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Trees with maximum multiplicative connectivity indices

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Abstract

The product-connectivity (also called Randić connectivity) index, sum-connectivity index and harmonic index are among the best-known and most successful vertex-degree-based topological indices in mathematical chemistry. The multiplicative versions of these graph invariants were proposed by Kulli in 2016. In this paper, we give the maximum values of the multiplicative product-connectivity, multiplicative sum-connectivity and multiplicative harmonic indices within the set of trees with a given order and maximum vertex degree and specify the maximal trees.

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1. Introduction

Throughout the paper, our graphs are considered to be simple, finite and connected. Let $\mathfrak{G}$ be a graph and $V(\mathfrak{G})$ and $E(\mathfrak{G})$ represent the set of

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its vertices and edges, respectively. The *open neighborhood* $N_{\mathfrak{G}}(\mathfrak{g})$ of $\mathfrak{g} \in V(\mathfrak{G})$ is the set of all $\mathfrak{g}' \in V(\mathfrak{G})$ for which $\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{G})$. The *degree* $d_{\mathfrak{G}}(\mathfrak{g})$ is the order of $N_{\mathfrak{G}}(\mathfrak{g})$. The *distance* $d_{\mathfrak{G}}(\mathfrak{g},\mathfrak{g}')$ between $\mathfrak{g},\mathfrak{g}' \in V(\mathfrak{G})$ is the number of edges in any shortest $\mathfrak{g}-\mathfrak{g}'$ path in $\mathfrak{G}$. For $\mathcal{E} \subseteq E(\mathfrak{G})$ ($\mathcal{E}' \nsubseteq E(\mathfrak{G})$, resp.), $\mathfrak{G}-\mathcal{E}$ ($\mathfrak{G}+\mathcal{E}'$, resp.) denotes the graph derived from $\mathfrak{G}$ by removing (adding, resp.) edges in $\mathcal{E}$, ($\mathcal{E}'$ resp.).

In chemical graph theory, the physico-chemical characteristics of molecular compounds are studied through structural descriptors called topological indices. A *topological index* is a parameter assigned to a chemical graph that characterizes the graph topology and remains invariant under isomorphism of graphs. Such indices are helpful in studying the structure-property relationships, structure-activity relationships, and structure-toxicity relationships (see, for example, [11, 37]). They are classified into different categories among which *vertex-degree-based* (VDB) indices are more well-known. These indices are helpful in examination of certain characteristics of molecular structures like entropy, viscosity, boiling point, gyrational radius, enthalpy of vaporization, etc. Lots of degree-related indices have been put forward to date with real or potential applications in science. Some of the most-known indices within this category are Zagreb indices [20, 21], augmented Zagreb index [10, 15], Randić connectivity index [30], harmonic index [14], sum-connectivity index [42], atom-bond connectivity index [4, 13] and geometric-arithmetic index [5, 39].

The *Zagreb indices*, put forward by Gutman and his coworkers in 1970's [20, 21], belong among the famous VDB indices whose formulae for a graph $\mathfrak{G}$ are given by

$$M_1(\mathfrak{G}) = \sum_{\mathfrak{g}\in V(\mathfrak{G})} d_{\mathfrak{G}}(\mathfrak{g})^2 = \sum_{\mathfrak{g}\mathfrak{g}'\in E(\mathfrak{G})} (d_{\mathfrak{G}}(\mathfrak{g}) + d_{\mathfrak{G}}(\mathfrak{g}')),$$

$$M_2(\mathfrak{G}) = \sum_{\mathfrak{g}\mathfrak{g}'\in E(\mathfrak{G})} d_{\mathfrak{G}}(\mathfrak{g}) d_{\mathfrak{G}}(\mathfrak{g}').$$

For results on their theory, applications and generalization, see the surveys [2, 8, 19] and the references quoted there in.

The product-connectivity, sum-connectivity and harmonic indices are among the best-known and well-investigated VDB indices in mathematical Chemistry. The *product-connectivity* (also called *Randić connectivity*) index was proposed by Randić [30] in 1975. This invariant is formulated for a graph $\mathfrak{G}$ as

$$R(\mathfrak{G}) = \sum_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{G})} \frac{1}{\sqrt{d_{\mathfrak{G}}(\mathfrak{g}) d_{\mathfrak{G}}(\mathfrak{g}')}}.$$

The Randić index is known as a useful measure for analyzing the amount of branching of the carbon atom structure in saturated hydrocarbons.

The *sum-connectivity index*, introduced by Zhou and Trinajstić [42] in 2009, is formulated by

$$\chi(\mathfrak{G}) = \sum_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{G})} \frac{1}{\sqrt{d_{\mathfrak{G}}(\mathfrak{g}) + d_{\mathfrak{G}}(\mathfrak{g}')}}.$$

It was shown in [27] that, the R and χ indices are well-correlated with each other and with the π -electron energy of benzenoid hydrocarbons.

The *harmonic index*, proposed by Fajtlowics [14] in 1987, is formulated by

$$H(\mathfrak{G}) = \sum_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{G})} \frac{2}{d_{\mathfrak{G}}(\mathfrak{g}) + d_{\mathfrak{G}}(\mathfrak{g}')}.$$

The harmonic index has a well correlation with the π -electron energy of benzenoid hydrocarbons. Also it was shown that its correlations with physical and chemical properties is some what better than that of the product connectivity index. Further results concerning mathematical properties and applications of the aforementioned connectivity indices can be found in [1, 3, 9, 18, 25, 26, 31, 32, 35, 38, 40, 41] and the references quoted therein.

The *first and second multiplicative Zagreb indices*, proposed by Todeschini *et al*. [36] in 2010, are formulated for a graph $\mathfrak{G}$ as

$$\Pi_1(\mathfrak{G}) = \prod_{\mathfrak{g} \in V(\mathfrak{G})} d_{\mathfrak{G}}(\mathfrak{g})^2, \ \Pi_2(\mathfrak{G}) = \prod_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{G})} d_{\mathfrak{G}}(\mathfrak{g}) d_{\mathfrak{G}}(\mathfrak{g}').$$

The *multiplicative-sum Zagreb index*, suggested by Eliasi *et al*. [12], is another multiplicative version of M_1 index which is formulated by

$$\Pi_1^*(\mathfrak{G}) = \prod_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{G})} (d_{\mathfrak{G}}(\mathfrak{g}) + d_{\mathfrak{G}}(\mathfrak{g}')).$$

Inspired by the definitions of multiplicative Zagreb indices, Kulli [22] proposed the multiplicative version of some VDB indices. Based on the Kulli's definition, the multiplicative version of R, χ and H indices are respectively formulated by

$$R\Pi(\mathfrak{G}) = \prod_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{G})} \frac{1}{\sqrt{d_{\mathfrak{G}}(\mathfrak{g}) d_{\mathfrak{G}}(\mathfrak{g}')}},$$

$$\chi\Pi(\mathfrak{S}) = \prod_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{S})} \frac{1}{\sqrt{d_{\mathfrak{S}}(\mathfrak{g}) + d_{\mathfrak{S}}(\mathfrak{g}')}},$$

$$H\Pi(\mathfrak{S}) = \prod_{\mathfrak{g}\mathfrak{g}' \in E(\mathfrak{S})} \frac{2}{d_{\mathfrak{S}}(\mathfrak{g}) + d_{\mathfrak{S}}(\mathfrak{g}')}.$$

The multiplicative connectivity indices have attracted considerable interest in the mathematical chemistry literature. See, for example, [16, 17, 23, 24] for their computation over nanotubes and nanotori, [6, 29] for investigation over dendrimers, [7, 28] for study under silicates networks and silicates layer, [33] for their value for block shift and hierarchical hypercube networks and [34] for calculation on molecular structure in anticancer drugs.

An important topic in extremal graph theory is to compute the extremal amounts of topological indices over special families of graphs such that certain parameters of the graphs are considered to be fixed. Our purpose is to examine the maximum amounts of the $R\Pi$, $\chi\Pi$ and $H\Pi$ indices over all trees on a given order and with a given maximum vertex degree and to characterize the maximal trees.

2. Main results

A tree (a connected acyclic graph) in which a special vertex is labeled as the *root* is said to be a *rooted tree*. Vertices with degree one in a tree are called its leaves. Any tree with at most a vertex of degree three or more is said to be a *spider*. The vertex of a spider possessing highest degree is called its *center*. The paths connecting the center and leaves of the spider are called its *legs*. A spider whose all legs are of length one is the star. Besides a path can be assumed as a spider with one or two leg/legs.

Hereafter, for positive integers $\mathfrak{y}$ and $\mathfrak{D}$, by $\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$ we mean the family of all trees on $\mathfrak{y}$ vertices whose maximum degree equals $\mathfrak{D}$.

Lemma 2.1: *Let $\Psi \in \mathcal{T}_{\mathfrak{y},\mathfrak{D}}$ be rooted at w, where w is a vertex with $d_{\Psi}(w) = \mathfrak{D}$. Let Ψ have a vertex except w of degree three or more. Then there is a tree $\Psi' \in \mathcal{T}_{\mathfrak{y},\mathfrak{D}}$ for that $R\Pi(\Psi') > R\Pi(\Psi)$, $\chi\Pi(\Psi') > \chi\Pi(\Psi)$, and $H\Pi(\Psi') > H\Pi(\Psi)$.*

Proof: Among the non-root vertices of Ψ with degree more than 2, let h have greatest distance from w. Let $d_{\Psi}(h) = \xi \geq 3$ and $N_{\Psi}(h) = \{h_1, h_2, \ldots, h_{\xi-1}, h_{\xi}\}$ where h_{ξ} lies on the $w-h$ path in Ψ. Then $d_{\Psi}(h_i) \in \{1,2\}$ when $1 \leq i \leq \xi - 1$. We consider the following cases.

Case 1: h is adjacent to more than one leaf.

We can suppose that h_1 and h_2 are two leaves. Let $\Psi' = (\Psi - \{hh_1\}) + \{h_1h_2\}$. Then

$$\mathcal{P}_1 = \prod_{i=3}^{\xi} \frac{\frac{1}{\sqrt{d_\Psi(h_i)+d_\Psi(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_i)+d_{\Psi'}(h)}}} = \prod_{i=3}^{\xi} \frac{\frac{1}{\sqrt{d_\Psi(h_i)+\xi}}}{\frac{1}{\sqrt{d_\Psi(h_i)+\xi-1}}} = \prod_{i=3}^{\xi} \sqrt{\frac{d_\Psi(h_i)+\xi-1}{d_\Psi(h_i)+\xi}} < 1,$$

$$\mathcal{P}_2 = \prod_{i=3}^{\xi} \frac{\frac{1}{\sqrt{d_\Psi(h_i)d_\Psi(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_i)d_{\Psi'}(h)}}} = \prod_{i=3}^{\xi} \frac{\frac{1}{\sqrt{\xi d_\Psi(h_i)}}}{\frac{1}{\sqrt{(\xi-1)d_\Psi(h_i)}}} = \prod_{i=3}^{\xi} \sqrt{\frac{\xi-1}{\xi}} < 1,$$

and

$$\mathcal{P}_3 = \prod_{i=3}^{\xi} \frac{\frac{2}{d_\Psi(h_i)+d_\Psi(h)}}{\frac{2}{d_{\Psi'}(h_i)+d_{\Psi'}(h)}} = \prod_{i=3}^{\xi} \frac{\frac{2}{d_\Psi(h_i)+\xi}}{\frac{2}{d_\Psi(h_i)+\xi-1}} = \prod_{i=3}^{\xi} \frac{d_\Psi(h_i)+\xi-1}{d_\Psi(h_i)+\xi} < 1.$$

Therefore

$$\frac{\chi\Pi(\Psi)}{\chi\Pi(\Psi')} = \mathcal{P}_1 \times \frac{\frac{1}{\sqrt{d_\Psi(h_1)+d_\Psi(h)}} \times \frac{1}{\sqrt{d_\Psi(h_2)+d_\Psi(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_1)+d_{\Psi'}(h_2)}} \times \frac{1}{\sqrt{d_{\Psi'}(h_2)+d_{\Psi'}(h)}}} < \frac{\frac{1}{\sqrt{\xi+1}} \times \frac{1}{\sqrt{\xi+1}}}{\frac{1}{\sqrt{3}} \times \frac{1}{\sqrt{\xi+1}}} = \sqrt{\frac{3}{\xi+1}} < 1,$$

$$\frac{R\Pi(\Psi)}{R\Pi(\Psi')} = \mathcal{P}_2 \times \frac{\frac{1}{\sqrt{d_\Psi(h_1)d_\Psi(h)}} \times \frac{1}{\sqrt{d_\Psi(h_2)d_\Psi(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_1)d_{\Psi'}(h_2)}} \times \frac{1}{\sqrt{d_{\Psi'}(h_2)d_{\Psi'}(h)}}} < \frac{\frac{1}{\sqrt{\xi}} \times \frac{1}{\sqrt{\xi}}}{\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2(\xi-1)}}} = \sqrt{\frac{4(\xi-1)}{\xi^2}} < 1,$$

and

$$\frac{H\Pi(\Psi)}{H\Pi(\Psi')} = \mathcal{P}_3 \times \frac{\frac{2}{d_\Psi(h_1)+d_\Psi(h)} \times \frac{2}{d_\Psi(h_2)+d_\Psi(h)}}{\frac{2}{d_{\Psi'}(h_1)+d_{\Psi'}(h_2)} \times \frac{2}{d_{\Psi'}(h_2)+d_{\Psi'}(h)}} < \frac{\frac{1}{\xi+1} \times \frac{1}{\xi+1}}{\frac{1}{3} \times \frac{1}{\xi+1}} = \frac{3}{\xi+1} < 1.$$

Case 2: h is adjacent to exactly one leaf.

We can assume that h_1 is a leaf and $hp_1p_2\ldots p_l$, $l \geq 2$ is a path in Ψ and $h_2 = p_1$. Let $\Psi' = (\Psi - \{hh_1\}) + \{h_1p_l\}$. Then

$$\mathcal{P}_1=\prod_{i=2}^{\xi}\frac{\frac{1}{\sqrt{d_{\Psi}(h_i)+d_{\Psi}(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_i)+d_{\Psi'}(h)}}}=\prod_{i=2}^{\xi}\frac{\frac{1}{\sqrt{d_{\Psi}(h_i)+\xi}}}{\frac{1}{\sqrt{d_{\Psi}(h_i)+\xi-1}}}=\prod_{i=2}^{\xi}\sqrt{\frac{d_{\Psi}(h_i)+\xi-1}{d_{\Psi}(h_i)+\xi}}<1,$$

$$\mathcal{P}_2=\prod_{i=3}^{\xi}\frac{\frac{1}{\sqrt{d_{\Psi}(h_i)d_{\Psi}(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_i)d_{\Psi'}(h)}}}=\prod_{i=3}^{\xi}\frac{\frac{1}{\sqrt{\xi d_{\Psi}(h_i)}}}{\frac{1}{\sqrt{(\xi-1)d_{\Psi}(h_i)}}}=\prod_{i=3}^{\xi}\sqrt{\frac{\xi-1}{\xi}}<1,$$

and

$$\mathcal{P}_3=\prod_{i=2}^{\xi}\frac{\frac{2}{d_{\Psi}(h_i)+d_{\Psi}(h)}}{\frac{2}{d_{\Psi'}(h_i)+d_{\Psi'}(h)}}=\prod_{i=2}^{\xi}\frac{\frac{2}{d_{\Psi}(h_i)+\xi}}{\frac{2}{d_{\Psi}(h_i)+\xi-1}}=\prod_{i=2}^{\xi}\frac{d_{\Psi}(h_i)+\xi-1}{d_{\Psi}(h_i)+\xi}<1.$$

Therefore

$$\frac{\chi\Pi(\Psi)}{\chi\Pi(\Psi')}=\mathcal{P}_1\times\frac{\frac{1}{\sqrt{d_{\Psi}(h_1)+d_{\Psi}(h)}}\times\frac{1}{\sqrt{d_{\Psi}(p_l)+d_{\Psi}(p_{l-1})}}}{\frac{1}{\sqrt{d_{\Psi'}(h_1)+d_{\Psi'}(p_l)}}\times\frac{1}{\sqrt{d_{\Psi'}(p_l)+d_{\Psi'}(p_{l-1})}}}<\frac{\frac{1}{\sqrt{\xi+1}}\times\frac{1}{\sqrt{3}}}{\frac{1}{\sqrt{3}}\times\frac{1}{\sqrt{4}}}=\sqrt{\frac{4}{\xi+1}}\le 1,$$

$$\frac{R\Pi(\Psi)}{R\Pi(\Psi')}=\mathcal{P}_2\times\frac{\frac{1}{\sqrt{d_{\Psi}(h_1)d_{\Psi}(h)}}\times\frac{1}{\sqrt{d_{\Psi}(h_2)d_{\Psi}(h)}}\times\frac{1}{\sqrt{d_{\Psi}(p_l)d_{\Psi}(p_{l-1})}}}{\frac{1}{\sqrt{d_{\Psi'}(h_1)d_{\Psi'}(p_l)}}\times\frac{1}{\sqrt{d_{\Psi'}(h_2)d_{\Psi'}(h)}}\times\frac{1}{\sqrt{d_{\Psi'}(p_l)d_{\Psi'}(p_{l-1})}}}<\frac{\frac{1}{\sqrt{\xi}}\times\frac{1}{\sqrt{2\xi}}\times\frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{2}}\times\frac{1}{\sqrt{2(\xi-1)}}\times\frac{1}{\sqrt{4}}}=\sqrt{\frac{4(\xi-1)}{\xi^2}}<1,$$

and

$$\frac{H\Pi(\Psi)}{H\Pi(\Psi')}=\mathcal{P}_3\times\frac{\frac{2}{d_{\Psi}(h_1)+d_{\Psi}(h)}\times\frac{2}{d_{\Psi}(p_l)+d_{\Psi}(p_{l-1})}}{\frac{2}{d_{\Psi'}(h_1)+d_{\Psi'}(p_l)}\times\frac{2}{d_{\Psi'}(p_l)+d_{\Psi'}(p_{l-1})}}<\frac{\frac{1}{\xi+1}\times\frac{1}{3}}{\frac{1}{3}\times\frac{1}{4}}=\frac{4}{\xi+1}\le 1.$$

Case 3: The vertices adjacent to h have degree two or more.

Let $hp_1p_2\dots p_t$, $hq_1q_2\dots q_l$ be two paths in Ψ such that $l,t\ge 2$, $h_1=p_1$ and $h_2=q_1$. Let Ψ' be the tree deduced from $\Psi-\{p_1,p_2,\dots,p_t\}$ by attaching the path $q_lp_1p_2\dots p_t$. Then

$$\mathcal{P}_1=\prod_{i=3}^{\xi}\frac{\frac{1}{\sqrt{d_{\Psi}(h_i)+d_{\Psi}(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_i)+d_{\Psi'}(h)}}}=\prod_{i=3}^{\xi}\frac{\frac{1}{\sqrt{d_{\Psi}(h_i)+\xi}}}{\frac{1}{\sqrt{d_{\Psi}(h_i)+\xi-1}}}=\prod_{i=3}^{\xi}\sqrt{\frac{d_{\Psi}(h_i)+\xi-1}{d_{\Psi}(h_i)+\xi}}<1,$$

$$\mathcal{P}_2=\prod_{i=3}^{\xi}\frac{\frac{1}{\sqrt{d_\Psi(h_i)d_\Psi(h)}}}{\frac{1}{\sqrt{d_{\Psi'}(h_i)d_{\Psi'}(h)}}}=\prod_{i=3}^{\xi}\frac{\frac{1}{\sqrt{\xi d_\Psi(h_i)}}}{\frac{1}{\sqrt{(\xi-1)d_\Psi(h_i)}}}=\prod_{i=3}^{\xi}\sqrt{\frac{\xi-1}{\xi}}<1,$$

and

$$\mathcal{P}_3=\prod_{i=3}^{\xi}\frac{\frac{2}{d_\Psi(h_i)+d_\Psi(h)}}{\frac{2}{d_{\Psi'}(h_i)+d_{\Psi'}(h)}}=\prod_{i=3}^{\xi}\frac{\frac{2}{d_\Psi(h_i)+\xi}}{\frac{2}{d_\Psi(h_i)+\xi-1}}=\prod_{i=3}^{\xi}\frac{d_\Psi(h_i)+\xi-1}{d_\Psi(h_i)+\xi}<1.$$

Therefore

$$\frac{\chi\Pi(\Psi)}{\chi\Pi(\Psi')}=\mathcal{P}_1\times\frac{\frac{1}{\sqrt{d_\Psi(h_1)+d_\Psi(h)}}\times\frac{1}{\sqrt{d_\Psi(h_2)+d_\Psi(h)}}\times\frac{1}{\sqrt{d_\Psi(q_l)+d_\Psi(q_{l-1})}}}{\frac{1}{\sqrt{d_{\Psi'}(h_1)+d_{\Psi'}(q_l)}}\times\frac{1}{\sqrt{d_{\Psi'}(h_2)+d_{\Psi'}(h)}}\times\frac{1}{\sqrt{d_{\Psi'}(q_l)+d_{\Psi'}(q_{l-1})}}}$$

$$<\frac{\frac{1}{\sqrt{\xi+2}}\times\frac{1}{\sqrt{\xi+2}}\times\frac{1}{\sqrt{3}}}{\frac{1}{\sqrt{4}}\times\frac{1}{\sqrt{\xi+1}}\times\frac{1}{\sqrt{4}}}=\sqrt{\frac{16(\xi+1)}{3(\xi+2)^2}}<1,$$

$$\frac{R\Pi(\Psi)}{R\Pi(\Psi')}=\mathcal{P}_2\times\frac{\frac{1}{\sqrt{d_\Psi(h_1)d_\Psi(h)}}\times\frac{1}{\sqrt{d_\Psi(h_2)d_\Psi(h)}}\times\frac{1}{\sqrt{d_\Psi(q_l)d_\Psi(q_{l-1})}}}{\frac{1}{\sqrt{d_{\Psi'}(h_1)d_{\Psi'}(q_l)}}\times\frac{1}{\sqrt{d_{\Psi'}(h_2)d_{\Psi'}(h)}}\times\frac{1}{\sqrt{d_{\Psi'}(q_l)d_{\Psi'}(q_{l-1})}}}$$

$$<\frac{\frac{1}{\sqrt{2\xi}}\times\frac{1}{\sqrt{2\xi}}\times\frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{4}}\times\frac{1}{\sqrt{2(\xi-1)}}\times\frac{1}{\sqrt{4}}}=\sqrt{\frac{4(\xi-1)}{\xi^2}}<1,$$

and

$$\frac{H\Pi(\Psi)}{H\Pi(\Psi')}=\mathcal{P}_3\times\frac{\frac{2}{d_\Psi(h_1)+d_\Psi(h)}\times\frac{2}{d_\Psi(h_2)+d_\Psi(h)}\times\frac{2}{d_\Psi(q_l)+d_\Psi(q_{l-1})}}{\frac{2}{d_{\Psi'}(h_1)+d_{\Psi'}(q_l)}\times\frac{2}{d_{\Psi'}(h_2)+d_{\Psi'}(h)}\times\frac{2}{d_{\Psi'}(q_l)+d_{\Psi'}(q_{l-1})}}$$

$$<\frac{\frac{1}{\xi+2}\times\frac{1}{\xi+2}\times\frac{1}{3}}{\frac{1}{4}\times\frac{1}{\xi+1}\times\frac{1}{4}}=\frac{16(\xi+1)}{3(\xi+2)^2}<1.$$

This complete the proof.

Lemma 2.2: *Let $\Psi\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$ be a spider with $\mathfrak{D}\geq 3$ and let Ψ have at least one leaf and one leg with length three or more. Then there exists a spider $\Psi'\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$ for which $\chi\Pi(\Psi')>\chi\Pi(\Psi)$ and $H\Pi(\Psi')>H\Pi(\Psi)$.*

Proof: Denote by w a vertex of Ψ with $d_\Psi(w)=\mathfrak{D}$ and wh_1, $wp_1p_2\ldots p_l$ be two legs in Ψ such that $l\geq 3$. Assume that Ψ' is the tree derived from $\Psi-\{p_lp_{l-1}\}$ by adding the path p_lh_1. Then

$$\frac{\chi\Pi(\Psi)}{\chi\Pi(\Psi')}=\frac{\frac{1}{\sqrt{d_\Psi(h_1)+d_\Psi(w)}}\times\frac{1}{\sqrt{d_\Psi(p_l)+d_\Psi(p_{l-1})}}\times\frac{1}{\sqrt{d_\Psi(p_{l-1})d_\Psi(p_{l-2})}}}{\frac{1}{\sqrt{d_{\Psi'}(h_1)d_{\Psi'}(p_l)}}\times\frac{1}{\sqrt{d_{\Psi'}(h_1)d_{\Psi'}(w)}}\times\frac{1}{\sqrt{d_{\Psi'}(p_{l-1})d_{\Psi'}(p_{l-2})}}}=\frac{\frac{1}{\sqrt{\mathfrak{D}+1}}\times\frac{1}{\sqrt{3}}\times\frac{1}{\sqrt{4}}}{\frac{1}{\sqrt{3}}\times\frac{1}{\sqrt{\mathfrak{D}+2}}\times\frac{1}{\sqrt{3}}}=\sqrt{\frac{3(\mathfrak{D}+2)}{4(\mathfrak{D}+1)}}<1,$$

and

$$\frac{H\Pi(\Psi)}{H\Pi(\Psi')}=\frac{\frac{1}{d_\Psi(h_1)+d_\Psi(w)}\times\frac{1}{d_\Psi(p_l)+d_\Psi(p_{l-1})}\times\frac{1}{d_\Psi(p_{l-1})+d_\Psi(p_{l-2})}}{\frac{1}{d_{\Psi'}(h_1)+d_{\Psi'}(p_l)}\times\frac{1}{d_{\Psi'}(h_1)+d_{\Psi'}(w)}\times\frac{1}{d_{\Psi'}(p_{l-1})+d_{\Psi'}(p_{l-2})}}<\frac{\frac{1}{\mathfrak{D}+1}\times\frac{1}{3}\times\frac{1}{4}}{\frac{1}{3}\times\frac{1}{\mathfrak{D}+2}\times\frac{1}{3}}=\frac{3(\mathfrak{D}+2)}{4(\mathfrak{D}+1)}<1,$$

so the claim follows.

Lemma 2.3: *For any spider Ψ with order $\mathfrak{y}\geq 3$ and maximum degree $\mathfrak{D}$,*

$$R\Pi(\Psi)=\left(\frac{1}{\sqrt{\mathfrak{D}}}\right)^{\mathfrak{D}}\left(\frac{1}{2}\right)^{\mathfrak{y}-\mathfrak{D}-1}.$$

Proof: If $\mathfrak{D}=2$, then $\Psi=P_{\mathfrak{y}}$ where $\mathfrak{y}\geq 3$, for which

$$R\Pi(P_{\mathfrak{y}})=\left(\frac{1}{2}\right)^{\mathfrak{y}-2}=\left(\frac{1}{\sqrt{\mathfrak{D}}}\right)^{\mathfrak{D}}\left(\frac{1}{2}\right)^{\mathfrak{y}-\mathfrak{D}-1}.$$

Now let $\mathfrak{D}\geq 3$. Assume that w is the center of Ψ and $N_\Psi(w)=\{w_1, w_2, \ldots, w_{\mathfrak{D}}\}$. Let $w_1, w_2, \ldots, w_s\in N_\Psi(w)$ with $d_\Psi(w_i)=1$ $(1\leq i\leq s)$ and $w_{s+1}, \ldots, w_{\mathfrak{D}}\in N_\Psi(w)$ with $d_\Psi(w_i)=2$ $(s+1\leq i\leq \mathfrak{D})$. Hence

$$R\Pi(\Psi)=\left(\frac{1}{\sqrt{\mathfrak{D}}}\right)^{s}\left(\frac{1}{\sqrt{2\mathfrak{D}}}\times\frac{1}{\sqrt{2}}\right)^{\mathfrak{D}-s}\left(\frac{1}{2}\right)^{\mathfrak{y}-2\mathfrak{D}+s-1}=\left(\frac{1}{\sqrt{\mathfrak{D}}}\right)^{\mathfrak{D}}\left(\frac{1}{2}\right)^{\mathfrak{y}-\mathfrak{D}-1}.$$

So the desired result holds.

Theorem 2.4: *For $\Psi\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$,*

$$R\Pi(\Psi)\leq\left(\frac{1}{\sqrt{\mathfrak{D}}}\right)^{\mathfrak{D}}\left(\frac{1}{2}\right)^{\mathfrak{y}-\mathfrak{D}-1},$$

and the equality happens if and only if Ψ is a spider.

Proof: Consider the tree Ψ' from $\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$ where $R\Pi(\Psi)\leq R\Pi(\Psi')$ for all $\Psi\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$. Let Ψ' be rooted at u, where $d_{\Psi'}(u)=\mathfrak{D}$. By Lemma 2.1, Ψ' must be a spider with center u and by Lemma 2.3,

$$R\Pi(\Psi')=\left(\frac{1}{\sqrt{\mathfrak{D}}}\right)^{\mathfrak{D}}\left(\frac{1}{2}\right)^{\mathfrak{y}-\mathfrak{D}-1}.$$

From which the proof is completed.

Theorem 2.5: *For* $\Psi\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$,

$$H\Pi(\Psi)\le\begin{cases}\left(\frac{2}{\mathfrak{D}+1}\right)^{2\mathfrak{D}-\mathfrak{y}+1}\times\left(\frac{4}{3(\mathfrak{D}+2)}\right)^{\mathfrak{y}-\mathfrak{D}-1} & \text{if } \mathfrak{D}>\frac{\mathfrak{y}-1}{2},\\ \left(\frac{4}{3(\mathfrak{D}+2)}\right)^{\mathfrak{D}}\times\left(\frac{1}{2}\right)^{\mathfrak{y}-2\mathfrak{D}-1} & \text{if } \mathfrak{D}\le\frac{\mathfrak{y}-1}{2},\end{cases}$$

in which the equality case happens if and only if Ψ *is a spider whose all legs have length less than or equal to two or all legs have length more than or equal to two.*

Proof: Let $\Psi'\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$ such that $H\Pi(\Psi')\ge H\Pi(\Psi)$ for all $\Psi\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$. Denote by u a vertex of Ψ' with $d_{\Psi'}(u)=\mathfrak{D}$ and root Ψ' at u. If $\mathfrak{D}=2$, then $\Psi\cong P_{\mathfrak{y}}$ for which $H\Pi(P_{\mathfrak{y}})=\frac{1}{9\times2^{\mathfrak{y}-5}}$. If $\mathfrak{D}>2$, then according to the Lemma 2.1, Ψ' must be a spider whose center is u. According to Lemma 2.2 and the choice of Ψ', we deduce that, all legs of Ψ' either have length less than or equal to two or have length more than or equal to two. We start with the case that the length of all legs of Ψ' is more than or equal to two. Then it is evident that $\mathfrak{D}\le\frac{\mathfrak{y}-1}{2}$ and

$$H\Pi(\Psi')=\left(\frac{2}{\mathfrak{D}+2}\right)^{\mathfrak{D}}\times\left(\frac{2}{3}\right)^{\mathfrak{D}}\times\left(\frac{1}{2}\right)^{\mathfrak{y}-2\mathfrak{D}-1}=\left(\frac{4}{3(\mathfrak{D}+2)}\right)^{\mathfrak{D}}\times\left(\frac{1}{2}\right)^{\mathfrak{y}-2\mathfrak{D}-1},$$

as desired. Now consider the other case when the length of all legs of Ψ' is less than or equal to two. Considering the previous case, it can be assumed that Ψ' contains a leg with length 1. If $\Psi'\cong S_{\mathfrak{y}}$, then the result is immediate. If $\Psi'\ncong S_{\mathfrak{y}}$, then $2\mathfrak{D}+1-\mathfrak{y}$ leaves are adjacent to u. Then

$$\begin{aligned}H\Pi(\Psi')&=\left(\frac{2}{\mathfrak{D}+1}\right)^{2\mathfrak{D}-\mathfrak{y}+1}\times\left(\frac{2}{\mathfrak{D}+2}\right)^{\mathfrak{y}-\mathfrak{D}-1}\times\left(\frac{2}{3}\right)^{\mathfrak{y}-\mathfrak{D}-1}\\&=\left(\frac{2}{\mathfrak{D}+1}\right)^{2\mathfrak{D}-\mathfrak{y}+1}\times\left(\frac{4}{3(\mathfrak{D}+2)}\right)^{\mathfrak{y}-\mathfrak{D}-1}.\end{aligned}$$

So the proof is complete.

By a same reasoning as that of Theorem 2.5, we arrive at:

Theorem 2.6: *For* $\Psi\in\mathcal{T}_{\mathfrak{y},\mathfrak{D}}$,

$$\chi\Pi(\Psi) \leq \begin{cases} \left(\frac{1}{\sqrt{\mathfrak{D}+1}}\right)^{2\mathfrak{D}-\mathfrak{y}+1} \times \left(\frac{1}{\sqrt{3(\mathfrak{D}+2)}}\right)^{\mathfrak{y}-\mathfrak{D}-1} & \text{if } \mathfrak{D} > \frac{\mathfrak{y}-1}{2}, \\ \left(\frac{1}{\sqrt{3(\mathfrak{D}+2)}}\right)^{\mathfrak{D}} \times \left(\frac{1}{2}\right)^{\mathfrak{y}-2\mathfrak{D}-1} & \text{if } \mathfrak{D} \leq \frac{\mathfrak{y}-1}{2}. \end{cases}$$

The equality case happens if and only if Ψ *is a spider whose all legs have length less than or equal to two or all legs have length more than or equal to two.*

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