

Some Bounds for the Steiner-Harary Index of a Graph

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Abstract The Steiner distance for the set $S \subseteq V(G)$ would simply be the number of edges in the minimal subtree connecting them and is denoted as $d_G(S)$. The Steiner-Harary index is $SH_k(G)$, defined as the sum of the reciprocal of the Steiner distance for all subsets with k vertices in G . In this article, we calculate the exact value of $SH_k(G)$ for specific graphs and establish new best possible lower and upper bounds and characterization. Furthermore, we explore the relationship between $SH_k(G)$ and other graph indices based on Steiner distance.

Keywords Harary index, Steiner index, Steiner-Harary index

MSC(2010) 05C05, 05C07, 05C12, 05C38.

1. Introduction

The graphs considered in this paper are undirected, simple, finite, and connected. The graph $G = (V, E)$ has p -vertices and q -edges, where $V = V(G)$ and $E = E(G)$ represent the vertex and edge collections, respectively. The degree of a vertex v_i is defined as the number of vertices adjacent to it and is denoted by $d_G(v_i)$. If a vertex is adjacent to only one edge, it is called a pendant vertex. The distance between two vertices in a graph is given by $d_G(v_i, v_j)$, the shortest path length between v_i and v_j . The greatest distance between any two vertices in a graph G is called the diameter of the graph and is denoted by $diam(G)$. For undefined notations in this paper, we refer to [2, 8].

In 1947, Harold Wiener [18] first introduced the distance-based graph invariant, revealing correlations between the molecular structure of paraffins and their boiling points. The Wiener index, denoted by $W(G)$, is defined by:

$$W(G) = \sum_{v_i, v_j \subseteq V(G)} d_G(v_i, v_j).$$

In 1989, Chartrand [4] introduced the Steiner distance of a connected graph G and is denoted by $d_G(S)$, where $S \subseteq V(G)$ and $2 \leq |S| \leq p$. In 2016, Li, et al. [9]

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introduced the Steiner k -Wiener index, which is defined by:

$$SW_k(G) = \sum_{S \subseteq V(G), |S|=k} d_G(S).$$

In 2016, Furtula, et al. [6] introduced the k -center Steiner Harary index or the Steiner Harary k -index or simply Steiner-Harary index, which is defined by:

$$SH_k(G) = \sum_{S \subseteq V(G), |S|=k} \frac{1}{d_G(S)}.$$

In 2018, Tratnik [17] introduced the Steiner k -hyper Wiener index, defined by:

$$SWW_k(G) = \sum_{S \subseteq V(G)} [d_G(S) + d_G(S)^2].$$

The use of graphical indices based on degree, distance, and Steiner distance has been extensively studied. For their history, applications, and mathematical properties, see [1, 3, 5, 7, 10, 12–16] and the references cited therein.

2. Specific families of graphs

Proposition 2.1. [11] *Let G be a specific families of graph with $2 \leq k \leq p$.*

(i) *If K_p is a complete graph, then*

$$SH_k(K_p) = \binom{p}{k} \frac{1}{k-1}.$$

(ii) *If P_p is a path, then*

$$SH_k(P_p) = \sum_{s=0}^{p-k} \binom{k+s-2}{k-2} (p-k-s+1) \frac{1}{k+s-1}.$$

(iii) *If S_p is a star, then*

$$SH_k(S_p) = \binom{p-1}{k} \frac{1}{k} + \binom{p-1}{k-1} \frac{1}{k-1}.$$

(iv) *If $K_{m,n}$ is a complete bipartite graph with $1 \leq m \leq n$, then*

$$SH_k(K_{m,n}) = \begin{cases} \frac{1}{k-1} \binom{p}{k} - \frac{1}{k(k-1)} \binom{m}{k} - \frac{1}{k(k-1)} \binom{n}{k}, & \text{if } 1 \leq k \leq m; \\ \frac{1}{k-1} \binom{p}{k} - \frac{1}{k(k-1)} \binom{n}{k}, & \text{if } m \leq k \leq n; \\ \frac{1}{k-1} \binom{p}{k}, & \text{if } n \leq k \leq p. \end{cases}$$

Proposition 2.2. *If W_p is a wheel and $S \subseteq V(W_p)$ with $p > 4$, then*

$$SH_k(W_p) = \left[\binom{p-1}{k-1} + (p-1) \right] \frac{1}{k-1} + \left[\binom{p-1}{k} - (p-1) \right] \frac{1}{k}.$$

Proof. Let W_p be a wheel and $S \subseteq V(W_p)$. If the vertices of S are connected, they form a path of length $k-1$. In such a case, $\frac{1}{d_G(S)} = \frac{1}{k-1}$. On the other hand, if the vertices of S are not connected, then they form a disconnected subgraph of W_p . In this scenario, $\frac{1}{d_G(S)} = \frac{1}{k}$.

$$SH_k(W_p) = \left[\binom{p-1}{k-1} + (p-1) \right] \frac{1}{k-1} + \left[\binom{p-1}{k} - (p-1) \right] \frac{1}{k}.$$

Further, if $p = 4$, then $W_4 = K_4$. \square

Proposition 2.3. Let $G \equiv K_{n_1, n_2, n_3, \dots, n_l}$ be a complete multipartite graph and $S \subseteq V(G)$ with $|S| = k$ and $n_1 \leq n_2 \leq \dots \leq n_{f-1} < k \leq n_f \dots \leq n_l$. Then

$$SH_k(G) = \binom{p}{k} \frac{1}{k-1} + \left[\binom{n_f}{k} + \binom{n_{f+1}}{k} + \dots + \binom{n_l}{k} \right] \left[\frac{1}{k} - \frac{1}{k-1} \right].$$

Proof. Let $G \equiv K_{n_1, n_2, n_3, \dots, n_l}$ be a complete multipartite graph with $|S| = k$, $n_1 \leq n_2 \leq \dots \leq n_{f-1} < k \leq n_f \dots \leq n_l$ and vertex partitions $V_1(G)$, $V_2(G), \dots, V_l(G)$ such that $V(G) = V_1(G) \cup V_2(G) \cup \dots \cup V_l$.

$$SH_k(G) = \sum_{v_i \in S; S \subseteq V_{f+h}; 0 \leq h \leq l-f} \frac{1}{d_G(S)} + \sum_{v_i \in S; S \not\subseteq V_i; \text{for all } i} \frac{1}{d_G(S)},$$

$$SH_k(G) = \left[\binom{n_f}{k} + \binom{n_{f+1}}{k} + \dots + \binom{n_l}{k} \right] \frac{1}{k} + \left[\binom{p}{k} - \binom{n_f}{k} - \binom{n_{f+1}}{k} - \dots - \binom{n_l}{k} \right] \frac{1}{k-1}.$$

On simplification, we have the desired result. \square

Proposition 2.4. Let $L_{m,n}$ be a lollipop graph and $S \subseteq V(L_{m,n})$ with $m \geq k > n$. Then

$$\begin{aligned} SH_k(L_{m,n}) &= \sum_{l=1}^{n+1} \binom{m-1}{k-l} \binom{n}{l-1} \frac{1}{k+n-l} \\ &+ \sum_{l=1}^n \binom{m-1}{k-l} \binom{n-1}{l-1} \frac{1}{k+n-l-1} \\ &+ \dots \\ &+ \sum_{l=1}^2 \binom{m-1}{k-l} \binom{1}{l-1} \frac{1}{k-l+1} \\ &+ \binom{m}{k-1} \frac{1}{k-1}, \end{aligned}$$

where the lollipop graph $L_{m,n}$ is the graph obtained by joining a complete graph K_m to pendant vertex of a path graph P_n with an edge.

Proof. Let $L_{m,n}$ be a lollipop graph with $m \geq k \geq n$. We prove the result by fixing the particular vertex in the path associated with the graph. First, we fix the pendant vertex in the set S and choose $(k-1)$ -vertices from the remaining $(p-1)$ -vertices, which yields a value of $SH_k(G)$ equal to $\sum_{l=1}^{n+1} \binom{m-1}{k-l} \binom{n}{l-1} \frac{1}{k+n-l}$. Next, we fix the vertex adjacent to the pendant vertex and choose $(k-1)$ -vertices from the remaining $(p-2)$ -vertices other than the pendant vertex. The corresponding value of $SH_k(G)$ is equal to $\sum_{l=1}^n \binom{m-1}{k-l} \binom{n-1}{l-1} \frac{1}{k+n-l-1}$. For n iterations, the value of $SH_k(G)$ for the last selection is $\sum_{l=1}^2 \binom{m-1}{k-l} \binom{1}{l-1} \frac{1}{k-l+1}$. Hence, the value of $SH_k(G)$ for choosing k -vertices from the complete graph associated with the graph is $\binom{m}{k-1} \frac{1}{k-1}$. Therefore, to obtain the $SH_k(G)$ value, we need to add up the terms mentioned earlier. Thus, the desired result follows. \square

Proposition 2.5. Let $S_{m,n}$ be a double star and $S \subseteq V(S_p)$ with $m \geq n > k \geq 2$ and $p \geq 7$. Then

$$\begin{aligned} SH_k(S_{m,n}) = & \left[\binom{m-1}{k-1} + \binom{m-1}{k-2} + \binom{n-1}{k-1} + \binom{n-1}{k-2} \right] \frac{1}{k-1} \\ & + \left[\binom{m-1}{k} + \binom{n-1}{k} + \binom{m-1}{k-1} + \binom{n-1}{k-1} \right] \frac{1}{k} \\ & + \left[\sum_{l=1}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} \right] \frac{1}{k-1} \\ & + \left[2 \sum_{l=1}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k} \\ & + \left[\sum_{l=1}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}, \end{aligned}$$

where the double star $S_{m,n}$ is a tree obtained by joining the center of two stars S_m and S_n with an edge.

Proof. Consider a double star $S_{m,n}$ with a vertex partition of m and n . This double star has a total of $p = m + n$ vertices, among which $m + n - 2$ are pendant vertices, one vertex of degree m and another of degree n .

$$SH_k(S_{m,n}) = X_1 + X_2 + X_3 + X_4 + X_5.$$

The values of X_1 , X_2 , X_3 , X_4 and X_5 , are as follows.

- (i) If X_1 is the value of $SH_k(S_{m,n})$ for which $(k-1)$ -vertices are chosen from either the pendant vertices adjacent to the vertex of degree m or the vertex of degree n including the corresponding vertex or $(k-2)$ -vertices are chosen from either the pendant vertices adjacent to the vertex of degree m or vertex of degree n and including both the vertices, then

$$X_1 = \left[\binom{m-1}{k-1} + \binom{m-1}{k-2} + \binom{n-1}{k-1} + \binom{n-1}{k-2} \right] \frac{1}{k-1}.$$

- (ii) If X_2 is the value of $SH_k(S_{m,n})$ for which k -vertices are chosen from the pendant vertices adjacent to a vertex of degree m including the vertex of degree n or k -vertices are chosen from the pendant vertices adjacent to a vertex of degree n including the vertex of degree m , then

$$X_2 = \left[\binom{m-1}{k} + \binom{n-1}{k} + \binom{m-1}{k-1} + \binom{n-1}{k-1} \right] \frac{1}{k}.$$

- (iii) If X_3 is the value of $SH_k(S_{m,n})$ for which, at least one vertex is chosen from pendant vertices adjacent to central vertices including both the central vertices, then

$$X_3 = \left[\sum_{l=1}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} \right] \frac{1}{k-1}.$$

- (iv) If X_4 is the value of $SH_k(S_{m,n})$ for which, at least one vertex is chosen from pendant vertices adjacent to central vertices with exactly one central vertex, then

$$X_4 = \left[2 \sum_{l=1}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k}.$$

- (v) If X_5 is the value of $SH_k(S_{m,n})$ for which, at least one vertex is chosen from pendant vertices adjacent to central vertices without central vertices, then

$$X_5 = \left[\sum_{l=1}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}.$$

From (i) to (v) of the above facts, the desired result follows. \square

By Proposition 2.5, we have the following.

Corollary 2.1. *Let $S_{m,n}$ be a double star with $k \geq n$.*

- (i) *If $m \geq n = k$, then*

$$\begin{aligned} SH_k(S_{m,n}) = & \left[\binom{m-1}{k-1} + \binom{m-1}{k-2} + \binom{n-1}{k-1} + \binom{n-1}{k-2} \right] \frac{1}{k-1} \\ & + \left[\binom{m-1}{k} + \binom{m-1}{k-1} + \binom{n-1}{k-1} \right] \frac{1}{k} \\ & + \left[\sum_{l=1}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} \right] \frac{1}{k-1} \\ & + \left[2 \sum_{l=1}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k} \\ & + \left[\sum_{l=1}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}. \end{aligned}$$

- (ii) *If $m = n = k$, then*

$$SH_k(S_{m,n}) = \left[\sum_{l=1}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} + 2k \right] \frac{1}{k-1}$$

$$\begin{aligned}
& + 2 \left[1 + \sum_{l=1}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k} \\
& + \left[\sum_{l=1}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}.
\end{aligned}$$

(iii) If $m > k = n + 1$, then

$$\begin{aligned}
SH_k(S_{m,n}) &= \left[\binom{m-1}{k} + \binom{m-1}{k-1} + 2 \sum_{l=1}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k} \\
&+ \left[\binom{m-1}{k-1} + \binom{m-1}{k-2} + 1 \right] \frac{1}{k-1} \\
&+ \sum_{l=1}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} \frac{1}{k-1} \\
&+ \left[\sum_{l=2}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}.
\end{aligned}$$

(iv) If $m > k = n + 2$, then

$$\begin{aligned}
SH_k(S_{m,n}) &= \left[\binom{m-1}{k} + \binom{m-1}{k-1} + 2 \sum_{l=2}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k} \\
&+ \left[\binom{m-1}{k-1} + \binom{m-1}{k-2} + 1 \right] \frac{1}{k-1} \\
&+ \sum_{l=1}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} \frac{1}{k-1} \\
&+ \left[\sum_{l=3}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}.
\end{aligned}$$

(v) If $m > k = n + 3$, then

$$\begin{aligned}
SH_k(S_{m,n}) &= \left[\binom{m-1}{k} + \binom{m-1}{k-1} + 2 \sum_{l=3}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k} \\
&+ \left[\binom{m-1}{k-1} + \binom{m-1}{k-2} \right] \frac{1}{k-1} \\
&+ \sum_{l=2}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} \frac{1}{k-1} \\
&+ \left[\sum_{l=4}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}.
\end{aligned}$$

(vi) If $m > k = n + a$ and $a > 3$, then

$$SH_k(S_{m,n}) = \left[\binom{m-1}{k} + \binom{m-1}{k-1} + 2 \sum_{l=a}^{k-2} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k}$$

$$\begin{aligned}
& + \left[\binom{m-1}{k-1} + \binom{m-1}{k-2} \right] \frac{1}{k-1} \\
& + \sum_{l=a-1}^{k-3} \binom{m-1}{l} \binom{n-1}{k-l-2} \frac{1}{k-1} \\
& + \left[\sum_{l=a+1}^{k-1} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}.
\end{aligned}$$

(vii) If $k = m + a \geq n + a$ and $a > 3$, then

$$\begin{aligned}
SH_k(S_{m,n}) &= \left[2 \sum_{l=a}^{k-a-1} \binom{m-1}{l} \binom{n-1}{k-l-1} \right] \frac{1}{k} \\
&+ \sum_{l=a-1}^{k-a-2} \binom{m-1}{l} \binom{n-1}{k-l-2} \frac{1}{k-1} \\
&+ \left[\sum_{l=a+1}^{k-a} \binom{m-1}{l} \binom{n-1}{k-l} \right] \frac{1}{k+1}.
\end{aligned}$$

Proposition 2.6. Let $G \equiv S_{n_1} \ominus K_1 \ominus S_{n_2}$ be a double broom graph with $p \geq 9$ and $n_1 \geq n_2 > k > 4$. Then

$$\begin{aligned}
SH_k(G) &= \left[\binom{n_1-1}{k-3} + \binom{n_2-1}{k-3} + \sum_{l=1}^{k-4} \binom{n_1-1}{l} \binom{n_2-1}{k-l-3} \right] \frac{1}{k-1} \\
&+ \left[\binom{n_1-1}{k-1} + \binom{n_2-1}{k-1} + \binom{n_1-1}{k-2} + \binom{n_2-1}{k-2} \right] \frac{1}{k-1} \\
&+ \left[\binom{n_1-1}{k} + \binom{n_2-1}{k} + \binom{n_1-1}{k-1} + \binom{n_2-1}{k-1} \right] \frac{1}{k} \\
&+ \left[2 \binom{n_1-1}{k-2} + 2 \binom{n_2-1}{k-2} + 3 \sum_{l=1}^{k-3} \binom{n_1-1}{l} \binom{n_2-1}{k-l-2} \right] \frac{1}{k} \\
&+ \left[\binom{n_1-1}{k-1} + \binom{n_2-1}{k-1} + 3 \sum_{l=1}^{k-2} \binom{n_1-1}{l} \binom{n_2-1}{k-l-1} \right] \frac{1}{k+1} \\
&+ \sum_{l=1}^{k-1} \binom{n_1-1}{l} \binom{n_2-1}{k-l} \frac{1}{k+2},
\end{aligned}$$

where the double broom graph $S_{n_1} \ominus K_1 \ominus S_{n_2}$ is a tree obtained by joining the centers of two stars S_{n_1} and S_{n_2} with edges from pendant vertices of K_1 .

Proof. Let G be a double broom graph with $n_1 + n_2 - 2$ pendant vertices and two vertices of degree n_1 and n_2 . Then

$$SH_k(G) = Y_1 + Y_2 + Y_3 + Y_4.$$

The values of Y_1 , Y_2 , Y_3 and Y_4 , are as follows.

- (i) If Y_1 is the value of $SH_k(G)$ for which, k -vertices of the set S are chosen from $n_1 + n_2 - 2$ pendant vertices, then

$$Y_1 = \sum_{l=1}^{k-1} \binom{n_1-1}{l} \binom{n_2-1}{k-l} \frac{1}{k+1} + \left[\binom{n_1-1}{k} + \binom{n_2-1}{k} \right] \frac{1}{k}.$$

- (ii) If Y_2 is the value of $SH_k(G)$ for which, $(k-1)$ -vertices of the set are chosen from $(n_1 + n_2 - 2)$ pendant vertices and one vertex are other than pendant vertices, then

$$Y_2 = \left[\binom{n_1-1}{k-1} + \binom{n_2-1}{k-1} \right] \left[\frac{1}{k-1} + \frac{1}{k} + \frac{1}{k+1} \right] + 3 \sum_{l=1}^{k-2} \binom{n_1-1}{l} \binom{n_2-1}{k-l-1} \frac{1}{k+1}.$$

- (iii) If Y_3 is the value of $SH_k(G)$ for which, $(k-2)$ -vertices of the set are chosen from $(n_1 + n_2 - 2)$ pendant vertices and two vertices are other than pendant vertices, then

$$Y_3 = \left[\binom{n_1-1}{k-2} + \binom{n_2-1}{k-2} \right] \left[\frac{1}{k-1} + 2\frac{1}{k} \right] + 3 \sum_{l=1}^{k-3} \binom{n_1-1}{l} \binom{n_2-1}{k-l-2} \frac{1}{k}.$$

- (iv) If Y_4 is the value of $SH_k(G)$ for which $(k-3)$ -vertices of the set are chosen from $(n_1 + n_2 - 2)$ pendant vertices and three vertices are other than pendant vertices, then

$$Y_4 = \sum_{l=1}^{k-4} \binom{n_1-1}{l} \binom{n_2-1}{k-l-3} \frac{1}{k-1} + \left[\binom{n_1-1}{k-3} + \binom{n_2-1}{k-3} \right] \frac{1}{k-1}.$$

From (i) to (iv) of the above facts, we obtain.

$$\begin{aligned} SH_k(G) &= \left[\binom{n_1-1}{k} + \binom{n_2-1}{k} \right] \frac{1}{k} + \sum_{l=1}^{k-1} \binom{n_1-1}{l} \binom{n_2-1}{k-l} \frac{1}{k+2} \\ &\quad + \left[\binom{n_1-1}{k-1} + \binom{n_2-1}{k-1} \right] \left[\frac{1}{k-1} + \frac{1}{k} + \frac{1}{k+1} \right] \\ &\quad + 3 \sum_{l=1}^{k-2} \binom{n_1-1}{l} \binom{n_2-1}{k-l-1} \frac{1}{k+1} \\ &\quad + \left[\binom{n_1-1}{k-2} + \binom{n_2-1}{k-2} \right] \left[\frac{1}{k-1} + 2\frac{1}{k} \right] \end{aligned}$$

$$\begin{aligned}
& + 3 \sum_{l=1}^{k-3} \binom{n_1-1}{l} \binom{n_2-1}{k-l-2} \frac{1}{k} \\
& + \left[\binom{n_1-1}{k-3} + \binom{n_2-1}{k-3} \right] \frac{1}{k-1} \\
& + \sum_{l=1}^{k-4} \binom{n_1-1}{l} \binom{n_2-1}{k-l-3} \frac{1}{k-1}.
\end{aligned}$$

On simplification, we have the desired result. \square

By Proposition 2.6, we have the following corollary.

Corollary 2.2. *Let $G \equiv S_{n_1} \ominus K_1 \ominus S_{n_2}$ be a double broom graph with $p \geq 9$ and $n_1 \geq n_2$.*

(i) *If $k = 4$, then*

$$\begin{aligned}
SH_4(G) &= \sum_{l=1}^3 \left[\binom{n_1-1}{l} + \binom{n_2-1}{l} \right] \frac{1}{3} + \sum_{l=1}^3 \left[\binom{n_1-1}{l+1} + \binom{n_2-1}{l+1} \right] \frac{1}{4} \\
&+ \left[\binom{n_1-1}{2} + \binom{n_2-1}{2} + (n_1-1)(n_2-1) \right] \frac{1}{4} \\
&+ \left[\binom{n_1-1}{3} + \binom{n_2-1}{3} + 3 \sum_{l=1}^2 \binom{n_1-1}{l} \binom{n_2-1}{3-l} \right] \frac{1}{5} \\
&+ \sum_{l=1}^3 \binom{n_1-1}{l} \binom{n_2-1}{4-l} \frac{1}{6}.
\end{aligned}$$

(ii) *If $k = 3$, then*

$$\begin{aligned}
SH_3(G) &= \sum_{l=1}^3 \left[\binom{n_1-1}{l-1} + \binom{n_2-1}{l-1} \right] \frac{1}{2} + \sum_{l=1}^3 \left[\binom{n_1-1}{l} + \binom{n_2-1}{l} \right] \frac{1}{3} \\
&+ (n_1-1)(n_2-1) \frac{1}{3} + \sum_{l=1}^2 \binom{n_1-1}{l} \binom{n_2-1}{3-l} \frac{1}{4} \\
&+ \left[\binom{n_1-1}{2} + \binom{n_2-1}{2} + 3(n_1-1)(n_2-1) \right] \frac{1}{5}.
\end{aligned}$$

(iii) *If $k = 2$, then*

$$\begin{aligned}
SH_k(G) &= (n_1 + n_2) + \left[\binom{n_1-1}{2} + \binom{n_2-1}{2} + n_1 + n_2 + 2 \right] \frac{1}{2} \\
&+ [n_1 + n_2 - 2] \frac{1}{3} + (n_1-1)(n_2-1) \frac{1}{4}.
\end{aligned}$$

3. Bounds and characterization

Theorem 3.1. *Let G be any connected graph with p -pendant vertices ($p > 1$) and $k = p - 1$. Then*

$$SH_k(G) = \eta \frac{1}{p-1} + (p-\eta) \frac{1}{p-2},$$

where η is the number of non-pendant vertices adjacent to at least one pendant vertex.

Proof. Let G be a connected graph with ρ -pendant vertices, η be the number of non-pendant vertices adjacent to at least one pendant vertex, and $k = p - 1$. To calculate $SH_k(G)$, we first choose all the vertices except one from the above mentioned η -vertices. Then, we choose all η -vertices adjacent to at least one pendant vertex, except for one vertex other than the η -vertices, which yields

$$\begin{aligned} SH_k(G) &= \rho \frac{1}{p-2} + \eta \frac{1}{p-1} + (p - \rho - \eta) \frac{1}{p-2} \\ &= \eta \frac{1}{p-1} + (p - \eta) \frac{1}{p-2}. \end{aligned}$$

□

Theorem 3.2. Let G be a connected r -regular graph with $r \geq \frac{p}{2}$. Then

$$\binom{p}{k} \frac{1}{k} \leq SH_k(G) \leq \binom{p}{k} \frac{1}{k-1}.$$

Proof. Let G be a connected r -regular graph with $r \geq \frac{p}{2}$. Then, the sum of degree of any two distinct vertices is equal to $2r \geq p$. The induced subgraph with vertex set S is either connected or disconnected, and the minimum size of the connected subgraph of G whose vertex set contains S is $k - 1$ or k , respectively, that is $\frac{1}{k} \leq \frac{1}{d_G(S)} \leq \frac{1}{k-1}$. Taking the sum for each S , we have the desired result. □

Theorem 3.3. Let P_p and $\overline{P_p}$ be the path and its complement graph with $p \geq 4$. Then

$$SH_k(P_p) \leq SH_k(\overline{P_p}).$$

Further, the equality holds if $p = 4$.

Proof. Let P_p and $\overline{P_p}$ be the path and its complement graph with $p \geq 4$. The path minimizes the $SH_k(G)$ value for any connected graph. Since $\overline{P_p}$ is also connected, we have

$$SH_k(P_p) \leq SH_k(\overline{P_p}).$$

Further, if $p = 4$, then $P_4 \cong \overline{P_4}$, resulting in equality. □

Theorem 3.4. Let G^* be a connected graph with $\text{diam}(G^*) = 2$, $p \geq 6$ and $k \geq 3$. Then

$$\binom{p-1}{k} \frac{1}{k} + \binom{p-1}{k-1} \frac{1}{k-1} \leq SH_k(G^*) \leq \binom{p}{k} \frac{1}{k-1}.$$

Proof. Let G^* be a connected graph with $\text{diam}(G^*) = 2$. The removal of an edge cannot decrease the value of $\frac{1}{d_{G^*}(S)}$. The graph attains its upper bound with the maximum possible edges. This graph is created by removing one edge from a complete graph. The corresponding inequality is

$$SH_k(G^*) \leq \binom{p}{k} \frac{1}{k-1}. \quad (3.1)$$

The star is a connected graph with a $\text{diam}(G^*) = 2$ that has the minimum number of edges, leading to the lower bound

$$SH_k(G^*) \geq \binom{p-1}{k} \frac{1}{k} + \binom{p-1}{k-1} \frac{1}{k-1}. \quad (3.2)$$

By equation (3.1) and equation (3.2), we have

$$\binom{p-1}{k} \frac{1}{k} + \binom{p-1}{k-1} \frac{1}{k-1} \leq SH_k(G^*) \leq \binom{p}{k} \frac{1}{k-1}.$$

□

Lemma 3.1. *Let G^{**} be a connected graph with $p \geq 7$ and maximum possible edges and $\text{diam}(G^{**}) = 3$. Then*

$$\begin{aligned} SH_k(G^{**}) = & \left[\binom{p-2}{k} + \binom{d_{G^{**}}(v_1)}{k-1} + \binom{d_{G^{**}}(v_2)}{k-1} + \binom{p-2}{k-2} \right] \frac{1}{k-1} \\ & + \left[\binom{d_{G^{**}}(v_2)}{k-1} + \binom{d_{G^{**}}(v_1)}{k-1} \right] \frac{1}{k} \\ & + \left[\binom{d_{G^{**}}(v_1)}{k-2} + \binom{d_{G^{**}}(v_2)}{k-2} \right] \left(\frac{1}{k} - \frac{1}{k-1} \right), \end{aligned}$$

where $d_{G^{**}}(v_1) + d_{G^{**}}(v_2) = p - 2$.

Proof. Consider a graph G^{**} with $\text{diam}(G^{**}) = 3$ and the maximum possible edges. Since the diameter of the graph G^{**} is 3, a pair of vertices (v_1, v_2) must exist such that the distance between them is 3. The remaining $(p-2)$ -vertices in the graph must be adjacent to each other, and each of these $(p-2)$ -vertices must be connected to the vertices of either v_1 or v_2 . The partition of $(p-2)$ -vertices into sets V_1 and V_2 is such that vertices in V_1 are adjacent to vertex v_1 with $|V_1| = d_{G^{**}}(v_1)$ and vertices in V_2 are adjacent to vertex v_2 with $|V_2| = d_{G^{**}}(v_2)$.

The value of $d_{G^{**}}(S)$ is $k-1$ for $S \subseteq V(G^{**})$ with $|S| = k$, if any of the following conditions hold:

- (i) The vertices in S are chosen from $(p-2)$ -vertices, excluding v_1 and v_2 .
- (ii) The vertices in S include v_1 and v_2 , along with at least one vertex from the partitions V_1 and V_2 .
- (iii) The vertices in S include v_1 but not v_2 , and at least one vertex from V_1 , and vice versa.

In all other cases, $d_{G^{**}}(S) = k$.

For $d_{G^{**}}(v_1) \geq d_{G^{**}}(v_2) \geq k = |S|$, then

$$\begin{aligned} SH_k(G^{**}) = & \sum_{S \subseteq V_1 \cup V_2} \frac{1}{d_{G^{**}}(S)} + \sum_{\substack{S \subseteq V_1 \cup \{v_1\}, \\ v_1 \in S}} \frac{1}{d_{G^{**}}(S)} + \sum_{\substack{S \subseteq V_2 \cup \{v_1\}, \\ v_1 \in S}} \frac{1}{d_{G^{**}}(S)} \\ & + \sum_{\substack{S \subseteq V_1 \cup \{v_2\}, \\ v_2 \in S}} \frac{1}{d_{G^{**}}(S)} + \sum_{\substack{S \subseteq V_2 \cup \{v_2\}, \\ v_2 \in S}} \frac{1}{d_{G^{**}}(S)} \end{aligned}$$

$$\begin{aligned}
& + \sum_{\substack{S \subseteq \{v_1, v_2\} \cup V_1 \cup V_2, \\ v_1, v_2 \in S}} \frac{1}{d_{G^{**}}(S)}. \\
SH_k(G^{**}) &= \binom{p-2}{k} \frac{1}{k-1} + \binom{d_{G^{**}}(v_1)}{k-1} \frac{1}{k-1} + \binom{d_{G^{**}}(v_2)}{k-1} \frac{1}{k-1} \\
& + \binom{p-2}{k-2} \frac{1}{k-1} + \binom{d_{G^{**}}(v_2)}{k-1} \frac{1}{k} + \binom{d_{G^{**}}(v_1)}{k-1} \frac{1}{k} \\
& + \left[\binom{d_{G^{**}}(v_1)}{k-2} + \binom{d_{G^{**}}(v_2)}{k-2} \right] \left(\frac{1}{k} - \frac{1}{k-1} \right).
\end{aligned}$$

On simplification, we have the desired result. \square

By Lemma 3.1, we have the following corollary.

Corollary 3.1. *Let G^{**} be a connected graph with maximum possible edges and $\text{diam}(G^{**}) = 3$.*

$$\begin{aligned}
(i) \quad SH_k(G^{**}) &= \left[\binom{p-2}{k} + \binom{d_{G^{**}}(v_1)}{k-1} + \binom{p-2}{k-2} \right] \frac{1}{k-1} \\
& + \left[\binom{d_{G^{**}}(v_2)}{k-1} \right] k^b + \left[\binom{d_{G^{**}}(v_2)}{k-2} \right] \left(\frac{1}{k} - \frac{1}{k-1} \right), \\
& \text{if } k-2 \leq d_{G^{**}}(v_1) \leq k < d_{G^{**}}(v_2) \text{ and } d_{G^{**}}(v_1) + d_{G^{**}}(v_2) = p-2. \\
(ii) \quad SH_k(G^{**}) &= \left[\binom{p-2}{k} + \binom{p-2}{k-2} \right] \frac{1}{k-1}, \\
& \text{if } d_{G^{**}}(v_1) \leq d_{G^{**}}(v_2) < k-1 \text{ and } d_{G^{**}}(v_1) + d_{G^{**}}(v_2) = p-2.
\end{aligned}$$

Observation 3.1. Let G be a connected graph with $\text{diam}(G) = 3$ and $p \geq 7$. Then the upper bound is attained for graph with the maximum number of edges and lower bound attained for the graph with minimum number of edges.

4. Comparison among Steiner related indices

Theorem 4.1. *Let G be a connected graph with $k \geq 2$. Then*

$$\begin{aligned}
kSW_k(G) + (k-1)SH_k(G) - \binom{p}{k} &\leq SWW_k(G) \\
&\leq pSW_k(G) + (p-1)SH_k(G) - \binom{p}{k}.
\end{aligned}$$

Further, both the equality hold if $k = p$.

Proof. Let G be a connected graph with $|S| = k \geq 2$. Then

$$\begin{aligned}
SW_k(G) + SH_k(G) &= \sum_{S \subseteq V(G)} \left(d_G(S) + \frac{1}{d_G(S)} \right) \\
&= \sum_{S \subseteq V(G)} \frac{1}{d_G(S)} ((d_G(S))^2 + d_G(S)) - d_G(S) + 1. \quad (4.1)
\end{aligned}$$

Now

$$\begin{aligned}
 \sum_{S \subseteq V(G)} \frac{1}{d_G(S)} ((d_G(S)^2 + d_G(S)) - d_G(S) + 1) &\leq \frac{(SWW_k(G) + \binom{p}{k})}{k-1} \\
 &\quad - \frac{SW_k(G)}{k-1}, \\
 \implies SW_k(G) + SH_k(G) &\leq \frac{(SWW_k(G) + \binom{p}{k})}{k-1} - \frac{SW_k(G)}{k-1} \\
 \implies kSW_k(G) + (k-1)SH_k(G) - \binom{p}{k} &\leq SWW_k(G). \quad (4.2)
 \end{aligned}$$

And

$$\begin{aligned}
 \sum_{S \subseteq V(G)} \frac{1}{d_G(S)} ((d_G(S)^2 + d_G(S)) - d_G(S) + 1) &\geq \frac{(SWW_k(G) + \binom{p}{k})}{p-1} \\
 &\quad - \frac{SW_k(G)}{p-1}, \\
 \implies SW_k(G) + SH_k(G) &\geq \frac{(SWW_k(G) + \binom{p}{k})}{p-1} - \frac{SW_k(G)}{p-1} \\
 \implies pSW_k(G) + (p-1)SH_k(G) - \binom{p}{k} &\leq SWW_k(G). \quad (4.3)
 \end{aligned}$$

By equation (4.2) and equation (4.3), we have the desired results.

Further, If $k = p$, then $d_G(S) = p - 1$, which leads to the equality. \square

Remark 4.1. In Theorem 4.1, the left equality holds if $d_G(S) = k - 1$ for all $S \subseteq V(G)$ and the right equality holds if $d_G(S) = p - 1$ for all $S \subseteq V(G)$.

5. Conclusion and open problems

The Steiner-Harary index of a graph lies on the claim that their particular cases, for pertinently chosen values of the parameter k , p , and q . Here, we have the following observations and open problems.

- (i) Among all connected graphs, the complete graph has the highest value, and the path attains the lowest value of $SH_k(G)$.
- (ii) Removing edges from a graph may decrease the value while adding edges may increase the value of $SH_k(G)$.
- (iii) The function corresponding to $SH_k(G)$ is strictly decreasing with the independent variable $d_G(S)$.
- (iv) If G is a tree with diameter $d \geq 4$, then the number of pendent vertices varies between $\lceil \frac{p}{d} \rceil$ and $p - d + 1$. But with diameter d , the bounds for the G are still unsolved.

- (v) Find the values of the Steiner-Harary index of certain class of chemical graphs and compare them with other distance-based graphical indices. Also, explore some results towards QSPR / QSAR / QSTR model.
- (vi) If G and \overline{G} are both connected regular graphs with $d_G(v_i) > \frac{p}{2}$, then $SH_k(G) \geq SH_k(\overline{G})$.

6. Conflicts of interest

The authors have declared that they have no conflicts of interest.

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