2}$.
The bounds for the Sombor index of a k-nested graph is given below.

Theorem 4.6: Let $G(\bigcup_{i=1}^{k} V_i, E)$ be a k-nested graph on n vertices with $|V_i| = p_i, 1 \leqslant i \leqslant k$. Then,

$$\sum_{i<j} \sqrt{(n-p_i)^2 + (n-p_j)^2} + \sum_{i=1}^{n} (n-p_i-k+1)\sqrt{(n-p_i)^2 + (k-1)^2} \leqslant S(G) \leqslant \sum_{i<j} p_i p_j \sqrt{(n-p_i)^2 + (n-p_j)^2}.$$

V. Concluding Remarks

Wiener index $W(G)$ of a graph G is a concept of primary significance in the field of chemical graph theory due to the correlation between $W(G)$ and physio-chemical properties of the paraffins i.e., hydrocarbons where G is taken to be the molecular graph of the corresponding chemical compound. The properties of a newly defined class of graphs namely, k-nested graphs is studied. We give the bounds for Wiener index and Szeged indices of k-nested graphs. We have also given the expressions for some degree based topological indices of k-nested graphs. An algorithm that returns a k-nested graph on n vertices (if exists) for a given Wiener index W could be a goal for future work on k-nested graphs. We know that a 2-nested graphs are recognized to be $(2K_2, C_5, C_3)-$ free graphs. Similar to 2-nested graphs, one can try to get the forbidden structure of a k-nested graphs.

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