A Quantitative Analysis of the Utilization of the Hyper-Weiner Index and the Steiner Distance for QSAR and QSPR

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Abstract — For a associated graph $\boldsymbol{G}$ Randić index is given as

$$\boldsymbol{R(G)} = \sum_{\{u,v\}\subseteq V(G)} \frac{}{\sqrt{d_G(u)d_G(v)}}$$

A expansion of the idea of graph distance, the Steiner Wiener index was first developed by Chartrand et al. in 1989. The Steiner distance d(S) of the vertices of S is the smallest size of a connected subgraph whose vertex set is S for a connected graph G of order n and S V (G). In this work, the Steiner Randi index Rk(G) is introduced, along with various characteristics and limitations for it, in the context of the Randic index and steiner distance-based indices..

Keywords — ***Graphs, Degree, Distance, Topological indices, steiner distance Randić index.***

I. Introduction

Let G be a simple connected graph with the properties |V (G)| = n and |E(G)| = m, which are referred to as the graph's order and size, respectively. The distance d(x, y) = dG(x, y) is the shortest path between u and v, and the degree degG(v) of a graph G is the cardinality of the first neighbours of the vertex u and x, y V (G). A extension of the historical graph distance, the Steiner distance of a connected graph was first described in 1989 by Chartrand et al. The Steiner distance d(S) of the vertices of S is the smallest size of a connected subgraph whose vertex set is S for a connected graph G of order at least 2 and S V (G). Li, Mao, and Gutman expanded the idea of a graph's G as the Steiner wiener index [12] denoted as wiener index in light of equation (1)

$$SW_k(G) = \sum_{\substack{S\subset V\ (G) \\ |\ |=}} d(S)$$

When $= \{\ ,\ \}, |\ | = 2$, then the stiener distance reduces to distance between a pair of vertices which is equal to the ordinary wiener index [14] that is

$$W(G) = SW_k(G) = \sum_{\substack{S\subset V\ (G) \\ |\ |=2}} d(S)$$

Further when $k = 0, SW(G) = 0$, and $k = n - 1, SW_k(G) = n - 1$. Among the several hundred presently existing graph-based molecular structure descriptors [2], the Randić index of a graph was introduced by the chemist Randić under the name of "branching index" in 1975 [3] as thesum of

$$R(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$

Also, it was designed in 1975 to measure the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. It was demonstrated that the Randić index is well correlated with a variety of physicochemical properties of alkanes, such as boiling point, enthalpy of formation, surface area, and

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solubility in water. The Randić index is certainly the most widely applied in chemistry and pharmacology, in particular for designing quantitative structure-property and structure-activity relations. Randić proposed this index to quantitatively characterize the degree of molecular branching. According to him, the degree of branching of the molecular skeleton is a critical factor for some molecular properties such as boiling points of hydrocarbons and the retention volumes and the retention times obtained from chromatographic studies (all citations are taken from [3]). Zhou et al. [4] obtained lower and upper bounds for the general Randić index, and Du et al. [5] obtained new lower and upper bounds for the Randić index in terms of other topology indices; for other bounds, see [6, 7]. Then, in this paper, we will obtain new lower and upper bounds for the Randić index. In this paper, we introduce Randić index and study some interesting properties and bounds.

II. Steiner Hyper Wiener index of Standard Graph Structures

Steiner Randić index of a simple connected graph G is the generalization of Randić index with k vertices. In view of equation (1) and (3), we introduce the following definition.

Definition 2.1. For any connected graph G the Steiner Randić index $R(G)$ of a graph G is defined as

$$R_k(G) = \sum_{\substack{S\subset V(G)\\ |\ |=}} \frac{1}{\sqrt{\sum_{v\in S} \deg_S(v)}}$$

Where $1 \le k \le n-1$ and when $k = 1$ then $R(G) = 0$. One can note that in the special case $k = 2$ of equation (5) implies Randić index $R(G)$.

Theorem 2.3. The Steiner Randić index index of the Star graph S_n is

$$(\ \ ) = \binom{n-1}{k}\left[\frac{1}{\sqrt{k}} + \frac{k}{(p-k)\sqrt{n+k-2}}\right]$$

where $2 \le k \le n-2$.

Proof. Let v_1 be the center vertex of the star graph S_n. Divide the vertex set $V(G)$ of S_n in to two partition as follows. For any $S \subset V(Sn)$ and $|S| = k$, if $v_1 \notin S$, then $\sum_{v\in S} \deg_S(v) = k$. If $v_1 \in S$, then $\sum_{v\in S} \deg_S(v) = n + k - 2$ Therefore

$$R_k(S_n) = \sum_{\substack{S\subset V(G)\\ v_1\notin S, |S|=k}} \frac{1}{\sqrt{\sum_{v\in S} \deg_S(v)}} + \sum_{\substack{S\subset V(G)\\ v_1\in S, |S|=k}} \frac{1}{\sqrt{\sum_{v\in S} \deg_S(v)}}$$
$$= \binom{n-1}{\ } \frac{1}{\sqrt{k}} + \binom{n-1}{k-1} \frac{1}{\sqrt{n+k-2}}$$

$$= \binom{n-1}{\ } \frac{1}{\sqrt{k}} + \frac{k}{p-k} \binom{n-1}{k} \frac{1}{\sqrt{n+k-2}}$$

$$= \binom{n-1}{\ } \left[\frac{1}{\sqrt{k}} + \frac{}{(p-k)\sqrt{n+k-2}} \right]$$

Theorem 2.4. For a complete graph K_n with n vertices and k be an integer $2 \leq k \leq n$ then $R(K_n) = \binom{n}{\ } k(n-1)$.

Proof. For any graph $S \subset V(K_n)$ and $|S| = k$ vertices of the K_n has degree $n-1$

$$\sum_{v \in S} \deg_S(v) = k(n-1)$$

There exist ( ) vertex subsets in ( )

Hence,

$$R(K_n) = \binom{\ }{r} k(n-1)$$

Theorem 2.5. The Steiner Hyper Wiener index of path of order is

$$(\ ) = \binom{n-1}{k-1} \frac{1}{\sqrt{2k-1}} + \binom{n-2}{k-2} \frac{1}{\sqrt{2k-2}} + \binom{n-2}{k} \frac{1}{\sqrt{2k}}$$

where $2 \leq k \leq n-2$.

Proof. Let $V(P_n) = \{v_1, v_2, \dots, v_n\}$ be the vertices of P_n where v_1 and v_n are pendent vertices. For any $S \subset V(Pn)$ and $|S| = k$. The vertex set can be partition into three sets as follows. (i) v_1 & $v_n \notin$,(ii) v_1 or $v_n \in S$,and (iii) v_1 & $v_n \in S$.

Case (i): If v_1 & $v_n \notin S$ then the vertices in S non pendent vertices and whose vertices are 2.

Therefore, $\sum_{v \in S} \deg_S(v) = 2k$.

Case (ii): v_1 or $v_n \in$. In a path graph P_n the vertices of $_1$and v_n are pendent vertices, therefore, $\sum_{v \in S} \deg_S(v) = 2k-1$.

Case (ii): v_1 & $v_n \in S$. . In a path graph P_n the vertices of $v_1$and v_n are pendent vertices, therefore, $\sum_{v \in S} \deg_S(v) = 2k-2$.

$$R_k(P_n) = \sum_{\substack{S \subset V(P_n) \\ v_1 \in S \text{ or } v_n \in S \\ |\ | =}} \frac{1}{\sqrt{\sum_{v \in S} \deg_S(v)}} + \sum_{\substack{S \subset V(P_n) \\ v_1 and \\ v_n \in S \\ |\ | =}} \frac{1}{\sqrt{\sum_{v \in S} \deg_S(v)}} + \sum_{\substack{S \subset V(P_n) \\ v_1 and \\ v_n \notin S \\ |\ | =}} \frac{1}{\sqrt{\sum_{v \in S} \deg_S(v)}}$$

Hence

$$R_k(P_n) = \sum_{\substack{S \subset V(P_n) \\ v_1 \in S \text{ or } v_n \in S \\ |\ | =}} \frac{1}{\sqrt{2k-1}} + \sum_{\substack{S \subset V(P_n) \\ v_1 and \\ v_n \in S \\ |\ | =}} \frac{1}{\sqrt{2k-2}} + \sum_{\substack{S \subset V(P_n) \\ v_1 and \\ v_n \notin S \\ |\ | =}} \frac{1}{\sqrt{2k}}$$

$$(\ \ ) = \binom{n-1}{k-1}\frac{1}{\sqrt{2k-1}} + \binom{n-2}{k-2}\frac{1}{\sqrt{2k-2}} + \binom{n-2}{k}\frac{1}{\sqrt{2k}}$$

Theorem 2.6. Let be the , be the complete bipartite graph with + vertices, and r being an integer such that $2 \leq r \leq m + n - 2$, then

$$= \begin{cases} 2(\ \ )\frac{1}{\sqrt{mk}} + (\ \ )\binom{}{x}\binom{}{k-x}\frac{1}{\sqrt{nx+m(k-x)}} & if\ 1 \leq r \leq m \\ \binom{}{k}\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{nx+m(k-x)}} \ \ {}_{=1} \ \ \binom{}{k-x} \\ \quad + (\ )\frac{1}{\sqrt{nx+mt-mx}} & if\ n < r \leq m+n \end{cases}$$

Proof. Let $G = K_{m,}$ and let $V_1 = \{x_1, x_2, x_3, \dots, x_m\}$ and $V_2 = \{y_1, y_2, y_3, \dots, y_n\}$ be the twopartition of vertices of G.

Case I. $1 \leq k \leq m$

For all $S \subset V(G)$ and $|S| = r$, we have the following three subcases (i) $S \cap V1 = \emptyset$ (ii) $S \cap V_2 = \emptyset$ (iii) $S \cap V_1 = \emptyset$ and $S \cup V_2 = \emptyset$. If $S \cap V_1 = \emptyset$ or $S \cap V_2 = \emptyset$ then $S \subset V_2$ suppose $S = \{y_1, y_2, \dots, y_r\}$. Then the Steiner tree containing the vertices $y_1, y_2, \dots, y_n$ has k edges therefore $d_G(S) = k$. Similarly, if $S \cap V_2 = \emptyset$ then $d(S) = k$ and suppose $S \cap V_1 = \emptyset$ and $S \cap V2 = \emptyset$ and let $S = \{x_1, x_2, \dots, x_a\ y_1, y_2, \dots, y_{(k-m)}$ then the Steiner tree induced by the edges

$x_1y_1, y_1x_2, y_1x_3, \dots, y_1x_a, x_1y_2, x_1y_3, \dots, x_1y_{(k-m)}\}$

Therefore $d(S) = k - 1$ Thus

$$R_k(K_{m,n}) = \sum_{\substack{S\subset(K_{m,n})\\ S\cap V_1=\emptyset}} \frac{1}{\sqrt{\sum_{v\in S}\deg_{S_n}(v)}} + \sum_{\substack{S\subset(K_{m,n})\\ S\cap V_2=\emptyset}} \frac{1}{\sqrt{\sum_{v\in S}\deg_{S_n}(v)}} + \sum_{\substack{S\subset V(K_{m,n})\\ S\cap V_1=\emptyset\, V_2\neq\emptyset}} \frac{1}{\sqrt{\sum_{v\in S}\deg_S(v)}}$$

$$R_k(K_{m,n}) = \sum_{\substack{S\subset V(K_{m,n})\\ S\cap V_1=\emptyset}} \frac{1}{\sqrt{mk}} + \sum_{\substack{S\subset V(K_{m,n})\\ S\cap V_2=\emptyset}} \frac{1}{\sqrt{mk}} + \sum_{\substack{S\subset V(K_{m,n})\\ S\cap V_1=\emptyset\, V_2\neq\emptyset}} \frac{1}{\sqrt{nx+m(k-x)}}$$

$$= \binom{}{k}\frac{1}{\sqrt{mk}} + \binom{}{k}\frac{1}{\sqrt{mk}} + \binom{}{x}\binom{}{k-x}\frac{1}{\sqrt{nx+m(k-x)}}$$

$$= 2(\ \ )\frac{1}{\sqrt{mk}} + \binom{}{x}\binom{}{k-x}\frac{1}{\sqrt{nx+m(k-x)}}$$

Case II: Consider $m < r \leq n$. For any $S \subset V(G)$ and $|S| = r$, we have $S \cap V_1 = \emptyset$ or $S \cap V_1 = \emptyset$. If $S \cap V_1 = \emptyset$ then $S \subset V2$ and suppose $S = \{y_1, y_2, \dots, y_r\}$ then the tree T induced by the edges is $\{x_1y_1, x_1y_2, \dots, x_1y_m\}$ is a Steiner tree containing S hence $d_G(S) = r$. If $S \cap V_1$ and let $S = \{x_1, x_2, \dots, x_a, y_1, y_2, y_{r-m}\}(a \leq r \leq n)$ then the tree induced by the vertices S has the edges

$\{x_1y_1, y_1x_2, y_1x_2, \dots, y_1x_m, x_1y_2, x_1y_3, \dots, x_1y_{r-m}\}$ is a steiner tree containing S. Therefore $d(S) = r - 1$.

$$R_k(K_{m,n}) = \sum_{\substack{S\subset(K_{m,n})\\ S\cap V_1=\emptyset}} \frac{1}{\sqrt{\sum_{v\in S} \deg_{S_n}(v)}} + \sum_{\substack{S\subset(K_{m,n})\\ S\cap V_2=\emptyset}} \frac{1}{\sqrt{\sum_{v\in S} \deg_{S_n}(v)}} +$$

$$R_k(K_{m,n}) = \sum_{\substack{S\subset V(K_{m,n})\\ S\cap V_1=\emptyset}} \frac{1}{\sqrt{m}} + \sum_{\substack{S\subset V(K_{m,n})\\ S\cap V_2\neq\emptyset}} \frac{1}{\sqrt{mk}} +$$

$$= (\ )_{k} \frac{1}{\sqrt{m}} + \frac{1}{\sqrt{nx + m(k-x)}} \sum_{=1} (\ )(\ _{k-x})$$

Case III: we consider the remaining case $n < r \leq m + n$. For any set $S \subset (G)$ with r vertices. If $S \cap V_1 \neq \emptyset$, and $S \cap V_2 \neq \emptyset$ suppose $S = \{x_1, x_2, \dots, x_x, y_1, y_2, \dots, y_{r-x}\}$. Then the steiner tree T induced by the edges is $\{x_1 y_1, y_1 x_2, \dots, y_1 x_x, x_1 y_2, x_1 y_3, \dots, x_1 y_{r-x}$ Therefore $d_G(S) = r - 1$ Thus

$$R_k(K_{m,n}) = \sum_{\substack{S\subset V(G)\\ |\ |=}} \frac{1}{\sqrt{\sum_{v\in S} \deg_S(v)}}$$

$$= (\ \ ^{+}\ \ ) \frac{1}{\sqrt{nx + mt - mx}}$$

Remarks 2.7 For a connected graph with vertices and edges then $(\ ) = \frac{1}{\sqrt{2q}}$

Theorem 2.8 let be a tree with vertices and having pendent vertices Thus

$$R_k(T) = \frac{l}{\sqrt{2p-3}} + (p - l)\frac{l}{\sqrt{2q}} - \frac{1}{\sqrt{2p-l-1}}.$$

Proof. For $r = n - 1$ we have the following two cases. Let v be the pendent vertices such that $v \in (G) \setminus S$ is pendent, Then the vertices contained in S from a tree of order $n - 1$ Therefore $d_T(S) = n - 2$ and $\sum_{v\in S} deg(v) = 2m - 1$. There are r such subsets with cardinality $n - 1$ in $(G) \setminus S$. If $(G)\setminus S$ is non pendent in S. Then the vertices contained in S cannot form a tree. Then the respective Steiner tree must contain all the n vertices of . Therefore $d(S) = n - 1$ and $\sum_{u\in S} deg_T(u) = 2m - \deg_T(u)$ where $v \in V(G)\setminus S$. There are $n - p$ such subsets. Hence

$$R_{n-1}(T) = \sum_{\substack{S\subset V(T)\\ v\in V(G)\setminus S}} \frac{1}{\sqrt{\sum_{v\in S} \deg_S(v)}} + \sum_{\substack{S\subset(T)\\ v\in S}} \frac{1}{\sqrt{\sum_{v\in S} \deg_{S_n}(v)}}$$

$$= \frac{}{\sqrt{2p-3}} + (p-l)\frac{}{\sqrt{2q}} - \sum_{\deg(W)\geq 2} \frac{1}{\sqrt{\deg_{S_n}(\ )}}$$

$$= \frac{}{\sqrt{2p-3}} + (p-l)\frac{}{\sqrt{2q}} - \frac{1}{\sqrt{2p-l-1}}$$

III. SOME BOUNDS FOR STEINER RECIPROCAL DEGREE DISTANCE INDEX

For a connected Graph G the greatest and smallest vertex degree of the graph G respectively denote by $\Delta(G)$ and $\delta(G)$. The following Proposition, follows immediately from the definitions of the Steiner Hyper Wiener Index, equation (2).

Observation 3.1. Let be a connected graph with vertices and let be the spanning tree

$$R_k(G) \leq R_k(T)$$

holds for all r, $2 \leq k \leq n$ with equality holds iff G is a tree. For a connected Tree T theorem 3.3 of 3 we have following bounds

$$\binom{n-1}{r-1}(n-1) \leq R(G) \leq \binom{n+1}{r+1} \quad (8)$$

Theorem 3.2: Let T be the tree with n vertices and let r $(2 \leq r \leq n)$ then

$$(r-1)\binom{}{r} \leq R_k(G) \leq r(r-1)\binom{+1}{r+1}$$

From the definition of ( ) we have

$$\binom{n}{r}(r-1) \leq R(G) \leq (r-1)\binom{n-1}{r-1}$$

And

$$\binom{n}{}(r-1) + \binom{n}{}(r-1)^2 \leq R\ (G) \leq (n-1)(n-1 \quad (\quad)^2 \binom{n-1}{}$$

Conclusions

Since it combines the Steiner distance and the Hyper Weiner index, the Steiner Randi index that is developed in this research will be useful in the study of QSAR (Quantitative Structure-Property Relationship) and QSPR (Quantitative Structure-Property Relationship). Finding the Steiner Randi index for the caterpillar, wheel, windmill, and Cartesian product of standard graphs is simple. Our upcoming study involves investigating the overall graph.

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