Research Article

Minimum Variable Connectivity Index of Trees of a Fixed Order

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The connectivity index, introduced by the chemist Milan Randić in 1975, is one of the topological indices with many applications. In the first quarter of 1990s, Randić proposed the variable connectivity index by extending the definition of the connectivity index. The variable connectivity index for graph G is defined as $\sum_{vw \in E(G)} ((d(v) + \gamma)(d(w) + \gamma))^{-1/2}$, where γ is a nonnegative real number, $E(G)$ is the edge set of G , and $d(t)$ denotes the degree of an arbitrary vertex t in G . Soon after the innovation of the variable connectivity index, its various chemical applications have been reported in different papers. However, to the best of the authors' knowledge, mathematical properties of the variable connectivity index, for $\gamma > 0$, have not yet been discussed explicitly in any paper. The main purpose of the present paper is to fill this gap by studying this topological index in a mathematical point of view. More precisely, in this paper, we prove that the star graph has the minimum variable connectivity index among all trees of a fixed order n , where $n \geq 4$.

1. Introduction

All the graphs that we discuss in the present study are simple, connected, undirected, and finite. For a graph $G = (V, E)$, the number $|V(G)|$ is called its order, and $|E(G)|$ is the size of G . Neighbor of a vertex $v \in V(G)$ is a vertex adjacent to v . The set of all neighbors of vertex v of G is denoted by $N(v)$. The number $|N(v)|$ is called the degree of a vertex, $v \in G$, and it is denoted by $d(v)$. If $d(v) = 1$, then v is called a pendent vertex or a leaf. A graph of order n is called an n -vertex graph. Denote by P_n and S_n the n -vertex path graph and the n -vertex star graph, respectively. The class of all n -vertex trees is denoted by T_n . For the (chemical) graph theoretical notation and terminology that are not defined in this paper, refer to [1, 2].

One of the fundamental ideas in CGT (chemical graph theory) is molecular connectivity. Chemical behavior of a compound is dependent upon its structure. QSPR/QSAR (quantitative structure-property/activity relationship)

studies are progressive fields of chemical research that focus on the behavior of this dependency. The quantitative relationships are mathematical models that either enable the prediction of a continuous variable (e.g., boiling point and LC_{50} toxicity) or the classification of a discrete variable (e.g., sweet/bitter and toxic/nontoxic) from structural parameters. Actually, CGT has provided many topological indices that have been and are being used in QSPR/QSAR studies for predicting the physicochemical properties of chemical compounds. Topological indices are those graph invariants that found some applications in chemistry [3–6]. For further details about the topological indices and their applications, refer to [3, 7–11] and the references therein.

Molecules can be modeled using graphs in which vertices correspond to atoms of the considered molecules, and the edges correspond to the covalent bonds between atoms [6]. To model the heteroatom molecules, it is better to use the vertex-weighted graphs, which are the graphs whose one or more vertices are distinguished in some way from the rest of

the vertices [12]. Let G be a vertex-weighted graph with the vertex set $\{v_1, v_2, \dots, v_n\}$, and let w_i be the weight of the vertex v_i for $i = 1, 2, \dots, n$. The augmented vertex-adjacency matrix of G is an $n \times n$ matrix denoted by ${}^{av}\mathbf{A}(G)$ and is defined as ${}^{av}\mathbf{A}(G) = [a_{i,j}]_{n \times n}$ where

$$a_{i,j} = \begin{cases} 1, & \text{if } v_i v_j \in E(G); \\ w_i, & \text{if } i = j; \\ 0, & \text{otherwise.} \end{cases} \quad (1)$$

The variable connectivity index [13, 14], proposed by Randić, for graph G is defined as

$${}^1\chi^f(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{(d(v_i) + w_i)(d(v_j) + w_j)}} \quad (2)$$

We associate this index's name with its inventor Randić by calling it as the variable Randić index. This index was actually introduced within the QSPR/QSAR studies of heteroatom molecules. If G is the molecular graph of a homoatomic molecule, then $w_1 = w_2 = \dots = w_n = \gamma$ (say), and hence, the variable Randić index ${}^1\chi^f(G)$ becomes

$${}^1\chi^f(G) = {}^vR_\gamma(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{(d(v_i) + \gamma)(d(v_j) + \gamma)}} \quad (3)$$

In the rest of this paper, we denote this index by ${}^vR_\gamma$ instead of ${}^1\chi^f$. Clearly, if we take $\gamma = 0$, then the invariant

${}^vR_\gamma(G)$ is the classical Randić index [10, 15]. Liu and Zhong [5] showed that the variable Randić index has more flexibility in characterizing polymers, which can lead to simpler correlations with better correlative accuracy. Details about the chemical applications of the variable Randić index can be found in [5, 7, 9, 12, 15–22] and related references listed therein. It needs to be mentioned here that the variable Randić index seems to have more chemical applications than the several well-known variable indices, for example, the indices considered in [23–33]. However, to the best of the authors' knowledge, mathematical properties of the variable Randić index, for $\gamma > 0$, have not yet been discussed explicitly in any paper. The main purpose of the present paper is to fill this gap by studying this topological index in a mathematical point of view. Since the trees (that are the connected graphs without cycles) form an important class of graphs both in chemical graph theory as well as in general graph theory, in this paper, we study an extremal problem related to the variable Randić index of the class of trees. We prove that the star graph S_n has the minimum variable Randić index among all trees of a fixed order n , where $n \geq 4$.

2. Main Result

To establish the main result, we prove a lemma first.

Lemma 1. *If $\gamma \geq 0$ and $s, t \geq 2$, then function f defined as*

$$f(\gamma, s, t) = (s + t - 1)\sqrt{s + t - 1 + \gamma} - (s - 1)\sqrt{s + \gamma} - (t - 1)\sqrt{t + \gamma} - \sqrt{\frac{(s + \gamma)(t + \gamma)}{1 + \gamma}}, \quad (4)$$

is positive-valued.

Proof. We note that the function $\partial f / \partial s$ is strictly increasing in t on the interval $(1, \infty)$ because

$$\begin{aligned} \frac{\partial f}{\partial s} &= \sqrt{s + t - 1 + \gamma} + \frac{s + t - 1}{2\sqrt{s + t - 1 + \gamma}} - \sqrt{s + \gamma} - \frac{s - 1}{2\sqrt{s + \gamma}} - \frac{\sqrt{t + \gamma}}{2\sqrt{(1 + \gamma)(s + \gamma)}}, \\ \frac{\partial}{\partial t} \left(\frac{\partial f}{\partial s} \right) &= \frac{3\sqrt{(1 + \gamma)(t + \gamma)(s + \gamma)} - \sqrt{s + t - 1 + \gamma}}{4\sqrt{(1 + \gamma)(t + \gamma)(s + \gamma)}\sqrt{s + t - 1 + \gamma}} + \frac{\gamma}{4(s + t - 1 + \gamma)^{3/2}} > 0, \end{aligned} \quad (5)$$

where the last inequality holds because

$$(\gamma + 1)(s + \gamma)(t + \gamma) \geq (s + \gamma)(t + \gamma) > (s + \gamma) + (t + \gamma) - 1 \geq s + t + \gamma - 1. \quad (6)$$

Also, note that the value of the function $\partial f / \partial s$ at $t = 1$ is 0, which implies that the function $\partial f / \partial s$ is positive-valued for $t > 1$, and hence, function f is strictly increasing in s on the interval $(1, \infty)$. Due to the identity $f(\gamma, s, t) = f(\gamma, t, s)$, function f is strictly increasing also in t on the interval

$(1, \infty)$. It holds that $f(\gamma, 1, t) = f(\gamma, t, 1) = 0$, and hence, $f(\gamma, s, t) > 0$ for all $s, t > 1$ and $\gamma \geq 0$. $\square$

Transformation 1. For $n \geq 4$, let T be a tree of order n containing at least two nonpendent vertices. Let $u \in V(T)$ be

a vertex of maximum degree, and let $N_T(u) = \{v, u_1, u_2, \dots, u_{s-1}\}$, where $d(v) \geq d(u_i)$ for $i = 1, 2, \dots, s-1$. Also, take $N_T(v) = \{u, v_1, v_2, \dots, v_{t-1}\}$. Note that $s \geq t \geq 2$. We transform T into another tree T' by removing the edges $vv_1, vv_2, \dots, vv_{t-1}$ and adding the edges $uv_1, uv_2, \dots, uv_{t-1}$.

Lemma 2. Let T and T' be the trees defined in Transformation 1. For $\gamma \geq 0$, it holds that

$${}^vR_\gamma(T') < {}^vR_\gamma(T). \quad (7)$$

Proof. By using the definition of the variable Randić index, one has

$$\begin{aligned} {}^vR_\gamma(T) - {}^vR_\gamma(T') &= \sum_{i=1}^{s-1} [f(s, d(u_i)) - f(s+t-1, d(u_i))] \\ &\quad + \sum_{i=1}^{t-1} [f(t, d(v_i)) - f(s+t-1, d(v_i))] \\ &\quad + f(s, t) - f(s+t-1, 1), \end{aligned} \quad (8)$$

where

$$f(a, b) = \frac{1}{\sqrt{(a+\gamma)(b+\gamma)}}. \quad (9)$$

Equation (8) gives

$$\begin{aligned} {}^vR_\gamma(T) - {}^vR_\gamma(T') &= \sum_{i=1}^{s-1} f(s, d(u_i)) \left[1 - \frac{f(s+t-1, d(u_i))}{f(s, d(u_i))} \right] \\ &\quad + \sum_{i=1}^{t-1} f(t, d(v_i)) \left[1 - \frac{f(s+t-1, d(v_i))}{f(t, d(v_i))} \right] \\ &\quad + f(s, t) - f(s+t-1, 1) \\ &= \sum_{i=1}^{s-1} f(s, d(u_i)) \left(1 - \frac{\sqrt{s+\gamma}}{\sqrt{s+t-1+\gamma}} \right) \\ &\quad + \sum_{i=1}^{t-1} f(t, d(v_i)) \left(1 - \frac{\sqrt{t+\gamma}}{\sqrt{s+t-1+\gamma}} \right) \\ &\quad - \frac{1}{\sqrt{(1+\gamma)(s+t-1+\gamma)}} + \frac{1}{\sqrt{(s+\gamma)(t+\gamma)}}. \end{aligned} \quad (10)$$

Since the vertex $u \in V(T)$ has the maximum degree, that is, $d(u) = s \geq d(w)$ for every $w \in V(T)$ and $d(v) = t \geq d(u_i)$ for $i = 1, 2, \dots, s-1$, thus, $f(s, d(u_i)) \geq f(s, t)$ and $f(t, d(v_i)) \geq f(t, s) = f(s, t)$. Hence, equation (10) yields

$$\begin{aligned} {}^vR_\gamma(T) - {}^vR_\gamma(T') &\geq \frac{s-1}{\sqrt{(s+\gamma)(t+\gamma)}} \left(1 - \frac{\sqrt{s+\gamma}}{\sqrt{s+t-1+\gamma}} \right) \\ &\quad + \frac{t-1}{\sqrt{(s+\gamma)(t+\gamma)}} \left(1 - \frac{\sqrt{t+\gamma}}{\sqrt{s+t-1+\gamma}} \right) \\ &\quad - \frac{1}{\sqrt{(1+\gamma)(s+t-1+\gamma)}} + \frac{1}{\sqrt{(s+\gamma)(t+\gamma)}} \\ &= \frac{s-1}{\sqrt{(s+\gamma)(t+\gamma)}} + \frac{t-1}{\sqrt{(s+\gamma)(t+\gamma)}} + \frac{1}{\sqrt{(t+\gamma)(s+\gamma)}} \\ &\quad - \frac{s-1}{\sqrt{(t+\gamma)(s+t-1+\gamma)}} - \frac{t-1}{\sqrt{(s+\gamma)(s+t-1+\gamma)}} \\ &\quad - \frac{1}{\sqrt{(1+\gamma)(s+t-1+\gamma)}} \\ &= \frac{1}{\sqrt{(s+\gamma)(t+\gamma)(s+t-1+\gamma)}} [(s+t-1)\sqrt{s+t-1+\gamma} \\ &\quad - (s-1)\sqrt{s+\gamma} - (t-1)\sqrt{t+\gamma} - \sqrt{\frac{(s+\gamma)(t+\gamma)}{1+\gamma}}]. \end{aligned} \quad (11)$$

By using Lemma 1 in (11), we get ${}^vR_\gamma(T) - {}^vR_\gamma(T') > 0$, as desired.

Next result is a direct consequence of Lemma 2. $\square$

Theorem 1. For $n \geq 4$ and $\gamma \geq 0$, among all trees of a fixed order n , star graph S_n is the unique tree with minimum variable Randić index ${}^vR_\gamma$, which is

$$\frac{n-1}{\sqrt{(n-1+\gamma)(1+\gamma)}}. \quad (12)$$

For $\gamma \geq 0$ and small values of n , we calculate the variable Randić index ${}^vR_\gamma$ of the trees of order n and find that the value of this index does not exceed from

$${}^vR_\gamma(P_n) = \frac{2}{\sqrt{(1+\gamma)(2+\gamma)}} + \frac{n-3}{2+\gamma}. \quad (13)$$

This suggests the following conjecture.

Conjecture 1. For $n \geq 4$ and $\gamma \geq 0$, among all trees of a fixed order n , path graph P_n is the unique tree with maximum variable Randić index ${}^vR_\gamma$, which is

$$\frac{2}{\sqrt{(1+\gamma)(2+\gamma)}} + \frac{n-3}{2+\gamma}. \quad (14)$$

Data Availability

There are no data concerning the present study except those presented in this manuscript.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

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