Inverse Harary Index Problem for Chain Graphs

Shahistha Hanif

Abstract—**A chain graph is a bigraph where the neighborhood of vertices in each part forms a chain under set inclusion. Chain graphs have received considerable attention from researchers in the field of spectral graph theory, as they have the maximum spectral radius among all the bigraphs of prescribed size and order. Nevertheless, the areas of some graph parameters remain untouched. The reciprocal Wiener index or the Harary index is one of the distance-based topological indices among several graph parameters designed to capture the different aspects of molecular structure. This article explores the Harary index of chain graphs, giving the bounds and other properties. Further, the Harary index of threshold graphs, a slight structural variant of chain graphs is also discussed. The main focus is on chain graphs with integer-valued Harary index. The article presents a quadratic time algorithm for the inverse Harary index problem for chain graphs and hence contributes significantly to the theory of inverse problems on topological indices.**

Index Terms—**Chain, Bipartite graph, Bi-star graph, Complete bipartite graph.**

I. Introduction

Several distance and degree-based topological indices have been introduced by chemists to correlate the structure of chemical compounds with empirically acquired data on their physico-chemical properties. The Harary index, introduced by Plavsic et al. [17] and by Ivanciuc et al. [10] in 1993, is one among the variety of such indices that are designed to analyze the molecular structure. It has been named in honor of Professor Frank Harary on the occasion of his 70^{th} birthday due to his influence on the development of graph theory and its application in chemistry. The Harary index of a graph G is denoted by $H(G)$ and is defined as follows.

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)}$$

The summation goes over all unordered pairs of vertices of G, $V(G)$ represents the vertex set of graph G and $d(u,v)$ denotes the distance between the vertices u and v. A great deal of knowledge on Harary index is accumulated in the literature [[2], [4], [5], [11], and [18]].

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

A chain graph is a bipartite graph with the property that the neighborhood of vertices of each part forms a chain with respect to set inclusion. Each of the parts of 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 $N_G(u) = V_{2,1} \cup ... \cup V_{2,h-i+1}$, 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). Further results concerned with chain graphs are available in the literature [3], [6], [9], [13], [14], [19], [20], and [21].

A split graph is a graph which admits a partition of its vertex set into two parts, say W_1 and W_2 so that W_1 induces an independent set and W_2 induces a clique. All other cross edges, join a vertex in W_1 with a vertex in W_2([14]). A threshold graph is a split graph where the subsets of vertices W_1 and W_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 $u \in W_{1,i}$, $1 \le i \le h$, $N_G(u) = W_{2,1} \cup ... \cup W_{2,h-i+1}$. 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], [7], [8], [12], [15], and [16] for more results on threshold graphs. The schematic representation of both DNGs, as well as NSGs, are given in Figure 1.

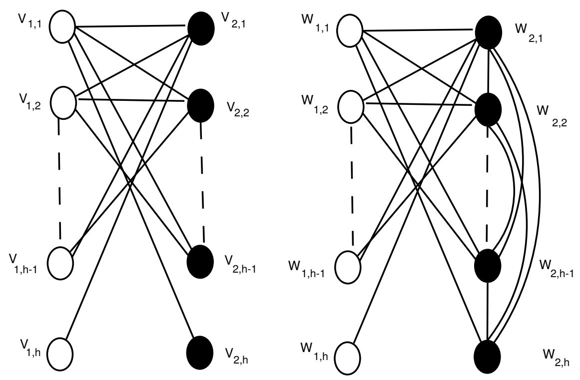

Fig. 1. Schematic diagram of chain and threshold graphs

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.

The outline of the remainder of this paper is as follows: In section 2, after the introduction, expressions and several bounds for Harary index of chain graphs are given. In the third section, further properties of Harary index of chain graphs are discussed. Using the results of section 3, an algorithm for the inverse Harary index problem is designed in section 4 limiting the domain only to chain graphs.

II. Harary index

In this section, we give an expression and bounds for Harary index of chain graphs. Some of the structural aspects

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of chain and threshold graphs, which are required to prove the key results of this article are listed below.

For any connected chain graph $G(V_1 \cup V_2, E)$, the following are true:

Remark 2.1: Each of V_i has at least one dominating vertex, which is adjacent with all the vertices of V_j $(i \neq j)$ $(i, j = 1, 2)$

Remark 2.2: Every connected chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = p$ and $|V_2| = q$ can be obtained from the bi-star graph $B(p; q)$ by successively adding edges, the procedure of which is given in [13]. Equivalently, every chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = p$ and $|V_2| = q$ can be obtained from the complete bipartite graph $K_{p,q}$ by successively deleting edges.

Remark 2.3: By the procedure given in [13], it is true that there exists at least one chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = p, |V_2| = q$ on $p + q$ vertices having m edges, for every $m \in [p + q - 1, pq]$. The bi-star graph $B(p, q)$ and the complete bipartite graph $K_{p,q}$ attain the lower and the upper bounds, respectively.

Similarly, if G is a threshold graph with split partition W_1, W_2, with W_1, W_2 inducing an independent set and a clique, respectively, then

Remark 2.4: The set W_2 has at least one vertex adjacent with every other vertices in the graph.

Remark 2.5: The set W_1 has at least one vertex which is adjacent with all the vertices of W_2.

The next theorem gives the expression for Harary index.

Theorem 2.1: Let $G(V_1 \cup V_2, E)$ be a chain graph of size m where $|V_1| = p, |V_2| = q$ $(p, q > 1)$ such that $p + q = n$. Then the Harary index $H(G)$ of G is given by

$$H(G) = \frac{3n^2 - 3n - 2pq + 8m}{12}.$$

Proof: Since each of the parts has at least one dominating vertex, let $u_1 \in V_1, v_1 \in V_2$ be the dominating vertices (without loss of generality,). Any two vertices that are in the same part are at a distance of two due to the existence of a dominating vertex in the other part. Between any non dominating vertex $v_i \in V_1$ and a vertex $u_j \in V_2$ with $u_j \nsim v_i$, there exists a shortest path $(v_i - u_1 - v_1 - u_j)$. Thus for any two vertices $u_i, v_j \in V(G)$,

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

The graph G has $\binom{p}{2} + \binom{q}{2}$ pairs of vertices having distance two between them(since $p, q > 1$). Since there are m edges, the rest of $(pq - m)$ pairs have distance three between them. Thus

$$\begin{aligned} H(G) &= \frac{1}{2}\binom{p}{2} + \frac{1}{2}\binom{q}{2} + m + \frac{1}{3}(pq - m) \\ &= \frac{3\left(p^2 + q^2\right) - 3(p + q) + 4pq + 8m}{12} \\ &= \frac{3n^2 - 3n - 2pq + 8m}{12}. \end{aligned}$$

$\blacksquare$

When both $p = q = 1$, $G = K_2$ and $H(G) = 1$. When either of p, q is 1, then $G = K_{1,n-1}$ and $H(G) = \frac{(n-1)(n+2)}{4}$.

The chain graph $G = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ with each of $m_i = n_i = 1$ for $1 \leq i \leq h$ is known as half graphs. The Harary index of a half graph is given below.

Corollary 2.2: Let G be a half graph given by $G = DNG(\underbrace{h\ times}1, 1, \ldots, 1; \underbrace{h\ times}1, 1, \ldots, 1)$ on n vertices and m edges. Then the Harary index of G is

$$H(G) = \frac{13n^2 + 2n}{24}$$

Proof: The number of vertices and edges in G are $n = 2h$ and $m = \frac{h(h+1)}{2}$, respectively. Further, on substituting $p = q = h = \frac{n}{2}$, the corollary follows. $\blacksquare$

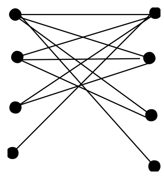

Fig. 2. The half graph $DNG(1, 1, 1, 1; 1, 1, 1, 1)$

From the expression for $H(G)$, one can note that the Harary index of a chain graph depends only on the number of vertices in both the parts and the number of edges. Further, the addition (deletion) of an edge increases $H(G)$ by $\frac{2}{3}$, irrespective of where the edges are added. Equivalently, the deletion of an edge decreases $H(G)$ by $\frac{2}{3}$, irrespective of which edges are deleted. The next theorems give lower and upper bounds for Harary index of chain graphs.

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

$$\frac{3n^2 + 5n - 2pq - 8}{12} \leq H(G) \leq \frac{n^2 - n + 2pq}{4}$$

Proof: From Theorem 2.1, a chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = p$ and $|V_2| = q$ has the maximum (minimum) Haray index when the number of edges m is maximum (minimum). A connected chain graph $G(V_1 \cup V_2, E)$ with $= |V_1| = p$ and $|V_2| = q$ has the minimum number of edges when it is a tree, that is a bi-star graph $B(p, q)$, where $m = p + q - 1$. Similarly, the number of edges is the maximum when $G = K(p, q)$, where $m = pq$. On substituting $m = p + q - 1$ and $m = pq$ in Theorem 2.1, the minimum and the maximum value of $H(G)$, respectively, are obtained. $\blacksquare$

Now, the values of p, q for which the Harary index $H(G)$ is optimum are investigated. In other words, the bounds for $H(G)$ in terms of a total number of vertices N (for even and odd separately) rather than the cardinalities of parts are obtained.

Theorem 2.4: Let $G(V_1 \cup V_2, E)$ be a chain graph on $N = 2n$ vertices. Then

$$\frac{5n^2 + 5n - 4}{6} \leq H(G) \leq \frac{3n^2 - n}{2}$$

Proof: Let $|V_1| = p, |V_2| = q$ such that $p + q = 2n$ and the bounds for $H(G)$ is given in the Theorem 2.3. Since $q = 2n - p$, the lower and the upper bounds, respectively are

$f(p) = \frac{12n^2+10n-4np+2p^2-8}{12}$ and $g(p) = \frac{4n^2-2n+4np-2p^2}{4}$. For given $2n$, the minima of the lower bound $f(p)$, maxima of the upper bound $g(p)$ are evaluated. It can be easily noted that $f(p)$ attains the minimum at the critical point $p = n$ and the minimum value is $\frac{5n^2+5n-4}{6}$. Similarly, the function $g(p)$ also attains the maxima at $p = n$ and the maximum value is $\frac{3n^2-n}{2}$. ■

The equalities in the above theorem are attained by the graphs $B(n,n)$(the lower bound) and $K_{n,n}$ (the upper bound). Similarly, the bounds when the number of vertices is odd are optimized.

Theorem 2.5: Let G be a chain graph on $N = 2n+1$ vertices. Then

$$\frac{5n^2+10n}{6} \leq H(G) \leq \frac{3n^2+2n}{2}.$$

Proof: The extreme values for both upper and lower bounds are attained at $p = n+1$ and $q = n$. ■

Similarly, the graphs $B(n+1,n)$ and $K_{n+1,n}$ attain the lower and upper bounds given in the above theorem, respectively. Any threshold graph can be obtained from a chain graph just by replacing either of the parts (independent set) with a clique. That is, a threshold graph $NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ can be obtained from an existing chain graph $G(V_1 \cup V_2, E) = DNG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ just by making V_2 complete. Hence, the distance between any two vertices is either one or two. The next theorem gives the Harary index of threshold graphs.

Theorem 2.6: Let G be a threshold graph with the split partition $\{W_1, W_2\}$, where W_1 induces an independent set of size p and W_2 a clique of size q such that $p+q = n$. Let m be the number of edges in G which connects the vertices of W_1 with W_2. Then the Harary index $H(G)$ of G is given by

$$H(G) = \frac{n^2-n+q^2-q+2m}{4}.$$

Proof: Without loss of generality, let $w_1 \in W_1$ be a vertex adjacent with every other vertices of W_2 and $w_2 \in W_2$ be the vertex adjacent with every other vertices in the entire graph. For any two vertices $w_i, w_j \in W_1 (i \neq j)$, there exists the shortest path $(w_i - w_2 - w_j)$. For $w_k \in W_1$, all the vertices $w_l \in W_2$ which are not adjacent to w_k have the shortest path $(w_k - w_2 - w_1)$. Thus for any two vertices $w_i, w_j \in V(G)$,

$$d(w_i, w_j) = \begin{cases} 1, & if\ w_i\ and\ w_j\ are\ adjacent \\ 2, & else \end{cases}.$$

The graph G has $\binom{q}{2} + m$ pairs of vertices having distance one between them. And the rest of $\binom{p}{2} + pq - m$ pairs of vertices have distance two between them. Thus

$$\begin{aligned} H(G) &= \frac{1}{2}\left(\binom{p}{2} + pq - m\right) + \binom{q}{2} + m \\ &= \frac{2q^2-2q+2m+p^2-p+2pq}{4} \\ &= \frac{n^2-n+q^2-q+2m}{4} \end{aligned}$$

■

Analogous to half graphs in the case of chain grphs, a special case of threshold graph $NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$ with each of $m_i = n_i = 1$ is considered in the next corollary.

Corollary 2.7: Let G be a theshold graph given by $G = NSG(\underbrace{h\ times}1, 1, \ldots, 1; \underbrace{h\ times}1, 1, \ldots, 1)$ on n vertices and m edges. Then the Harary index of G is

$$H(G) = \frac{3n^2-2n}{8}$$

Proof: Clearly, the number of vertices and edges in $G$is $n = 2h$. The number of edges are given by, $m = \frac{h(h+1)}{2} + \frac{h(h-1)}{2} = h^2$. But, among h^2 edges, only $\frac{h(h+1)}{2}$ edges connects the vertices of W_1 with the vertices of W_2. Further, on substituting $p = q = h = \frac{n}{2}$, the corollary follows. ■

The next theorem gives the relation between a chain graphs and a threshold graph.

Theorem 2.8: Let $G_1(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of size m where $|V_1| = p, |V_2| = q$ $(p, q > 1)$ such that $p+q = n$. Let $G_2 = NSG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a threshold graph ontained from G_1 by making V_2 complete. Given $H(G_1) = k_1$, then the Harary index of G_2 is given by

$$H(G_2) = \frac{12k_1+q^2-3q+2nq-2m}{12}$$

The proof of the above theorem follows directly from the Theorem 2.6 and Theorem 2.1.

Example 2.1: Consider the following graphs where $p = 5, q = 4$ and $m = 12$,

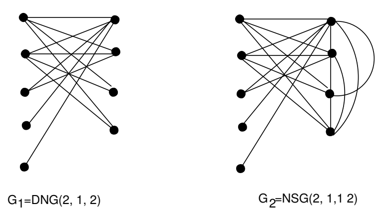

Fig. 3. Graphs G_1 and G_2 illustrating Theorem 2.8

The Harary indices are given by $H(G_1) = \frac{68}{3}$ and $H(G_2) = 27$.

III. Further results

In this section, further properties of Harary index are given. The main focus is on graphs with integral valued Harary indices.

Theorem 3.1: Let $G(V_1 \cup V_2, E)$ be a chain graph on $N = 4k-1$ vertices for some positive integer k. Then $H(G)$ is never an integer.

Proof: When the number of vertices $N = 4k-1$, by Theorem 2.1, $H(G) = \frac{24k^2-18k+3-pq+4m}{6}$, where $p = |V_1|$ and $q = |V_2|$. One can note that $\big(24k^2-18k+3-pq+4m\big) \not\equiv 0 (mod\, 6)$, that is $(3-pq+4m) \not\equiv 0(mod\, 6)$. Since $p+q = N = 4k-1$ is an odd integer, exactly one of p and q is odd. In either of the cases, the product pq is even. Further, since $4m$ is even, $(3-pq+4m)$, in turn $\big(24k^2-18k+3-pq+4m\big)$ is odd and hence not divisible by 6. ■

From Remark 2.2, it is noted that one can add edges successively and obtain any graph $G(V_1 \cup V_2, E)$ with $|V_1| = p$ and

$|V_2| = q$ from the bi-star $B(p,q)$. If $G_2(V_1 \cup V_2, E)$ is a chain graph obtained from an existing chain graph $G_1(V_1 \cup V_2, E^{'})$ by adding an edge, then $H(G_2) = H(G_1) + \frac{2}{3}$. Further, if $G_1(V_1 \cup V_2, E)$ has an integer Harary index, say $H(G_1) = n$ and $G_2(V_1 \cup V_2, E^{'})$ is a chain graph obtained from G_1 by adding three edges, then $H(G_2) = H(G_1) + 2$. That is, the addition (removal) of three edges increases(decreases) the Harary index by 2. Equivalently, the removal of three edges decreases the Harary index by 2.

Theorem 3.2: Let $N = 4k + 1$ for some positive integer k. Further, let $a = \frac{10(k^2+k)}{3}$ and $b = 2(3k^2 + k)$. Then for every integer $h \in [a, b]$, there exists at least one chain graph G on N vertices with $H(G) = h$.

Proof: Since $N = 4k + 1$ is odd, from Theorem 2.5, the Harary index $H(G)$ for any graph G is bounded as $a = \frac{10(k^2+k)}{3} \leq H(G) \leq b = 2(3k^2 + k)$. The lower and the upper bounds are attained by the bi-star graph $B(2k, 2k + 1)$ and the complete bipartite graph $K_{2k,2k+1}$, respectively. It is clear that $H(K_{2k,2k+1}) = b$ is an even integer. Also, any chain graph obtained from $K_{2k,2k+1}$ by removing three edges has the Harary index $b-2$. In general, any chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = 2k$, $|V_2| = 2k + 1$ obtained from $K_{2k,2k+1}$ by deleting $3n$ edges (for some positive integer n) has the Harary index $H(G) = b - 2n$, an even integer such that $b - 2n \geq a$. Further, by Remarks 2.2 and 2.3, every chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = 2k, |V_2| = 2k + 1$ can be obtained from the complete bipartite graph $K_{2k,2k+1}$ by successively deleting edges, but also the existence of at least one such graph having m edges is guaranteed, for every $m \in [4k, 4k(k + 1)]$. Thus for all even integers $h \in [a, b]$, there exists at least one chain graph G with $H(G) = h$.
Suppose the graph G has the $|V_1| = 2k - 1, |V_2| = 2k + 2$, then by Theorem 2.3, $a \leq \frac{10k^2+10k+1}{3} \leq H(G) \leq 6k^2 + 2k - 1 \leq b$. Let $a' = \frac{10k^2+10k+1}{3}$ and $b' = 6k^2 + 2k - 1$. The bounds a', b' are attained by the graphs $B(2k-1, 2k+2)$ and $K_{2k-1,2k+2}$, respectively. Every chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = 2k - 1, |V_2| = 2k + 2$ can be obtained from $K_{2k-1,2k+2}$ by successively deleting edges, and if $G(V_1 \cup V_2, E)$ is obtained by deleing $3n$ edges from $K_{2k-1,2k+2}$ (for some positive integer n), then $H(G) = b' - 2n$,an odd integer such that $b' - 2n \geq a'$. Since b' is odd, $a < a'$ and $b' < b$, it is clear that, for all odd integers $h \in [a, b]$, there exists at least one chain graph G with $H(G) = h$. ■

Theorem 3.3: Let $N = 4k$ for some positive integer k. Further, let $a = \frac{10k^2+5k-2}{3}$ and $b = 6k^2 - k$. If k is even, then for every even integer $h \in [a, b]$, there exists at least one chain graph G on N vertices such that $H(G) = h$. If k is odd, then for every odd integer $h \in [a, b]$, there exists at least one chain graph G on N vertices such that $H(G) = h$.

Proof: Since $N = 4k$ is even, from Theorem 2.4, the Harary index $H(G)$ for any graph G is bounded as $a = \frac{10k^2+5k-2}{3} \leq H(G) \leq b = 6k^2 - k$. The lower and the upper bounds are attained by the bi-star graph $B(2k, 2k)$ and the complete bipartite graph $K_{2k,2k}$, respectively. Clearly, the upper bound b is even or odd depending on k. Suppose k is even, then so is b. Every chain graph $G(V_1 \cup V_2, E)$ with $|V_1| = |V_2| = 2k$ can be obtained from $K_{2k,2k}$ by successively deleting edges, and if $G(V_1 \cup V_2, E)$ is obtained by deleing $3n$ edges (for some positive integer n), then $H(G) = b - 2n$, an even integer such that $b - 2n \geq a$. Thus for all even integers $h \in [a, b]$, there is at least one chain graph G with $H(G) = h$. The proof is similar when k is odd. ■

From the steps used in the above theorem, one can note that if k is even, then the upper bound b is also even. Thus, if there exists a chain graph G on $4k$ vertices with $H(G) = h$ for some integer $h \in [a, b]$, then h is even. Similarly, if k is odd and if there exists a graph G on $4k$ vertices with $H(G) = h$ for some integer $h \in [a, b]$, then h is also odd.

Corollary 3.4: Let $N = 4k$. If k is even, then there is no chain graph on N vertices with an odd Harary index. Similarly, if k is odd, then there is no chain graph on N vertices with even Harary index

Similarly, we have the next theorem and the corresponding corollary.

Theorem 3.5: Let $N = 4k + 2$ for some positive integer. Further, let k $a = \frac{10k^2+15k+3}{3}$ and $b = 6k^2 + 5k + 1$. If k is odd, then for every even integer $h \in [a, b]$, there exists at least one chain graph G on N vertices such that $H(G) = h$. If k is even, then for every odd integer $h \in [a, b]$, there exists at least one chain graph G on N vertices such that $H(G) = h$.

Corollary 3.6: Let $N = 4k + 2$. If k is even, then there exists no chain graph on N vertices with an even Harary index. Similarly, if k is odd, then there exists no chain graph on N vertices with odd Harary index

The results in this section lead to further conclusions about Harary index when it is an integer. Also, they contribute significantly to writing an algorithm for the inverse Harary index problem among chain graphs.

IV. Inverse Harary index problem for chain graphs

Limiting the domain to chain graphs, the inverse Harary index problem for integers is addressed in this section. Given an integer h, the inverse Harary index problem demands a graph (if possible) from a prescribed class (chain graph in this article) that attains this value.

The algorithm is written based on the theorems and the corollaries given in the previous section. The integer value h and the number of vertices N are the inputs. The main algorithm consists of 3 functions, among which the first two are to check and identify the existence of the required graph and the last one is just to construct the corresponding graph as per the instruction received from the previous functions. The main algorithm *inv_hry_index* directs to one of the functions *fun_1* or *fun_2* depending on the value of N. Once the respective part is executed, it will redirect to the last function *get_graph* to construct the required graph, if exists.

Algorithm 1 function inv_hry_index(h, N)

Input: h, N

Output: A chain graph G with $H(G) = h$, if exists

if $N \equiv 3(mod\ 4)$ **then**
  Print "No chain graph G exists on N vertices having $H(G) = h$."
else if $N \equiv 1(mod\ 4)$ **then**
  goto *fun_1*(h, N)
else
  goto *fun_2*(h, N)
end if

The functions referred above are given below.

Algorithm 2 function fun_1(h, N)

Input: h, N

Output: The arguments G, c, p, q for the function *get_graph*, if chain graph G with $H(G) = h$ exists

if $N \equiv 0(mod\ 4)$ **then**
  $k = \frac{N}{4}$
  if $\left[k \equiv 1(mod\ 2)\right.$ **and** $\left.h \equiv 0(mod\ 2)\right]$ **or** $\left[k \equiv 0(mod\ 2)\right.$ **and** $\left.h \equiv 1(mod\ 2)\right]$ **then**
    Print "No chain graph G exists on N vertices having $H(G) = h$."
  else
    $a = \frac{10k^2+5k-2}{3}$
    $b = 6k^2 - k$
    $p = q = 2k$
  end if
else
  $k = \frac{N-2}{4}$
  if $\left[k \equiv 1(mod\ 2)\right.$ **and** $\left.h \equiv 1(mod\ 2)\right]$ **or** $\left[k \equiv 0(mod\ 2)\right.$ **and** $\left.h \equiv 0(mod\ 2)\right]$ **then**
    Print "No chain graph G exists on N vertices having $H(G) = h$."
  else
    $a = \frac{10k^2+15k+3}{3}$
    $b = 6k^2 + 5k + 1$
    $p = q = 2k + 1$
  end if
  if $h \notin [a, b]$ **then**
    Print "No chain graph G exists on N vertices having $H(G) = h$."
  else
    $c = \frac{3(b-h)}{2}$
    $G = K_{p,q}$
    if $c == 0$ **then**
      return G
    else
      goto *get_graph*(G, c, p, q)
    end if
  end if
end if

Algorithm 3 function fun_2(h, N)

Input: h, N

Output: The arguments G, c, p, q for the function *get_graph*, if chain graph G with $H(G) = h$ exists

$k = \frac{N-1}{4}$
$a = \frac{10k^2+10k}{3}$
$b = 6k^2 + 2k$
if $h \notin [a, b]$ **then**
  Print ""No chain graph G exists on N vertices having $H(G) = h$."
else if $h \equiv 0(mod\ 2)$ **then**
  $p = 2k$
  $q = 2k + 1$
  $m = b$
else
  $p = 2k - 1$
  $q = 2k + 2$
  $m = b - 1$
end if
$G = k_{p,q}$
$c = \frac{3(m-h)}{2}$
if $c == 0$ **then**
  return G
else
  goto *get_graph*(G, c, p, q)
end if

One of the arguments G in the function *get_graph*(G, c, p, q) is the complete bipartite graph $G = K_{p,q}$ with parts $V(G) = V_1 \cup V_2$ with vertices labeled as follows: $V_1 = \{1, 2, \ldots, p-1, p\}$ and $V_2 = \{1', 2', \ldots, (q-1)', q'\}$. The rest of the values p, q, c are recieved from either *fun_1*(h, N) or *fun_2*(h, N). Specifically, this function *get_graph*(G, c, p, q) constructs the required graph G from $K_{p,q}$ by removing c edges, sequentially. Whenever the required chain graph exists, it is noted that $c = \frac{3(b-h)}{2}$ is an integer, in all the cases. Finally, the procedure to construct the required chain graph from the inputs obtained from the previous functions is given below.

Algorithm 4 function get_graph(G, c, p, q)

Input: G, c, p, q

Output: The chain graph G with $H(G) = h$, if exists

if $q - 1 \geq c$ **then**
  for $j = 2' : c$ **do**
    $E(G) = E(G) \setminus (j, p)$
  end for
  return G
else
  for $j = 2' : q'$ **do**
    $E(G) = E(G) \setminus (j, p)$
  end for
  $p = p - 1$
  $c = c - (q - 1)$
  $get\_graph(G, p, q, c)$
end if

A. Complexity

The main algorithm *inv_hry_index* directs to one of the functions *fun_1* or *fun_2* depending on the value of N. The computations and comparisions in the main algorithm and the two functions involve only if loops and hence the constant time. Once the respective part (either *fun_1* or *fun_2*) is executed, it will redirect to the last function *get_graph* to construct the required graph, if exists. The function *get_graph*(G, c, p, q) contains a for loop with $(q-1)$ iterations (line 7), which is executed as long as $c \leq (q-1)$. It takes $\lceil \frac{c}{q-1} - 1 \rceil$ steps for c satisfy $c \leq (q-1)$. Thus, until this point, the total number of steps is $(q-1)\lceil \frac{c}{q-1} - 1 \rceil \leq c+q-2$. Then, in line 3, the for loop is executed c times where $c \leq (q-1)$. Therefore, the total time taken by function *get_graph*(G, c, p, q) is at most $c + 2q - 3$. The expressions for c is $c = \frac{3(b-h)}{2}$ in *fun_1* and $c = \frac{3(m-h)}{2}$ in *fun_2*. On substituting the expressions for b, q, m in c, it is noted that c is a quadratic exprression in N. Hence the total complexity of the above proposed algorithm is $O(N^2)$.

V. Conclusion

The Harary index has noteworthy applications in the field of molecular studies. This article extends the study of Harary index of structured graphs, namely chain and threshold graphs. Further, a significant contribution to the existing knowledge on inverse problems for topological indices is made by the article.

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