International J.Math. Combin. Vol.4(2015), 92-98

Relation Between
Sum-Connectivity Index and Average Distance of Trees

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Abstract: The sum-connectivity index of a simple graph G is defined in mathematical chemistry as

$$R^{+}(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}}$$

where $E(G)$ is the edge set of G and d_u is the degree of vertex u in G. We report relation between Sum connectivity index and Average distance $ad(T)$ of tree T.

Key Words: Sum connectivity index, average distance, tree.

AMS(2010): 05C20.

§1. Introduction and Preliminaries

Let G be a simple graph, the vertex-set and edge-set of which are represented by $V(G)$ and $E(G)$ respectively. The connectivity index introduced in 1975 by Milan Randic [9], who has shown this index to reflect molecular branching. The *Randic index* was defined as follows:

$$\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u d_v}}.$$

It is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies [4], [9]. Mathematical properties of this descriptor as summarized in [2] and its generalizations/variants [8] have also been studied extensively. We also call the $R(G)$ index as the product-connectivity index of G.

Motivated by Randics definition of the product-connectivity index, the sumconnectivity

[1]Received April 8, 2015, Accepted December 5, 2015.

index was recently proposed in [9]. The *sum-connectivity index* of the graph G is defined as

$$R^+(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

It is interesting to note that various kinds of variants and extension of the product connectivity index have been reported, but there is not a single one on the additive version of the connectivity index before the sum-connectivity index was proposed [17].

The product-connectivity index and the sum-connectivity index are highly inter-correlated quantities. For example, the correlation coefficient between the product connectivity index and the sum-connectivity index for 137 alkane-trees [6] is 0.9996.

The Wiener index is a distance-based topological index defined as the sum of distances between all pairs of vertices in a graph and is denoted by $W(G)$. It was the first topological index in chemistry [15], introduced in 1945. Since then, the Wiener index has been used to explain various chemical and physical properties of molecules. However the Wiener index can be cubic in the number of vertices of a graph, hence for the sake of simplicity we use the average distance instead [1],[5], [10],[12], [14],[16.

$$ad(G) = \frac{W(G)}{\binom{n}{2}}.$$

In order to state the results of this paper let us introduce some notation. By $distG(u, v)$ we denote the length of the shortest path between vertices u and v in a connected graph G. The length $max_{u,v}\ distG(u, v)$ is a diameter of a graph G, which we denote by $diam(G)$. In particular for trees the diameter is the length of the longest simple path. A star is a tree where at most one vertex is of degree greater than one. Note that a tree with at most three vertices is a star. Also notice that stars are precisely the trees with diameter at most two. The thorn graph of the graph G, with parameters $p_1, p_2, \cdots, p_n$, is obtained by attaching p_i new vertices of degree one to the vertex u_i of the graph G, $i = 1, 2, \cdots, n$. ([3])

In [7] author defined special class of thorn tree named as as *Double comet*. It is defined as $\tau_{n,p}$ which denotes a set of all trees with exactly n nodes and p pendent vertices. For $a, b \geq 1$, $n \geq a + b + 2$ Double Comet $DC(n, a, b)$, is a tree composed of a path containing $n - a - b$ vertices with a pendent vertices attached to one of the ends of the path and b pendent vertices attached to the other end of the path. Thus, $DC(n, a, b)$ has n vertices and $a + b$ leaves, i.e.,$DC(n, a, b) \in \tau_{n,a+b}$.

In this paper we present a relation between sum-connectivity index and average distance of a trees. This paper is motivated from [7].

§2. Relation Between Sum-Connectivty Index and Average Distance of a Tree

The main result of this paper is the following theorem.

Theorem 2.1 *For any tree T with n vertices and p leaves the following inequality holds:*

$$R^+(T) \geq ad(T) + min(0, \sqrt{p} - 2), when\ p = 2.$$
$$R^+(T) \geq ad(T) + max(0, \frac{p-1}{\sqrt{p+1}} - 2), when\ p \geq 3.$$

The inequality is sharp for stars, if we consider the limit when n goes to infinity.

Proof Let $\tau_{n,p}$ be the set of all trees with exactly n nodes and p pendent vertices.

First we prove a theorem for stars and path in the following lemma.

Lemma 2.1 *Let $\tau_{n,p}$ be a tree such that $p \leq 2$ (a path) or $p = n-1$ (a star).Then*

$$R^+(T) \geq ad(T) + min(0, \sqrt{p} - 2), when\ p = 2,$$
$$R^+(T) \geq ad(T) + max(0, \frac{p-1}{\sqrt{p+1}} - 2), when\ p \geq 3.$$

Proof If $n \leq 2$ then the inequality trivially holds, hence we assume $n \geq 3$.

If T is a star then by calculation we obtain $ad(T) = 2 - \frac{2}{n}$ and $R^+(T) = \frac{(n-1)}{\sqrt{n}}$.

If T is a path then by calculation we obtain $ad(T) = \frac{(n+1)}{3}$ and $R^+(T) = \frac{2}{\sqrt{3}} + \frac{(n-3)}{2}$.

In both cases the lemma holds. □

Now we assume that $T \in \tau_{n,p}$ and $3 \leq p \leq n-2$, for this we make use of the following lemma [18], [19].

Lemma 2.2([19]) *Let T be a tree with n vertices and p pendant vertices, where $3 \leq p \leq n-2$. Then*

$$R^+(T) \geq \frac{n-p-2}{2} + \frac{1}{\sqrt{p+2}} + \frac{p-1}{\sqrt{p+1}} + \frac{1}{\sqrt{3}}.$$

From this lemma we obtain

Corollary 2.1 *Let T be a tree with n vertices and p pendant vertices, where $3 \leq p \leq n-2$.*

$$R^+(T) \geq \frac{n-p-2}{2} + \frac{p-1}{\sqrt{p+1}} + 1.025.$$

Since each tree can be transformed into a double comet without decreasing the average distance and simultaneously preserving the number of vertices and leaves(lemma 2.4 in [7]) and in Corollary 2.1 we only use n and p disregarding the actual structure of a tree it is enough to show that for double comets we have

$$\frac{p-1}{\sqrt{p+1}} + \frac{n-p-2}{2} + 1.025 \geq ad(T) + max(0, \frac{p-1}{\sqrt{p+1}} - 2).$$

Lemma 2.3 *Let $\tau_{n,p}$ be a double comet $DC(n,a,b)$ for $a,b \geq 1$, where $3 \leq p \leq n-2$. Then*

$$\frac{p-1}{\sqrt{p+1}} + \frac{n-p-2}{2} + 1.025 \geq ad(T) + max(0, \frac{p-1}{\sqrt{p+1}} - 2).$$

Proof To prove this lemma first we have to find average distance of double comet $ad(G) = \frac{W(G)}{\binom{n}{2}}$, i.e to find the wiener index of the double comet.

In order to compute $W(DC(n,a,b))$ we distinguish four types of pairs of vertices of

TYPE 1. Distance between inner vertices;

TYPE 2. Distance between leaves and inner vertices;

TYPE 3. Distance between the leaves from a to b;

TYPE 4. Distance between leaves with the distance 2.

Let the contributions of all such vertex pairs to $DC(n,a,b)$ be denoted by F_1 , F_2 , F_3 and F_4, respectively. Then,

$$W(DC(n,a,b)) = F_1 + F_2 + F_3 + F_4. \tag{2.1}$$

There are $n-(a+b)$ vertices of Type 1. So

$$F_1 = \binom{n-p+1}{3}.$$

There are $p_i = a, b$ vertices of Type 2. Whence

$$F_2 = \frac{(a+b)(n-p)(n-p+1)}{2}.$$

There are ab vertex pair of Type 3, each of them separated by distance $(n-p+1)$. Thus

$$F_3 = ab(n-p+1).$$

There are $\binom{p_i}{2}$, $p_i = a, b$ vertex pairs of Type 4, each of them at distance 2. Consequently

$$F_4 = 2\binom{a}{2} + 2\binom{b}{2}.$$

Substituting the above relations back into Eq.(2.1) we arrive at the wiener index of the Double comet. i.e

$$W(DC(n,a,b)) = \binom{n-p+1}{3} + \frac{(a+b)(n-p)(n-p+1)}{2} + ab(n-p+1) + 2\binom{a}{2} + 2\binom{b}{2}.$$

Therefore

$$\begin{aligned}\binom{n}{2} ad(T) &= W(T)\\ &= \binom{n-p+1}{3} + \frac{(a+b)(n-p)(n-p+1)}{2} + ab(n-p+1) + 2\binom{a}{2} + 2\binom{b}{2}.\end{aligned}$$

Using following inequalities:

$$2ab + 2\binom{a}{2} + 2\binom{b}{2} \leq (a+b)^2 = p^2,$$
$$ab \leq \frac{p^2}{4},$$
$$\binom{n-p+1}{3} \leq \frac{(n-p)^3}{6},$$

we obtain

$$\binom{n}{2}ad(T) \leq \frac{(n-p)^3}{6} + \frac{p(n-p)(n-p+1)}{2} + \frac{p^2(n-p+1)}{4} + p^2$$
$$= \frac{(n-p)^3}{6} + \frac{p(n-p)^2}{2} + \frac{p(n-p)}{2} + \frac{p^2(n-p)}{4} + \frac{5p^2}{4}.$$

For the sake of simplicity we put $x = p$, $y = n - p$.

$$\binom{n}{2}ad(T) \leq \frac{y^3}{6} + \frac{xy^2}{2} + \frac{xy}{2} + \frac{x^2y}{4} + \frac{5x^2}{4}.$$

In order to prove the lemma it is enough to show the following inequality:

$$(\binom{n}{2})(\frac{n-p-2}{2} + \frac{p-1}{\sqrt{p+1}} + 1.025 - max(0, \frac{p-1}{\sqrt{p+1}} - 2) - ad(T)) \geq 0.$$

Now multiply the expression by 4 , put x, y instead of $p, n-p$ and use the previously obtained inequality for $\binom{n}{2}ad(T)$

$$4(\binom{n}{2})(\frac{n-p-2}{2} + \frac{p-1}{\sqrt{p+1}} + 1.025 - max(0, \frac{p-1}{\sqrt{p+1}} - 2) - ad(T))$$
$$= 2(x+y)(x+y-1)(\frac{y-2}{2} + min(\frac{x-1}{\sqrt{x+1}} + 1.025, 3.025)) - 4ad(T)\binom{n}{2}$$
$$\geq 2(x^2 + y^2 + 2xy - x - y)(min(\frac{x-1}{\sqrt{x+1}} + 1.025, 3.025)) - 7xy - 3y^2 - 7x^2 + 2x$$
$$+ 2y + \frac{y^3}{3}.$$

We consider two cases. Either $p = x = 3$ or $p = x \geq 4$. If $x = 3$ from the above expression we obtain

$$2(y^2 + 5y + 6)(min(\frac{2}{\sqrt{4}} + 1.025, 3.025)) - 19y - 3y^2 + \frac{y^3}{3} - 57$$
$$\geq 4(y^2 + 5y + 6) + \frac{y^3}{3} - 3y^2 - 19y - 57$$
$$= \frac{y^3}{3} + y^2 + y + 9.$$

Using the assumption $p \leq n-2$ which is equivalent to $y \geq 2$, we obtain

$$\frac{y^3}{3} + y^2 + y + 9 \geq \frac{53}{3} \geq 0.$$

Now we assume $x \geq 4$. Hence $min(\frac{x-1}{\sqrt{x+1}} + 1.025, 3.025) \geq 2.4$. Since $x, y \geq 2$, then $xy \geq x+y$, so we have

$$\begin{aligned}&(2x^2 + 2y^2 + 4xy - 2x - 2y)2.4 - 7xy - 3y^2 - 7x^2 + 2x + 2y + \frac{y^3}{3} \\ &= \frac{y^3}{3} - 2.2x^2 - 1.2y^2 + 2.6xy - (2.8x + 6y) \geq 0.\end{aligned}$$

This the proof of the lemma. □

In Lemma 2.1 we proved Theorem 2.1 for paths and stars whereas by Lemmas 2.2 and 2.3 together with Corollary 2.2 we obtain the inequality for all other trees, thus completing the proof of Theorem 2.1. □

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