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Maximum Variable Connectivity Index of n-Vertex Trees

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ABSTRACT

In QSAR and QSPR studies the most commonly used topological index was proposed by chemist Milan Randić in 1975 called Randić branching index or path-one molecular connectivity index, 1χ and it has many applications. In the extension of connectivity indices, in early 1990s, chemist Milan Randic´ introduced variable Randić index defined as

$$\sum_{v_1v_2\in E(G)}\left((\mathrm{d}_{v_1}+\vartheta_*)(\mathrm{d}_{v_2}+\vartheta_*)\right)^{-1/2},$$

where ϑ_* is a non-negative real number and d_{v_1} is the degree of vertex v_1 in G. The main objective of the present study is to prove the conjecture proposed in [19]. In this study, we will show that the P_n (path graph) has the maximum variable connectivity index among the collection of trees whose order is n, where $n \geq 4$.

1. INTRODUCTION

In the present study, graphs under discussion are connected, finite, without loops and undirected. The number of vertices and number of edges in a graph $G = (V, E)$ are defined as order and size, respectively. A vertex adjacent to a vertex t is called neighbor of

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$t \in V(G)$ and $N(t)$ represents the collection of all neighbor vertices of t. $N(t)$ is called degree of the vertex $t \in G$ and we denote it by d_t. The vertex t is said to be pendent vertex or a leaf if $d_t = 1$. n-vertex graph means a graph whose order is n. P_n and S_n are well-known n-vertex path graph and the n-vertex star graph, respectively. T_n presents the collection of all n-vertex trees. For the relevant (chemical graph theoretical) symbols and undefined terms in this study, we suggest the reader to relevant book, as [8].

The variable Randić index [15, 14], introduced by Randić, for the graph H is defined as:

$$^{1}\chi^{f}(H) = {}^{v}\mathrm{R}_{\vartheta_*}(H) = \sum_{v_i v_j \in E(H)} \frac{1}{\sqrt{(\mathrm{d}_{v_i} + \vartheta_*)(\mathrm{d}_{v_j} + \vartheta_*)}},$$

where d_{v_1} is the degree of vertex v_1 in H and ϑ_* is a non-negative real number.Clearly, the topological index ${}^{v}\mathrm{R}_{\vartheta_*}(G)$ is the classical Randić index if we consider $\vartheta_* = 0$[16, 17]. Detailed chemical properties of the variable Randić index can be seen in [11, 12, 13, 16, 6, 18, 19] and related references therein. It is important to mention that the invariant ${}^{v}\mathrm{R}_{\vartheta_*}$ has more chemical applications than the various popular variable indices [3, 9, 10, 4, 7, 5, 2, 1].

Conjecture 1.1. [19] 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 ${}^{v}\mathrm{R}_{\gamma}$, which is

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

Since trees are important molecular structures in chemistry, in the following we only deal with trees i.e. connected graphs without cycles. Recently, Yousaf et al. [19] determined the graph with maximum ${}^{v}\mathrm{R}_{\vartheta_*}$ value among all the class of trees is path and thereby confirmed the Conjecture 1.1. We prove the Conjecture 1.1 by determining that the path graph P_n has the maximum variable Randić index among the collection of trees of a fixed order n, where $n \geq 4$.

2. MAIN RESULTS

To establish the main results, we prove some lemmas first. A vertex of graph is said to be a claw if all of its neighbors, except one, are leaves.

Theorem 2.1. [19] 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 ${}^{v}R_{\gamma}$, which is

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

Lemma 2.1. For $\vartheta_* \geq 0$, it holds that

$$\Phi(3,s,\vartheta_*) = \frac{1}{\sqrt{3+\vartheta_*}}\left(\frac{1}{\sqrt{1+\vartheta_*}} + \frac{1}{\sqrt{3+\vartheta_*}}\right) - \frac{2}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} < 0.$$

Proof. Since $\Phi(3,s,\vartheta_*) = \frac{1}{\sqrt{3+\vartheta_*}}\left(\frac{1}{\sqrt{1+\vartheta_*}} + \frac{1}{\sqrt{3+\vartheta_*}}\right) - \frac{2}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}$,

$$\begin{aligned}\Phi(3,s,\vartheta_*) &= \frac{1}{(2+\vartheta_*)\sqrt{(1+\vartheta_*)(3+\vartheta_*)}}\left(\frac{1}{(2+\vartheta_*)+\sqrt{(1+\vartheta_*)(3+\vartheta_*)}} - \frac{\sqrt{1+\vartheta_*}}{\sqrt{3+\vartheta_*}}\right)\\ &= \frac{1}{(2+\vartheta_*)\sqrt{(1+\vartheta_*)(3+\vartheta_*)}}\left(\frac{\sqrt{3+\vartheta_*}-\vartheta_*\sqrt{1+\vartheta_*}-2\sqrt{1+\vartheta_*}-(1+\vartheta_*)\sqrt{3+\vartheta_*}}{\sqrt{3+\vartheta_*}\left\{(2+\vartheta_*)+\sqrt{(1+\vartheta_*)(3+\vartheta_*)}\right\}}\right)\\ &= \frac{1}{(2+\vartheta_*)\sqrt{(1+\vartheta_*)(3+\vartheta_*)}}\left(\frac{-\vartheta_*\sqrt{1+\vartheta_*}-2\sqrt{1+\vartheta_*}-\vartheta_*\sqrt{3+\vartheta_*}}{\sqrt{3+\vartheta_*}\left\{(2+\vartheta_*)+\sqrt{(1+\vartheta_*)(3+\vartheta_*)}\right\}}\right) < 0,\end{aligned}$$

proving the lemma. ∎

Lemma 2.2. If $\vartheta_* \geq 0$ and $r \geq 3$ then the function Ψ defined as

$$\Psi(\vartheta_*,r) = 4(r+\vartheta_*)^{3/2}(r-1+\vartheta_*)^{3/2} - 4(r+\vartheta_*)(r-1+\vartheta_*)^2 - (r-1)(2r-1+2\vartheta_*)$$

gives positive real numbers.

Proof. Let $\Psi(\vartheta_*,r) = 4(r+\vartheta_*)^{3/2}(r-1+\vartheta_*)^{3/2} - 4(r+\vartheta_*)(r-1+\vartheta_*)^2 - (r-1)(2r-1+2\vartheta_*)$. We have to show that $\Psi(\vartheta_*,r) > 0$ implies that

$$4(r+\vartheta_*)^{3/2}(r-1+\vartheta_*)^{3/2} - 4(r+\vartheta_*)(r-1+\vartheta_*)^2 - (r-1)(2r-1+2\vartheta_*) > 0,$$

which can be rewritten as

$$16(r+\vartheta_*)^3(r-1+\vartheta_*)^3 - \{4(r+\vartheta_*)(r-1+\vartheta_*)^2 - (r-1)(2r-1+2\vartheta_*)\}^2 > 0.$$

Let

$$\begin{aligned}\Psi_1(\vartheta_*,r) &= 16(r+\vartheta_*)^3(r-1+\vartheta_*)^3\\ &\quad -(4(r+\vartheta_*)(r-1+\vartheta_*)^2 - (r-1)(2r-1+2\vartheta_*))^2.\end{aligned}$$

Then,

$$\begin{aligned}\Psi_1(\vartheta_*,r) &= 16r^4\vartheta_* + 64r^3{\vartheta_*}^2 + 96r^2{\vartheta_*}^3 + 64r{\vartheta_*}^4 + 16{\vartheta_*}^5 + 4r^4\\ &\quad -16r^3\vartheta_* - 76r^2{\vartheta_*}^2 - 88r{\vartheta_*}^3 - 32{\vartheta_*}^4 - 12r^3 - 20r^2\vartheta_* + 8{\vartheta_*}^3\\ &\quad +11r^2 + 24r\vartheta_* + 12{\vartheta_*}^2 - 2r - 4\vartheta_* - 1.\\ &= (r-1)^2\{4r(r-1)-1\} + 4{\vartheta_*}^2(r-1)(16r^2-3r-3)\\ &\quad +8r{\vartheta_*}^3(12r-11) + 4r^2\vartheta_*\{(2r-1)^2-6\} + 4\vartheta_*(6r-1)\\ &\quad +16{\vartheta_*}^5 + 8{\vartheta_*}^3 > 0.\end{aligned}$$

Hence the lemma is proved. ∎

Lemma 2.3. If $\vartheta_* \geq 0$ and $r \geq 3$, then the function Θ_1 defined as

$$\Theta_1(\vartheta_*, r) = 2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}-\frac{r-1}{r-1+\vartheta_*}-\frac{r-1}{2(r-1+\vartheta_*)^2}$$

gives positive real numbers.

Proof. Let $\Theta_1(\vartheta_*, r) = 2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}-\frac{r-1}{r-1+\vartheta_*}-\frac{r-1}{2(r-1+\vartheta_*)^2}$. Then,

$$\begin{aligned}\Theta_1(\vartheta_*, r) &= \frac{2(r+\vartheta_*)^{3/2}(r-1+\vartheta_*)^{3/2}}{(r-1+\vartheta_*)^2}+2(r+\vartheta_*)-\frac{r-1}{r-1+\vartheta_*}-\frac{r-1}{2(r-1+\vartheta_*)^2}\\ &= \frac{4(r+\vartheta_*)^{3/2}(r-1+\vartheta_*)^{3/2}-4(r+\vartheta_*)(r-1+\vartheta_*)^2-4(r-1)(2r-1+2\vartheta_*)}{2(r-1+\vartheta_*)^2}\\ &= \frac{1}{2(r-1+\vartheta_*)^2}[\Psi(\vartheta_*, r)] > 0,\end{aligned}$$

where $\Psi(\vartheta_*, r) = 4(r+\vartheta_*)^{3/2}(r-1+\vartheta_*)^{3/2}-4(r+\vartheta_*)(r-1+\vartheta_*)^2-4(r-1)(2r-1+2\vartheta_*)$. Now by Lemma 2.2, one can see that $\Psi(\vartheta_*, r) > 0$. ■

Lemma 2.4. If $\vartheta_* \geq 0$ and $r, s \geq 3$, then the function Θ_2 defined as $\Theta_2(\vartheta_*, r, s) = 1-\frac{r-1}{2(r-1+\vartheta_*)}-\frac{s-1}{2(s-1+\vartheta_*)}$ gives non-negative real numbers.

Proof. Note that $\Theta_2(\vartheta_*, r, s) = 1-\frac{r-1}{2(r-1+\vartheta_*)}-\frac{s-1}{2(s-1+\vartheta_*)}$ $\Theta_2(\vartheta_*, r, s) = \frac{\vartheta_*(r+s-2+2\vartheta_*)}{2(r-1+\vartheta_*)(s-1+\vartheta_*)}$ ≥ 0, proving the lemma. ■

Lemma 2.5. If $\vartheta_* \geq 0$ and $r, s \geq 3$, then the function g defined as

$$\begin{aligned}g(r,s,\vartheta_*) &= 2\sqrt{s-1+\vartheta_*}\left\{\sqrt{r+\vartheta_*}-\sqrt{r-1+\vartheta_*}\right\}\\ &\quad+(r-1)\sqrt{s-1+\vartheta_*}\left\{\frac{\sqrt{r-1+\vartheta_*}}{r+\vartheta_*}-\frac{\sqrt{r+\vartheta_*}}{r-1+\vartheta_*}\right\}\\ &\quad-\frac{(s-1)\sqrt{r-1+\vartheta_*}}{r+\vartheta_*}\left\{\sqrt{s+\vartheta_*}-\sqrt{s-1+\vartheta_*}\right\}\\ &\quad+\frac{1}{r+\vartheta_*}\left\{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}\right\},\end{aligned}$$

is positive-valued.

Proof. Let

$$\begin{aligned}g(r,s,\vartheta_*) &= 2\sqrt{s-1+\vartheta_*}\left\{\sqrt{r+\vartheta_*}-\sqrt{r-1+\vartheta_*}\right\}\\ &\quad+(r-1)\sqrt{s-1+\vartheta_*}\left\{\frac{\sqrt{r-1+\vartheta_*}}{r+\vartheta_*}-\frac{\sqrt{r+\vartheta_*}}{r-1+\vartheta_*}\right\}\end{aligned}$$

$$-\frac{(s-1)\sqrt{r-1+\vartheta_*}}{r+\vartheta_*}\left\{\sqrt{s+\vartheta_*}-\sqrt{s-1+\vartheta_*}\right\}$$
$$+\frac{1}{r+\vartheta_*}\left\{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}\right\}.$$

Then, one can see that

$$g(r,s,\vartheta_*)=\frac{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}}{r+\vartheta_*}\left[2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}+(r-1)\left\{1-\left(\frac{r+\vartheta_*}{r-1+\vartheta_*}\right)^{3/2}\right\}-(s-1)\left\{\sqrt{\frac{s+\vartheta_*}{s-1+\vartheta_*}}-1\right\}+1\right].$$
$$=\frac{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}}{r+\vartheta_*}\left[2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}+(r-1)\left\{1-\left(1+\frac{1}{r-1+\vartheta_*}\right)\left(1+\frac{1}{r-1+\vartheta_*}\right)^{1/2}\right\}-(s-1)\left\{\sqrt{1+\frac{1}{s-1+\vartheta_*}}-1\right\}+1\right].$$

Since $\sqrt{1+\frac{1}{r-1+\vartheta_*}}\le 1+\frac{1}{2(r-1+\vartheta_*)}$,

$$g(r,s,\vartheta_*)\ge\frac{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}}{r+\vartheta_*}\left[2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}+(r-1)\left\{1-\left(1+\frac{1}{r-1+\vartheta_*}\right)\left(1+\frac{1}{2(r-1+\vartheta_*)}\right)\right\}-(s-1)\left\{1+\frac{1}{2(s-1+\vartheta_*)}-1\right\}+1\right]$$

and so

$$g(r,s,\vartheta_*)\ge\frac{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}}{r+\vartheta_*}\left[2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}-\frac{3(r-1)}{2(r-1+\vartheta_*)}-\frac{r-1}{2(r-1+\vartheta_*)^2}-\frac{s-1}{2(s-1+\vartheta_*)}+1\right].$$

Therefore,

$$g(r,s,\vartheta_*)\ge\frac{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}}{r+\vartheta_*}\left[2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}-\frac{r-1}{r-1+\vartheta_*}-\frac{r-1}{2(r-1+\vartheta_*)}-\frac{r-1}{2(r-1+\vartheta_*)^2}-\frac{s-1}{2(s-1+\vartheta_*)}+1\right]$$

which implies that $g(r,s,\vartheta_*)\ge\frac{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}}{r+\vartheta_*}\left[\Theta_1(r,\vartheta_*)+\Theta_2(r,s,\vartheta_*)\right]>0$, where $\Theta_1(\vartheta_*,r)$ and $\Theta_2(r,s,\vartheta_*)$ are defined as follows:

$$\Theta_2(\vartheta_*,r,s)=1-\frac{r-1}{2(r-1+\vartheta_*)}-\frac{s-1}{2(s-1+\vartheta_*)},$$

and

$$\Theta_1(\vartheta_*,r)=2(r+\vartheta_*)\left\{\sqrt{\frac{r+\vartheta_*}{r-1+\vartheta_*}}-1\right\}-\frac{r-1}{r-1+\vartheta_*}-\frac{r-1}{2(r-1+\vartheta_*)^2}.$$

There quantities are greater than or equal to zero by Lemma 2.3 and Lemma 2.4. ■

Lemma 2.6. If $\vartheta_* \geq 0$ and $r, s \geq 3$, then the function h defined as

$$h(r,s,\vartheta_*) = \frac{r-1}{\sqrt{s+\vartheta_*}}\left(\frac{1}{\sqrt{r-1+\vartheta_*}} - \frac{1}{\sqrt{r+\vartheta_*}}\right) + \frac{s-1}{\sqrt{r+\vartheta_*}}\left(\frac{1}{\sqrt{s-1+\vartheta_*}} - \frac{1}{\sqrt{s+\vartheta_*}}\right) - \frac{1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}} + \frac{3}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} - \frac{2}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}$$

is positive-valued.

Proof. Let

$$h(r,s,\vartheta_*) = \frac{r-1}{\sqrt{s+\vartheta_*}}\left(\frac{1}{\sqrt{r-1+\vartheta_*}} - \frac{1}{\sqrt{r+\vartheta_*}}\right) + \frac{s-1}{\sqrt{r+\vartheta_*}}\left(\frac{1}{\sqrt{s-1+\vartheta_*}} - \frac{1}{\sqrt{s+\vartheta_*}}\right) - \frac{1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}} + \frac{3}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} - \frac{2}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}.$$

We compute the partial derivative to prove the desired inequality.

$$\frac{\partial h}{\partial r} = \frac{1}{\sqrt{s+\vartheta_*}}\left(\frac{1}{\sqrt{r-1+\vartheta_*}} - \frac{1}{\sqrt{r+\vartheta_*}}\right) + \frac{r-1}{2\sqrt{s+\vartheta_*}}\left(\frac{1}{(r+\vartheta_*)^{3/2}} - \frac{1}{(r-1+\vartheta_*)^{3/2}}\right) - \frac{s-1}{2(r+\vartheta_*)^{3/2}}\left(\frac{1}{\sqrt{s-1+\vartheta_*}} + \frac{1}{\sqrt{s+\vartheta_*}}\right) + \frac{1}{2(r+\vartheta_*)^{3/2}\sqrt{(s+\vartheta_*)}}.$$

$$\frac{\partial h}{\partial r} = \frac{1}{2\sqrt{(s+\vartheta_*)(r+\vartheta_*)(r-1+\vartheta_*)(s-1+\vartheta_*)}}\Big[2\sqrt{s-1+\vartheta_*}\left\{\sqrt{r+\vartheta_*} - \sqrt{r-1+\vartheta_*}\right\} + (r-1)\sqrt{s-1+\vartheta_*}\left\{\frac{\sqrt{r-1+\vartheta_*}}{r+\vartheta_*} - \frac{\sqrt{r+\vartheta_*}}{r-1+\vartheta_*}\right\} - \frac{(s-1)\sqrt{r-1+\vartheta_*}}{r+\vartheta_*}\left\{\sqrt{s+\vartheta_*} - \sqrt{s-1+\vartheta_*}\right\} + \frac{1}{r+\vartheta_*}\left\{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}\right\}\Big].$$

$$\frac{\partial h}{\partial r} = \frac{1}{2\sqrt{(s+\vartheta_*)(r+\vartheta_*)(r-1+\vartheta_*)(s-1+\vartheta_*)}}[g(r,s,\vartheta_*],$$

where

$$g(r,s,\vartheta_*) = 2\sqrt{s-1+\vartheta_*}\left\{\sqrt{r+\vartheta_*} - \sqrt{r-1+\vartheta_*}\right\} + (r-1)\sqrt{s-1+\vartheta_*}\left\{\frac{\sqrt{r-1+\vartheta_*}}{r+\vartheta_*} - \frac{\sqrt{r+\vartheta_*}}{r-1+\vartheta_*}\right\} - \frac{(s-1)\sqrt{r-1+\vartheta_*}}{r+\vartheta_*}\left\{\sqrt{s+\vartheta_*} - \sqrt{s-1+\vartheta_*}\right\} + \frac{1}{r+\vartheta_*}\left\{\sqrt{r-1+\vartheta_*}\sqrt{s-1+\vartheta_*}\right\}.$$

Using Lemma 2.5, one can see that $\frac{\partial h}{\partial r} > 0$. Similarly $\frac{\partial h}{\partial s} > 0$. Also, it can be easily investigated that $h(3,2) > h(2,2) = 0$ which completes the proof. ■

Transformation 2.1. Let T be a tree of order $n \geq 4$ and $u_1 \in V(T)$ is a claw such that $d(u_1) = r \geq 3$. Define $N(u_1) = \{u_0, u_2, v_1, v_2, \dots, v_{r-2}\}$ such that $d(u_0) = 1$ and

, $d(v_i) = 1$, for each $1 \le i \le r-2$ and $d(u_2) = q \ge 1$. Construct $\acute{T} = T - \{u_0u_1, u_1v_1, u_1v_2, \dots, u_1v_{r-2}\} + \{v_1v_2, v_2v_3, \dots, u_0v_{r-2}, u_0u_1\}$.

Lemma 2.7. Let $\acute{T}$ be a graph obtained from T by applying Transformation 2.1. Then for $\vartheta_* \ge 0$, ${}^{v}\mathrm{R}_{\vartheta_*}(T) < {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T})$.

Proof. For $n = 4$, there are only two trees namely S_4 (star graph) and P_4 (path graph), and hence the result follows from Theorem 2.1. In what follows, take $n \ge 5$. Since $d(u_1) = r \ge 3$. Let $N(u_1) = \{u_0, u_2, v_1, v_2, \dots, v_{r-2}\}$ such that $d(v_i) = 1$ for each $i \in \{1, 2, \dots, r-2\}$ and $d(u_2) = q \ge 1$. If T' is the tree deduced from T by applying Transformation 2.1, then we have,

$$\begin{aligned} {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = & \sum_{i=2}^{r-2}\left[\Gamma\big(d(u_1), d(v_i)\big) - \Gamma(2, d(v_i) + 1)\right] \\ & + [\Gamma(d(u_1), d(v_1)) - \Gamma(2, d(v_1))] \\ & + [\Gamma(d(u_1), d(u_0)) - \Gamma(2, d(u_0))] \\ & + \left[\Gamma\big(d(u_1), d(u_2)\big) - \Gamma\big(2, d(u_2)\big)\right] \end{aligned} \tag{1}$$

where $\Gamma(a,b) = \frac{1}{\sqrt{(a+\vartheta_*)(b+\vartheta_*)}}$. Equation (1) gives

$$\begin{aligned} {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = & \frac{r-3}{\sqrt{(r+\vartheta_*)(1+\vartheta_*)}} - \frac{r-3}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(r+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(1+\vartheta_*)}} \\ & + \frac{1}{\sqrt{(r+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(r+\vartheta_*)(2+\vartheta_*)}} - \frac{1}{\sqrt{(q+\vartheta_*)(2+\vartheta_*)}} \end{aligned} \tag{2}$$

In the following, we show that ${}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(T') < 0$. We note that Equation (2) can be re-written as

$$\begin{aligned} {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(T') = & \frac{(r-2)\left(\vartheta_* + 2 - \sqrt{(r+\vartheta_*)(1+\vartheta_*)}\right)}{(\vartheta_* + 2)\sqrt{(r+\vartheta_*)(1+\vartheta_*)}} \\ & + \left(\frac{1}{\sqrt{r+\vartheta_*}} - \frac{1}{\sqrt{2+\vartheta_*}}\right)\left(\frac{1}{\sqrt{1+\vartheta_*}} + \frac{1}{\sqrt{q+\vartheta_*}}\right) \end{aligned} \tag{3}$$

It can be easily observed that right hand side of Equation (3) is negative for all $r \ge 4$ and $\vartheta_* \ge 0$. Finally, for $r = 3$ and $\vartheta_* \ge 0$, Equation (2) yields

$$ {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(T') < \frac{\sqrt{3+\vartheta_*}\left\{1 - \sqrt{(2+\vartheta_*)(1+\vartheta_*)}\right\} - \sqrt{(2+\vartheta_*)}(1+\vartheta_*)}{\varsigma(\vartheta_*)} < 0. $$

where

$$\varsigma(\vartheta_*) = (2+\vartheta_*)\sqrt{(3+\vartheta_*)(1+\vartheta_*)}\left\{\sqrt{(2+\vartheta_*)} + \sqrt{(3+\vartheta_*)}\right\}\left\{(2+\vartheta_*) + \sqrt{(3+\vartheta_*)(1+\vartheta_*)}\right\}.$$

This completes the proof. ∎

Remark 2.1. If T is a tree with maximum variable connectvity index, then by repeating Transformation 2.1, any claw can be converted into a vertex of degree 2.

Lemma 2.8. If $T \in T_n$ is a tree with the maximum variable Randić index, then the neighbor of any pendent vertex must be of degree 2.

Proof. Let w be a pendent vertex of T and u_4 be its neighbor. Let $P = u_0u_1u_2\dots u_k$ be the longest path of T passing through u_4 with one end vertex is u_k and $u_{k-1}u_k \epsilon E(P)$. Lemma 2.7 implies that $d(u_{k-1}) = 2$. Let $d(u_4) = t \geq 3$, then there will be two cases as follows:

Case 1. $t > 3$**.** Construct the tree $\acute{T} = T - u_4w + wu_k$. Denote by $\acute{N}(u_4)$ the set of all neighbors of u_4 other than w and S_{u_4} the sum of the weights of all edges incident to u_4 other than wu_4. Then we have,

$$\begin{aligned} {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) &= \textstyle\sum_{x\in \acute{N}(\mathrm{u}_4)}\left[\Gamma\big(d(u_4), d(x)\big) - \Gamma\big(d(u_4)-1, d(x)\big)\right] \\ &\quad + \left[\Gamma(d(u_4), d(w)) - \Gamma(d(u_k)+1, d(w))\right] \\ &\quad + \left[\Gamma\big(d(u_k), d(u_{k-1})\big) - \Gamma(d(u_k)+1), d(u_{k-1}))\right], \end{aligned} \tag{4}$$

where $\Gamma(a,b) = \frac{1}{\sqrt{(a+\vartheta_*)(b+\vartheta_*)}}$. Equation (4) gives

$$\begin{aligned} {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) &= \textstyle\sum_{x\in \acute{N}(\mathrm{u}_4)}\left[\Gamma\big(d(u_4), d(x)\big)\left\{1 - \frac{\Gamma(d(u_4)-1, d(x))}{\Gamma(d(u_4), d(x))}\right\}\right] \\ &\quad + \left[\Gamma(d(u_4), d(w)) - \Gamma(d(u_k)+1, d(w))\right] \\ &\quad + \left[\Gamma\big(d(u_k), d(u_{k-1})\big) - \Gamma(d(u_k)+1), d(u_{k-1}))\right]. \end{aligned} \tag{5}$$

Equation (5) yields

$$\begin{aligned} {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) &= \mathrm{S}_{\mathrm{u}_4}\left(1 - \frac{\sqrt{t+\vartheta_*}}{\sqrt{t-1+\vartheta_*}}\right) + \frac{1}{\sqrt{(t+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}} \\ &\quad + \frac{1}{\sqrt{(2+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}. \end{aligned}$$

Hence,

$${}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = \mathrm{S}_{\mathrm{u}_4}\left(1 - \frac{\sqrt{t+\vartheta_*}}{\sqrt{t-1+\vartheta_*}}\right) + \frac{1}{\sqrt{(t+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}.$$

Since $t \geq 4$, we have $1 - \frac{\sqrt{t+\vartheta_*}}{\sqrt{t-1+\vartheta_*}} < 0$, also $\frac{1}{\sqrt{(t+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} < 0$. Thus, ${}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) < 0$. This contradicts our supposition.

Case 2. $t = 3$**.** Denote the neighbors of u_4 by $N(u_4) = \{u_3, u_5, w\}$ such that $d(u_3) = r \geq 2$ and $d(u_5) = s \geq 2$.

Sub-case 2(a). $r = 2$ or $s = 2$. Suppose $r = 2$ and u_2 be another neighbor of u_3 with $d(u_2) = l$. Define $\acute{T} = T - \{u_2u_3, u_3u_4\} + \{u_2u_4, u_3w\}$. Then T and $\acute{T}$ will be isomorphic if $l = 1$, so consider $l \geq 2$.

$$\begin{aligned} &{}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) \\ &\quad = \textstyle\sum_{x\in \acute{N}(\mathrm{u}_4)}\left[\Gamma\big(d(u_3), d(u_4)\big) - \Gamma(d(u_3)-1, d(w)+1)\right] \\ &\quad + \left[\Gamma(d(u_4), d(w)) - \Gamma(d(u_4), d(w)+1)\right] \\ &\quad + \left[\Gamma\big(d(u_2), d(u_3)\big) - \Gamma\big(d(u_2), d(u_4)\big)\right] \end{aligned} \tag{6}$$

where $\Gamma(a,b) = \frac{1}{\sqrt{(a+\vartheta_*)(b+\vartheta_*)}}$. Equation (6) gives

$$^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = \frac{1}{\sqrt{(r+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(r-1+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(3+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(3+\vartheta_*)}} + \frac{1}{\sqrt{(l+\vartheta_*)(r+\vartheta_*)}} - + \frac{1}{\sqrt{(l+\vartheta_*)(3+\vartheta_*)}}.$$

$$^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = \frac{1}{\sqrt{(2+\vartheta_*)(3+\vartheta_*)}} - \frac{1}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(3+\vartheta_*)(1+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(3+\vartheta_*)}} + \frac{1}{\sqrt{(l+\vartheta_*)(2+\vartheta_*)}} - \frac{1}{\sqrt{(l+\vartheta_*)(3+\vartheta_*)}}.$$

Thus,

$$^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = \frac{1}{\sqrt{l+\vartheta_*}}\left(\frac{1}{\sqrt{2+\vartheta_*}} - \frac{1}{\sqrt{3+\vartheta_*}}\right) + \frac{1}{\sqrt{1+\vartheta_*}}\left(\frac{1}{\sqrt{3+\vartheta_*}} - \frac{1}{\sqrt{2+\vartheta_*}}\right).$$

Since $l \geq 2$, $\quad {}^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = \left(\frac{1}{\sqrt{1+\vartheta_*}} - \frac{1}{\sqrt{l+\vartheta_*}}\right)\left(\frac{1}{\sqrt{3+\vartheta_*}} - \frac{1}{\sqrt{2+\vartheta_*}}\right) < 0,$

which is again a contradiction to our supposition.

Sub-case 2(b). If $r \geq 3$ and $s \geq 3$. Construct $\acute{T}$ from T by deleting the vertices $\{u_4, w\}$, adding the new edge u_3u_5 and a $2 - path$ to the end vertex of P, we get

$$\begin{aligned} ^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = & \left[\Gamma\big(d(u_3), d(u_4)\big) - \Gamma(2{,}2)\right] \\ & + [\Gamma(d(u_5), d(u_4)) - \Gamma(d(u_5), d(u_3))] \\ & + \left[\Gamma\big(d(w), d(u_4)\big) - \Gamma(2{,}2)\right] \end{aligned} \tag{7}$$

where $\Gamma(a,b) = \frac{1}{\sqrt{(a+\vartheta_*)(b+\vartheta_*)}}$. Equation (7) gives

$$^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) = \frac{1}{\sqrt{(r+\vartheta_*)(3+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(3+\vartheta_*)(s+\vartheta_*)}} - \frac{1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}} + \frac{1}{\sqrt{(1+\vartheta_*)(3+\vartheta_*)}} - \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}.$$

Let

$$\varphi(r,s,\vartheta_*) = \frac{1}{\sqrt{(r+\vartheta_*)(3+\vartheta_*)}} - \frac{2}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(3+\vartheta_*)(s+\vartheta_*)}} - \frac{1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}} + \frac{1}{\sqrt{(1+\vartheta_*)(3+\vartheta_*)}}.$$

By computing $\frac{\partial\varphi}{\partial r}$ and simplifying our calculations, we get

$$\frac{\partial\varphi}{\partial r} = \frac{-1}{2\sqrt{3+\vartheta_*}(r+\vartheta_*)^{\frac{3}{2}}} + \frac{1}{2\sqrt{s+\vartheta_*}(r+\vartheta_*)^{\frac{3}{2}}}$$

$$\frac{\partial\varphi}{\partial r} = \frac{1}{2(r+\vartheta_*)^{\frac{3}{2}}}\left(\frac{1}{\sqrt{s+\vartheta_*}} - \frac{1}{\sqrt{3+\vartheta_*}}\right) \leq 0, \text{ for } s \geq 3.$$

by Lemma 2.1, $\varphi(3,s,\vartheta_*) = \frac{1}{\sqrt{3+\vartheta_*}}\left(\frac{1}{\sqrt{1+\vartheta_*}} + \frac{1}{\sqrt{3+\vartheta_*}}\right) - \frac{2}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} < 0$,.

Hence, $^{v}\mathrm{R}_{\vartheta_*}(T) - {}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) < 0.$

This completes the proof. ∎

Transformation 2.2. Let $uv \epsilon E(T)$ such that $|T| = n$ and $P = u_0 u_1 u_2 \dots u_i u_{i+1} \dots u_k$ is the longest path of T where $d(u_i) = r \geq 3$ and $d(u_{i+1}) = s \geq 3$. Construct $\acute{T}$ from T by deleting the edge $u_i u_{i+1}$ and joining the end vertices of the longest path by an edge (join u_0 and u_k by an edge).

Lemma 2.9. Let $\acute{T}$ be a tree that is obtained after applying Transformation 2.2, for $\vartheta_* \geq 0$, it holds that ${}^{v}\mathrm{R}_{\vartheta_*}(\acute{T}) - {}^{v}\mathrm{R}_{\vartheta_*}(T) > 0$.

Proof. Choose an edge $u_i u_{i+1}$ such that $d(u_i) + d(u_{i+1})$ is maximum in T. Let v_j, $1 \leq j \leq r-1$ be the neighbors of u_i other than u_{i+1}. Similarly, $w_{\acute{j}}$, $1 \leq \acute{j} \leq s-1$ be the neighbors of u_{i+1} other than u_i. Since u_1 and u_{k-1} are neighbors of u_0 and u_k respectively; therefore, from Lemma 2.7 and 2.8, we know that $d(u_1) = d(u_{k-1}) = 2$. By the definition of the variable Randić index, one must have

$$
\begin{aligned}
{}^{v}R_{\vartheta_*}(\acute{T}) - {}^{v}R_{\vartheta_*}(T) = & \sum_{j=1}^{r-1} \left[\Gamma\left(\mathrm{d}(u_i) - 1, \mathrm{d}(v_j)\right) - \Gamma\left(d(u_i), d(v_j)\right)\right] \\
& + \sum_{\acute{j}=1}^{s-1} \left[\Gamma\left(d(u_{i+1}) - 1, d(w_{\acute{j}})\right) - \Gamma\left(d(u_{i+1}), d(w_{\acute{j}})\right)\right] \\
& + \Gamma\big(d(u_0) + 1, d(u_1)\big) - \Gamma\big(d(u_0), d(u_1)\big) \\
& + \Gamma\big(d(u_k) + 1, d(u_{k-1})\big) - \Gamma\big(d(u_k), d(u_{k-1})\big) \\
& + \Gamma(d(u_0) + 1, d(u_k) + 1) - \Gamma(r, s),
\end{aligned} \tag{9}
$$

where $\Gamma(a, b) = \frac{1}{\sqrt{(u+\vartheta_*)(b+\vartheta_*)}}$. Equation (9) gives

$$
\begin{aligned}
{}^{v}R_{\vartheta_*}(\acute{T}) - {}^{v}R_{\vartheta_*}(T) = & \sum_{j=1}^{r-1} \Gamma\left(d(u_i), d(v_j)\right) \left[\frac{\Gamma\left(d(u_i) - 1, d(v_i)\right)}{\Gamma\left(d(u_i), d(v_j)\right)} - 1\right] \\
& + \sum_{\acute{j}=1}^{s-1} \Gamma\left(d(u_{i+1}), d(w_{\acute{j}})\right) \left[\frac{\Gamma\left(d(u_{i+1}) - 1, d(w_{\acute{j}})\right)}{\Gamma\left(d(u_{i+1}), d(w_{\acute{j}})\right)} - 1\right] \\
& + \Gamma\big(d(u_0) + 1, d(u_1)\big) - \Gamma\big(d(u_0), d(u_1)\big) \\
& + \Gamma\big(d(u_k) + 1, d(u_{k-1})\big) - \Gamma\big(d(u_k), d(u_{k-1})\big) \\
& + \Gamma(d(u_0) + 1, d(u_k) + 1) - \Gamma(r, s)
\end{aligned}
$$

So,

$$
\begin{aligned}
R_{\vartheta_*}(\acute{T}) - {}^{v}R_{\vartheta_*}(T) = & \sum_{j=1}^{r-1} \Gamma\left(r, d(v_j)\right) \left[\frac{\sqrt{r+\vartheta_*}}{\sqrt{r-1+\vartheta_*}} - 1\right] \\
& + \sum_{\acute{j}=1}^{s-1} \Gamma\left(s, d(w_{\acute{j}})\right) \left[\frac{\sqrt{s+\vartheta_*}}{\sqrt{s-1+\vartheta_*}} - 1\right] \\
& + \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} - \frac{1}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} \\
& - \frac{1}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}} + \frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}} - \frac{1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}}.
\end{aligned} \tag{10}
$$

Since $u_i\ u_{i+1}$ be an edge such that $d(u_i)+d(u_{i+1})$ is maximum in T; therefore for $j=1,2,\dots,r-1, f(r,d(v_j))\geq f(r,s)$ and $j=1,2,\dots,s-1, f(s,d(w_j))\geq f(r,s)$. Hence, Equation (10) yields

$$\begin{aligned}{}^{v}R_{\vartheta_*}(\acute{T})-{}^{v}R_{\vartheta_*}(T) &= \frac{r-1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}}\left[\frac{\sqrt{r+\vartheta_*}}{\sqrt{r-1+\vartheta_*}}-1\right]+\frac{s-1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}}\left[\frac{\sqrt{s+\vartheta_*}}{\sqrt{s-1+\vartheta_*}}-1\right]\\ &+\frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}-\frac{1}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}\\ &+\frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}-\frac{1}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}\\ &+\frac{1}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}-\frac{1}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}.\end{aligned}$$

$$\begin{aligned}{}^{v}R_{\vartheta_*}(\acute{T})-{}^{v}R_{\vartheta_*}(T) &\geq \frac{r-1}{\sqrt{(s+\vartheta_*)(r-1+\vartheta_*)}}-\frac{r-1}{\sqrt{(s+\vartheta_*)(r+\vartheta_*)}}-\frac{1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}}+\frac{s-1}{\sqrt{(r+\vartheta_*)(s-1+\vartheta_*)}}\\ &-\frac{s-1}{\sqrt{(s+\vartheta_*)(r+\vartheta_*)}}+\frac{3}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}-\frac{2}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}.\end{aligned}$$

$$\begin{aligned}{}^{v}R_{\vartheta_*}(\acute{T})-{}^{v}R_{\vartheta_*}(T) &\geq \frac{r-1}{\sqrt{(s+\vartheta_*)}}\left(\frac{1}{\sqrt{(r-1+\vartheta_*)}}-\frac{1}{\sqrt{(r+\vartheta_*)}}\right)+\frac{s-1}{\sqrt{(r+\vartheta_*)}}\left(\frac{1}{\sqrt{(s-1+\vartheta_*)}}-\frac{1}{\sqrt{(s+\vartheta_*)}}\right)\\ &-\frac{1}{\sqrt{(r+\vartheta_*)(s+\vartheta_*)}}+\frac{3}{\sqrt{(2+\vartheta_*)(2+\vartheta_*)}}-\frac{2}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}.\end{aligned} \tag{11}$$

Using Lemma 2.3–2.6, one can see that (11) holds. Hence, ${}^{v}R_{\vartheta_*}(\acute{T})-{}^{v}R_{\vartheta_*}(T)>0$. ■

Theorem 2.2. For $n\geq 4$ *and* $\vartheta_*\geq 0$, among all trees of a fixed order n, path graph P_n is the unique tree with maximum variable Randić index ${}^{v}\mathrm{R}_{\vartheta_*}$, which is $\frac{2}{\sqrt{(1+\vartheta_*)(2+\vartheta_*)}}+\frac{n-3}{2+\vartheta_*}$.

3. Conclusion

In the present study, we proved the conjecture proposed in [19]. More precisely, we prove that the P_n (path graph) has the maximum variable connectivity index among all trees of fixed order n, where $n\geq 4$.

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