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Article

# The Extremal Trees for Logarithmic VDB Topological Indices

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**Abstract:** Vertex-degree-based (VDB) topological indices have been applied in QSPR/QSAR. As an important category, the general logarithmic VDB topological index  $T_{lnf}(G)$ , is defined as the summation of  $lnf(d(u), d(v))$ , where the summation over all  $uv \in E(G)$ . In this paper, we give the sufficient conditions for that (1) the path  $P_n$  is the only tree with the minimal  $T_{lnf}$ ; (2) the star  $S_n$  is the only tree with the maximal and the minimal  $T_{lnf}$ , respectively. As applications, the minimal and maximal trees of some logarithmic VDB indices are determined.

**Keywords:** tree; extreme value; logarithmic VDB topological indices

**MSC:** 05C05, 05C09, 05C92

## 1. Introduction

Topological indices (or graphical indices, or chemical indices) have an important role in studying the structures and properties of a molecular compound. Related studies have shown that topological indices are closely related to physico-chemical properties or biological activity [1,2]. Vertex-degree-based (VDB shortly) topological indices, as an important type of topological index, have long been considered and applied in QSPR/QSAR research [3,4]. Due to its importance in the field of chemistry, a large number of mathematical and chemical literature for the extremal values and extremal graphs have been published, and they are often considered and verified to have some excellent chemical properties. For relevant research, see [5–7].

Throughout the whole paper, all graphs we considered are simple, undirected and connected. Let  $G$  is a graph of order  $n$ , the vertex set and edge set are  $V(G)$  and  $E(G)$ , respectively. We use  $d_G(u)$ , or shortly by  $d(u)$  to represent the degree of vertex  $v$ . A vertex  $v$  is said to be *pendant* if  $d(v) = 1$ . If the edge  $uv \in E(G)$ , then the two vertices  $u$  and  $v$  in  $G$  are said to be *adjacent*. The vertex set adjacent to  $v$  is known as its *neighbors*, which denoted by  $N_G(v)$  or  $N(v)$ . If  $uv \notin E(G)$ , the graph  $G + uv$  represents the resulting graph by adding the edge  $uv$  from  $G$ . Meanwhile, we use  $G - uv$  represents the resulting graph by deleting the edge  $uv$  in  $G$  for the edge  $uv \in E(G)$ . We use  $S_n$ ,  $P_n$ , and  $\mathbb{T}_n$  to denote the star, the path, and the set of trees with order of  $n$ , respectively. Denote  $S_{r,n-r}$  to represent the double star with the degrees of two centers being  $r$  and  $n - r$ , where  $2 \leq r \leq \lfloor \frac{n}{2} \rfloor$ .

A general VDB (vertex-degree-based) index of a connected graph  $G$  is defined as

$$T_f = T_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)),$$

where  $f(x, y) = f(y, x)$  is a real symmetric function for  $x \geq 1$  and  $y \geq 1$ . To learn more about the relevant results, readers can refer to [8–10]. Especially, Gutman in [8] collected some important and well-studied VDB topological indices.

In 2019, the exponential of  $T_f$ , was first introduced in [11] by Rada, is defined as

$$T_{ef} = T_{ef}(G) = \sum_{uv \in E(G)} e^{f(d(u), d(v))} = \sum_{uv \in E(G)} \beta(d(u), d(v)),$$

where  $\beta(x, y) = e^{f(x, y)}$ . The notation  $T_{e^f}$  is known as an exponential VDB topological index, or abbreviated as exponential VDB index.

The study of VDB topological index has attracted increasing attention, especially, to find the extremal values of  $T_f$  or  $T_{e^f}$  for some special types of graphs. The authors in [12] provides a general way to obtain whether the star  $S_n$  or the path  $P_n$  are extremal trees of the VDB topological index. Also, if  $f(x, y)$  is concave upwards and increasing relative to the variable  $x$ , the maximum trees of  $T_f$  were determined in [13]. Gao in [14] provided some conditions for the function  $f(x, y)$ . If  $f(x, y)$  satisfies some conditions, then the necessary and sufficient conditions for a chemical tree to be a maximal  $T_f$  are attained. Very recently, the authors [15] gave sufficient conditions for  $P_n$  is the only tree with the smallest  $T_{e^f}$ , the sufficient conditions for  $S_n$  or  $S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}$  is the only tree with the largest  $T_{e^f}$ . For research on  $T_f$  or  $T_{e^f}$ , readers can refer to [16–18].

Inspired by [11], we introduce a new VDB topological indices, the logarithmic topological index, it is defined as

$$T_{\ln f} = T_{\ln f}(G) = \sum_{uv \in E(G)} \ln f(d(u), d(v)) = \sum_{uv \in E(G)} \gamma(d(u), d(v)),$$

where  $\gamma(x, y) = \ln f(x, y)$ , and  $f(x, y) = f(y, x)$  is a real symmetric function for  $x \geq 1$  and  $y \geq 1$ . As a VDB topological indices corresponding to exponential of  $T_f$ , the study for logarithmic of  $T_{\ln f}$  is of great significance.

In this paper, we mainly studied the extremal trees for logarithmic VDB topological indices. In section 3, we give the sufficient conditions for that the path  $P_n$  is the only tree with the minimal  $T_{\ln f}$ . In section 4, we obtain the sufficient conditions for that the star  $S_n$  is the only tree with the maximal and minimal  $T_{\ln f}$ . In addition, as applications, the minimal and maximal trees of some logarithmic VDB indices are determined in section 5.

## 2. Preliminaries

In the remainder of the paper, assume that  $\gamma(x, y) = \ln f(x, y)$ , and  $f(x, y) = f(y, x)$  is the real symmetric function, where  $x \geq 1$  and  $y \geq 1$ . In this section, we give the some lemmas firstly.

**Lemma 1.** *If  $\frac{\partial f}{\partial x} > 0$ , then  $\gamma(x, y)$  is strictly increasing on  $x \geq 1$ .*

**Proof.** Since  $\frac{\partial \gamma}{\partial x} = (\ln f(x, y))'_x = \frac{f'_x(x, y)}{f(x, y)}$ , thus  $\gamma(x, y)$  is strictly increasing on  $x \geq 1$  under the condition  $\frac{\partial f}{\partial x} > 0$ .  $\square$

**Lemma 2.** *Let  $\gamma(x, y) = \ln f(x, y)$ , where  $f(x, y) > 0$  for  $x, y \geq 1$ . For any positive integer  $r \geq 1$ , if  $f(x_1, y_1) \cdot f(x_2, y_2) \cdots f(x_r, y_r) \geq f(x'_1, y'_1) \cdot f(x'_2, y'_2) \cdots f(x'_r, y'_r)$ , then*

$$\gamma(x_1, y_1) + \gamma(x_2, y_2) + \cdots + \gamma(x_r, y_r) \geq \gamma(x'_1, y'_1) + \gamma(x'_2, y'_2) + \cdots + \gamma(x'_r, y'_r).$$

**Proof.** Since  $\gamma(x, y) = \ln f(x, y)$ , according to the condition of lemma, we have

$$\begin{aligned} & \gamma(x_1, y_1) + \gamma(x_2, y_2) + \cdots + \gamma(x_r, y_r) - \left( \gamma(x'_1, y'_1) + \gamma(x'_2, y'_2) + \cdots + \gamma(x'_r, y'_r) \right) \\ &= \ln \frac{f(x_1, y_1) \cdot f(x_2, y_2) \cdots f(x_r, y_r)}{f(x'_1, y'_1) \cdot f(x'_2, y'_2) \cdots f(x'_r, y'_r)} \geq \ln 1 = 0. \end{aligned}$$

So, the lemma is proved.  $\square$

**Lemma 3.** *Let  $f(x, y) = (xy)^\alpha$  ( $\alpha > 0$ ), then  $f(x, y) = g(x)h(y)$ , and  $g(s+1)^{s+1} \cdot g(t+1)^{t+1} < g(1) \cdot g(s+t+1)^{s+t+1}$ , where  $s, t \geq 1$ .*

**Proof.** Clearly,  $f(x, y) = (xy)^\alpha = g(x)h(y)$ , where  $g(x) = x^\alpha$ , and  $h(y) = y^\alpha$ . In the following, we will verify that  $g(s+1)^{s+1} \cdot g(t+1)^{t+1} < g(1) \cdot g(s+t+1)^{s+t+1}$ .

Without loss of generality, assuming  $s \leq t$ . Note that

$$\begin{aligned} g(s+t+1)^{s+t+1} &= (s+t+1)^{\alpha(s+t+1)} \\ &= (t+1)^{\alpha(t+1)} \cdot \left(\frac{s+t+1}{t+1}\right)^{\alpha(t+1)} \cdot (s+t+1)^{\alpha s} \\ &= g(t+1)^{t+1} \cdot \left(\frac{s+t+1}{t+1}\right)^{\alpha(t+1)} \cdot (s+t+1)^{\alpha s}, \end{aligned}$$

thus, lemma is true if the equality  $g(s+1)^{s+1} = (s+1)^{\alpha(s+1)} < \left(\frac{s+t+1}{t+1}\right)^{\alpha(t+1)} \cdot (s+t+1)^{\alpha s}$  holds, i.e.

$$\left(\frac{s+t+1}{t+1}\right)^{t+1} \cdot \left(\frac{s+t+1}{t+1}\right)^{s+1} > 1+s.$$

If  $s = 1, 2$ , then

$$\left(\frac{s+t+1}{t+1}\right)^{t+1} \cdot \left(\frac{s+t+1}{s+1}\right)^s = \begin{cases} \left(\frac{3}{2}\right)^2 \left(\frac{3}{2}\right) > 1+1=2, & \text{if } t=s=1, \\ \left(\frac{5}{3}\right)^2 \left(\frac{5}{3}\right) > 1+2=3, & \text{if } t=s=2. \end{cases}$$

and

$$\begin{aligned} \left(\frac{s+t+1}{t+1}\right)^{t+1} \cdot \left(\frac{s+t+1}{s+1}\right)^s &> \left(\frac{s+t+1}{s+1}\right)^s \\ &= \begin{cases} \left(\frac{1+2+1}{2}\right)^1 = 2 \geq 1+1=2, & \text{if } t > s=1, \\ \left(\frac{2+3+1}{2}\right)^2 = 4 \geq 1+2=3, & \text{if } t > s=2. \end{cases} \end{aligned}$$

If  $s \geq 3$ , and because  $t \geq s$ , then

$$\begin{aligned} \left(\frac{s+t+1}{t+1}\right)^{t+1} \cdot \left(\frac{s+t+1}{s+1}\right)^s &> \left(\frac{s+t+1}{s+1}\right)^s \geq \left(\frac{2s+1}{s+1}\right)^s = \left(1 + \frac{s}{s+1}\right)^s \\ &\geq C_s^0 + C_s^1 \frac{s}{s+1} + C_s^2 \left(\frac{s}{s+1}\right)^2 + C_s^3 \left(\frac{s}{s+1}\right)^3 \\ &= 1 + \frac{s^2}{s+1} + \frac{s(s-1)s^2}{2(s+1)^2} + \frac{s(s-1)(s-2)s^3}{6(s+1)^3} \\ &\geq 1 + \frac{s^2}{s+1} + \frac{s^3}{(s+1)^2} + \frac{s^3(s-2)}{(s+1)^3} \\ &> 1 + s \left[ \frac{s(s+1)^2 + (s+1)^2}{(s+1)^3} \right] \\ &= 1 + s. \end{aligned}$$

So, the lemma is proved.  $\square$

**Lemma 4.** Let binary function  $f(x, y) = \frac{xy}{x+y}$ , where  $x \geq 1$  and  $y \geq 1$ . Then,

- (1)  $\frac{\partial f}{\partial x} < 0$ ,  $f''_{xx}f - f_x'^2 < 0$ ; and
- (2)  $f(d, 1)^{d-1} \cdot f(n-d, 1)^{n-d-1} \cdot f(d, n-d) > f(n-1, 1)^{n-1}$ , where  $2 \leq d \leq \lfloor \frac{n}{2} \rfloor$ .

**Proof.** (1) Since  $\frac{\partial f}{\partial x} = \frac{y-xy}{(x+y)^2}$ , and  $x, y \geq 1$ , thus  $\frac{\partial f}{\partial x} < 0$ . Note that

$$f''_{xx} = \left( \frac{y-xy}{(x+y)^2} \right)' = \frac{-y^2 + xy - 2y}{(x+y)^3},$$

and therefore,

$$f''_{xx}f - f'^2_x = \frac{(-y^2 + xy - 2y)xy}{(x+y)^4} - \frac{(y-xy)^2}{(x+y)^4} = \frac{-xy^3 - y^2}{(x+y)^4} < 0.$$

(2) Substituting  $f(x, y) = \frac{xy}{x+y}$  into  $f(d, 1)^{d-1} \cdot f(n-d, 1)^{n-d-1} \cdot f(d, n-d) > f(n-1, 1)^{n-1}$  yields that

$$\left( \frac{d}{d+1} \right)^{d-1} \cdot \left( \frac{n-d}{n-d+1} \right)^{n-d-1} \cdot \frac{d(n-d)}{n} > \left( \frac{n-1}{n} \right)^{n-1},$$

i.e.,

$$\frac{d^d \cdot (n-d+1)}{(d+1)^{d-1} \cdot n} \cdot \left( \frac{n-d}{n-d+1} \right)^{n-d} > \left( \frac{n-1}{n} \right)^{n-1}.$$

Therefore, to complete the proof of the lemma, it is only necessary to prove that

$$\frac{d^d \cdot (n-d+1)}{(d+1)^{d-1} \cdot n} > 1, \text{ and } \left( \frac{n-d}{n-d+1} \right)^{n-d} > \left( \frac{n-1}{n} \right)^{n-1}.$$

Let us first consider  $\frac{d^d \cdot (n-d+1)}{(d+1)^{d-1} \cdot n} > 1$ . Note that

$$\begin{aligned} \left( \frac{d}{d+1} \right)^{d-1} &= \left( 1 - \frac{1}{d+1} \right)^{d-1} \\ &= C_{d-1}^0 - C_{d-1}^1 \frac{1}{d+1} + C_{d-1}^2 \left( \frac{1}{d+1} \right)^2 - \dots + C_{d-1}^{d-1} \left( -\frac{1}{d+1} \right)^{d-1} \\ &> 1 - \frac{d-1}{d+1} = \frac{2}{d+1}. \end{aligned}$$

And thus, we obtain

$$\frac{d^d \cdot (n-d+1)}{(d+1)^{d-1} \cdot n} = \left( \frac{d}{d+1} \right)^{d-1} \cdot \frac{d(n-d+1)}{n} > \frac{2}{d+1} \cdot \frac{d(n-d+1)}{n}.$$

In the following, we only need to prove that  $\frac{2}{d+1} \cdot \frac{d(n-d+1)}{n} \geq 1$ . Let  $f(d) = 2d(n-d+1) - n(d+1)$ , where  $2 \leq d \leq \lfloor \frac{n}{2} \rfloor$ . Since  $f'(d) = 2(n-d+1) - 2d - n = n - 4d + 2$ , then  $f_{\min} = \{f(2), f(\frac{n}{2})\} = f(\frac{n}{2}) = 0$ . This implies that  $2d(n-d+1) \geq n(d+1)$ , and therefore,

$$\frac{d^d \cdot (n-d+1)}{(d+1)^{d-1} \cdot n} > \frac{2}{d+1} \cdot \frac{d(n-d+1)}{n} \geq 1.$$

Now, let us turn to prove  $\left( \frac{n-d}{n-d+1} \right)^{n-d} > \left( \frac{n-1}{n} \right)^{n-1}$ . Let  $y = \left( \frac{n-x}{n-x+1} \right)^{n-x}$ , where  $2 \leq x \leq \lfloor \frac{n}{2} \rfloor$ . Since

$$y' = \left( \frac{n-x}{n-x+1} \right)^{n-x} \left( -\ln \frac{n-x}{n-x+1} - \frac{1}{n-x+1} \right),$$

and

$$g'(x) = \left(-\ln \frac{n-x}{n-x+1} - \frac{1}{n-x+1}\right)' = \frac{1}{(n-x+1)^2(n-x)} > 0,$$

thus, we have

$$g(x) \geq g(1) = \ln \frac{n}{n-1} - \frac{1}{n} \geq \ln \frac{4}{3} - \frac{1}{4} > 0.$$

This is to say,  $y$  is an increasing function, and hence,

$$\left(\frac{n-d}{n-d+1}\right)^{n-d} > y(1) = \left(\frac{n-1}{n}\right)^{n-1}.$$

Therefore, combining the above two inequations, the lemma proof is completed.  $\square$

### 3. Sufficient Conditions for $P_n$ Being the Minimal Tree

In this section, we give sufficient conditions for the path  $P_n$  being the minimal tree of  $T_{lnf}$ . We present the following transformation at first.

**Transformation 1.** Assume  $T \in \mathbb{T}_n$ , let  $x$  be the vertex in tree  $T$ .  $T_1$  is the graph obtained from  $T$  by adding two pendant paths,  $P_1$  and  $P_2$  attached at  $x$ , where  $P_1 = xu_1u_2 \cdots, u_a$ , and  $P_2 = xv_1v_2 \cdots, v_b$ ,  $a \geq b \geq 1$ ,  $d_{T_1}(x) \geq 3$ .  $T_2$  is the resulting graph obtained from  $T_1$  by deleting the edge  $xv_1$  and connecting an edge  $u_av_1$ , i.e.,  $T_2 = T_1 - xv_1 + u_av_1$ .  $T_1$  and  $T_2$  are depicted in Figure 1. Clearly,  $T_1, T_2 \in \mathbb{T}_n$ .

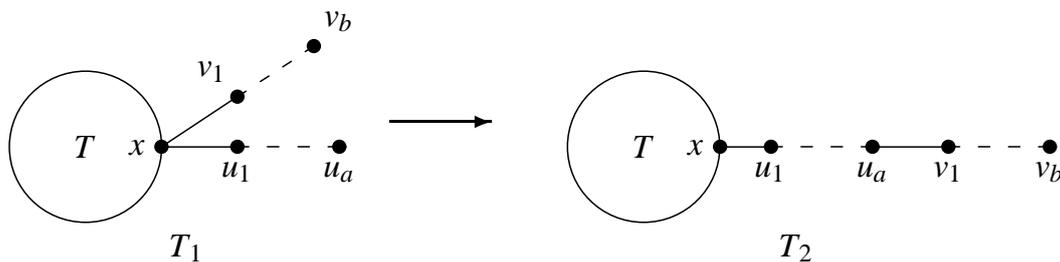


Figure 1. Trees  $T_1$  and  $T_2$  in Transformation 1.

**Lemma 5.** Let  $T_1$  and  $T_2$  be the graphs in Transformation 1 (see Figure 1), where  $a = b = 1$ . If  $f(x, y)$  matches the conditions  $\frac{\partial f}{\partial x} > 0$ , and  $f^2(1, x+2) \geq f(2, x+1) \cdot f(2, 1)$ , then  $T_{lnf}(T_1) > T_{lnf}(T_2)$ .

**Proof.** Denote  $d_{T_1}(x) = p+2$ ,  $p \geq 1$ , and  $N_T(x) = N_{T_1}(x) \setminus \{u_1, u_2\} = \{w_1, w_2, \dots, w_p\}$ . Since  $a = b = 1$ , then  $d_{T_1}(u_1) = d_{T_1}(v_1) = 1$ . And thus, we have

$$\begin{aligned} & T_{lnf}(T_1) - T_{lnf}(T_2) \\ &= 2\gamma(p+2, 1) + \sum_{i=1}^p \gamma(p+2, d_T(w_i)) - \left( \gamma(p+1, 2) + \gamma(2, 1) + \sum_{i=1}^p \gamma(p+1, d_T(w_i)) \right) \\ &= \sum_{i=1}^p \left( \gamma(p+2, d_T(w_i)) - \gamma(p+1, d_T(w_i)) \right) + 2\gamma(p+2, 1) - \gamma(p+1, 2) - \gamma(2, 1). \end{aligned}$$

As  $\frac{\partial f}{\partial x} > 0$ , and Lemma 1, we obtain  $\sum_{i=1}^p \left( \gamma(p+2, d_T(w_i)) - \gamma(p+1, d_T(w_i)) \right) > 0$ . Using Lemma 2, we have

$$T_{lnf}(T_1) - T_{lnf}(T_2) > 2\gamma(p+2, 1) - \gamma(p+1, 2) - \gamma(2, 1) \geq 0.$$

So, the lemma is proved.  $\square$

**Lemma 6.** Let  $T_1$  and  $T_2$  be the graphs in Transformation 1 (see Figure 1), where  $a > b = 1$ . If  $f(x, y)$  matches the conditions  $\frac{\partial f}{\partial x} > 0$ , and  $f(1, x+2) \cdot f(2, x+2) \geq f(2, x+1) \cdot f(2, 2)$ , then  $T_{lnf}(T_1) > T_{lnf}(T_2)$ .

**Proof.** Denote  $d_{T_1}(x) = p + 2$ ,  $p \geq 1$ , and  $N_T(x) = N_{T_1}(x) \setminus \{u_1, u_2\} = \{w_1, w_2, \dots, w_p\}$ . Since  $a > b = 1$ , then  $d_{T_1}(u_1) = 2$ , and  $d_{T_1}(v_1) = 1$ . Therefore, we have

$$\begin{aligned} & T_{Inf}(T_1) - T_{Inf}(T_2) \\ &= \gamma(p+2, 1) + \gamma(p+2, 2) + \gamma(2, 1) + \sum_{i=1}^p \gamma(p+2, d_T(w_i)) \\ &- \left( \gamma(p+1, 2) + \gamma(2, 2) + \gamma(2, 1) + \sum_{i=1}^p \gamma(p+1, d_T(w_i)) \right) \\ &= \sum_{i=1}^p \left( \gamma(p+2, d_T(w_i)) - \gamma(p+1, d_T(w_i)) \right) \\ &+ \gamma(p+2, 1) + \gamma(p+2, 2) - \gamma(p+1, 2) - \gamma(2, 2). \end{aligned}$$

According to  $\frac{\partial f}{\partial x} > 0$ , and Lemma 1,  $\sum_{i=1}^p \left( \gamma(p+2, d_T(w_i)) - \gamma(p+1, d_T(w_i)) \right) > 0$ . This, together with Lemma 2, implies that

$$T_{Inf}(T_1) - T_{Inf}(T_2) > \gamma(p+2, 1) + \gamma(p+2, 2) - \gamma(p+1, 2) - \gamma(2, 2) \geq 0.$$

Hence, we finished the proof.  $\square$

**Lemma 7.** Let  $T_1$  and  $T_2$  be the graphs in Transformation 1 (see Figure 1), where  $a \geq b > 1$ . If  $f(x, y)$  matches the conditions  $\frac{\partial f}{\partial x} > 0$ , and  $f^2(2, x+2) \cdot f(2, 1) \geq f(2, x+1) \cdot f^2(2, 2)$ , then  $T_{Inf}(T_1) > T_{Inf}(T_2)$ .

**Proof.** Denote  $d_{T_1}(x) = p + 2$ ,  $p \geq 1$ , and  $N_T(x) = N_{T_1}(x) \setminus \{u_1, u_2\} = \{w_1, w_2, \dots, w_p\}$ . Since  $a \geq b > 1$ , then  $d_{T_1}(u_1) = d_{T_1}(v_1) = 2$ . Hence, we have

$$\begin{aligned} & T_{Inf}(T_1) - T_{Inf}(T_2) \\ &= 2\gamma(p+2, 2) + 2\beta(2, 1) + \gamma(2, 1) + \sum_{i=1}^p \gamma(p+2, d_T(w_i)) \\ &- \left( \gamma(p+1, 2) + 2\gamma(2, 2) + \gamma(2, 1) + \sum_{i=1}^p \gamma(p+1, d_T(w_i)) \right) \\ &= \sum_{i=1}^p \left( \gamma(p+2, d_T(w_i)) - \gamma(p+1, d_T(w_i)) \right) \\ &+ 2\gamma(p+2, 2) + \gamma(2, 1) - \gamma(p+1, 2) - 2\gamma(2, 2). \end{aligned}$$

By  $\frac{\partial f}{\partial x} > 0$ , and Lemma 1, have  $\sum_{i=1}^p \left( \gamma(p+2, d_T(w_i)) - \gamma(p+1, d_T(w_i)) \right) > 0$ . Now, applying Lemma 2, we have

$$T_{Inf}(T_1) - T_{Inf}(T_2) > 2\gamma(p+2, 2) + \gamma(2, 1) - \gamma(p+1, 2) - 2\gamma(2, 2) \geq 0.$$

So, the proof is done.  $\square$

With the above lemmas, we now present the following theorem.

**Theorem 8.** Let  $T \in \mathbb{T}_n$ , suppose  $f(x, y)$  meets the conditions:

- (1)  $\frac{\partial f}{\partial x} > 0$ ,
- (2)  $f^2(1, x+2) \geq f(2, x+1) \cdot f(2, 1)$ ,
- (3)  $f(1, x+2) \cdot f(2, x+2) \geq f(2, x+1) \cdot f(2, 2)$ , and
- (4)  $f^2(2, x+2) \cdot f(2, 1) \geq f(2, x+1) \cdot f^2(2, 2)$ ,

then  $T_{Inf}(T) \geq T_{Inf}(P_n)$ , if and only if  $T \cong P_n$ .

**Proof.** The conditions (1)-(4) are satisfied for the results of Lemma 5, 6, and 7. If  $T \not\cong P_n$ , then, using Transformation 1 repeatedly,  $T'$  is attained from  $T$ . Moreover, according to Lemma 5, 6, and 7, we have  $T_{Inf}(T) > T_{Inf}(T')$ . Therefore,  $T_{Inf}(T) \geq T_{Inf}(P_n)$ , if and only if  $T \cong P_n$ , the equality holds. This completes the proof.  $\square$

#### 4. Sufficient Conditions for $S_n$ Being Extremal Trees

In this section, we provide sufficient conditions for the star  $S_n$  being the extremal trees of  $T_{lnf}$ . We introduce a transformation which is very useful to prove our results.

**Transformation 2.** Assume  $T \in \mathbb{T}_n$ ,  $\{xy, yz\} \in E(T)$ , and  $d_T(x) \leq d_T(z) \leq 2$ . Denote  $N_1 = N(x) \setminus \{y\}$ ,  $N_2 = N(y) \setminus \{x, z\}$ , and  $N_3 = N(z) \setminus \{y\}$ . Let  $T'$  be a tree obtained from  $T$  by replacing the edge  $xu$  by a new edge  $yu$  for each vertex  $u \in N_1$ .  $T$  and  $T'$  are depicted in Figure 2. Clearly,  $T' \in \mathbb{T}_n$ .

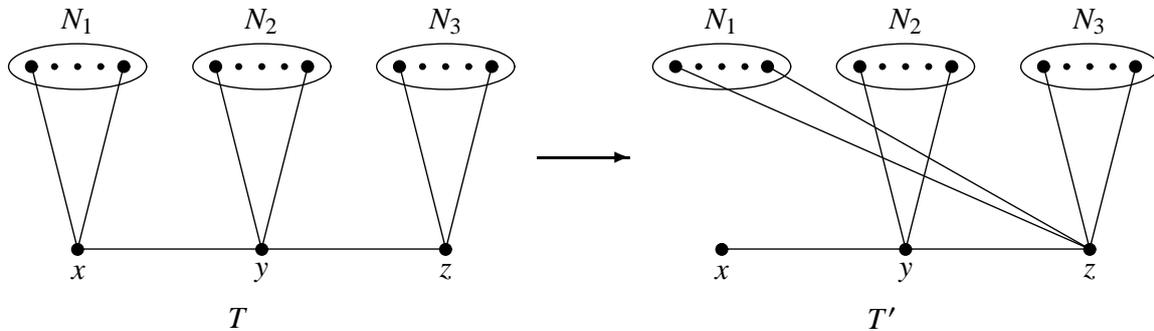


Figure 2. Trees  $T$  and  $T'$  in Transformation 2.

With the help of Transformation 2, we firstly give sufficient conditions for the star  $S_n$  being the maximal tree of  $T_{lnf}$ .

**Lemma 9.** Let  $T$  and  $T'$  be the graphs in Transformation 2 (see Fig. 2). If  $f(x, y) = g(x)h(y)$  is a real symmetric function with  $x, y \geq 1$ , and meets the condition  $g(s+1)^{s+1} \cdot g(t+1)^{t+1} < g(1) \cdot g(s+t+1)^{s+t+1}$ , then  $T_{lnf}(T) < T_{lnf}(T')$ .

**Proof.** Without loss of generality, we assume  $N_1 = \{u_1, u_2, \dots, u_s\}$  and  $N_3 = \{v_1, v_2, \dots, v_t\}$ , where  $s \leq t$ . Thus, we have  $d_T(x) = s+1, d_T(z) = t+1$ , and

$$\begin{aligned} T_{lnf}(T) - T_{lnf}(T') &= \sum_{i=1}^s \left( \gamma(s+1, d_T(u_i)) - \gamma(s+t+1, d_T(u_i)) \right) + \sum_{i=1}^t \left( \gamma(t+1, d_T(v_i)) - \gamma(s+t+1, d_T(v_i)) \right) \\ &+ \gamma(s+1, d_T(w)) + \gamma(t+1, d_T(w)) - \gamma(1, d_T(w)) - \gamma(s+t+1, d_T(w)) \\ &= \ln \prod_{i=1}^s \frac{f(s+1, d_T(u_i))}{f(s+t+1, d_T(u_i))} \cdot \prod_{i=1}^t \frac{f(t+1, d_T(v_i))}{f(s+t+1, d_T(v_i))} \cdot \frac{f(s+1, d_T(w)) \cdot f(t+1, d_T(w))}{f(1, d_T(w)) \cdot f(s+t+1, d_T(w))}. \end{aligned}$$

Since the same expressions  $d_T(u_i)$ ,  $d_T(v_i)$ , and  $d_T(w)$  are included in the above equation, therefore, under the condition  $f(x, y) = g(x)h(y)$ , the above equation can be simplified as

$$\begin{aligned} T_{lnf}(T) - T_{lnf}(T') &= \ln \prod_{i=1}^s \frac{g(s+1)}{g(s+t+1)} \cdot \prod_{i=1}^t \frac{g(t+1)}{g(s+t+1)} \cdot \frac{g(s+1) \cdot g(t+1)}{g(1) \cdot g(s+t+1)} \\ &= \ln \frac{g(s+1)^{s+1} \cdot g(t+1)^{t+1}}{g(1) \cdot g(s+t+1)^{s+t+1}}. \end{aligned}$$

Furthermore, if  $g(s+1)^{s+1} \cdot g(t+1)^{t+1} < g(1) \cdot g(s+t+1)^{s+t+1}$ , we can easily obtain  $T_{lnf}(T) - T_{lnf}(T') < \ln 1 = 0$ . Hence, the lemma is proved.  $\square$

**Theorem 10.** Suppose  $f(x, y) = g(x)h(y)$  is a real symmetric function with  $x, y \geq 1$ , and meets the condition  $g(s+1)^{s+1} \cdot g(t+1)^{t+1} < g(1) \cdot g(s+t+1)^{s+t+1}$ , then among all trees of order  $n$ , the maximum index  $T_{lnf}$  is the star  $S_n$ .

**Proof.** Let  $T$  be a tree with  $n$  vertices, and  $|p(T)|$  be the number of pendent vertices of  $T$ . Then  $2 \leq |p(T)| \leq n - 1$ . If  $|p(T)| = n - 1$  or  $n - 2$ , then  $T$  is the star  $S_n$  or double star  $S_{d,n-d}$ , where  $2 \leq d \leq \lfloor \frac{n}{2} \rfloor$ . Thus assume  $|p(T)| \leq n - 3$  for the rest of the proof.

Let  $T_0$  be the graph obtained by removing all pendant vertices from  $T$ . Then  $T_0$  is a subtree of  $T$  with  $n - |p(T)|$  vertices, where  $n - |p(T)| \geq 3$ , and  $d_T(v) \geq 2$  hold for all  $v \in V(T_0)$ . Take two adjacent edges in  $T_0$ , such as  $uwvw$ , thus  $\{uw, vw\} \subseteq E(T)$ ,  $d_T(v) \geq 2$ , and  $d_T(u) \geq 2$ . Without loss of generality, let  $d_T(v) \geq d_T(u)$ . By transformation 2, we obtain a new tree  $T'$  from the tree  $T$ , and have  $|p(T')| = |p(T)| + 1$ . According to Lemma 9,  $T_{lnf}(T) < T_{lnf}(T')$ .

If  $|p(T')| \neq n - 2$ , then using Transformation 2 again for  $T'$ , we can finally obtain the double star  $S_{d,n-d}$ . Therefore, applying Lemma 9, have  $T_{lnf}(T) < T_{lnf}(T')$ .

To complete the proof of theorem, we only need to prove that  $T_{lnf}(S_{d,n-d}) < T_{lnf}(S_n)$ . Note that

$$\begin{aligned} T_{lnf}(S_{d,n-d}) &= (d-1)lnf(d,1) + (n-d-1)lnf(n-d,1) + lnf(d,n-d) \\ &= lnf(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d). \\ T_{lnf}(S_n) &= (n-1)lnf(n-1,1) = lnf(n-1,1)^{n-1}. \end{aligned}$$

And thus,

$$\begin{aligned} T_{lnf}(S_{d,n-d}) - T_{lnf}(S_n) &= lnf(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d) - lnf(n-1,1)^{n-1} \\ &= ln \frac{f(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d)}{f(n-1,1)^{n-1}}. \end{aligned}$$

By substituting the condition into above equation, we can obtain that

$$\begin{aligned} T_{lnf}(S_{d,n-d}) - T_{lnf}(S_n) &= ln \frac{g(d)^{d-1} \cdot g(n-d)^{n-d-1} \cdot g(d) \cdot g(n-d) \cdot g(1)^{n-2}}{g(n-1)^{n-1} g(1)^{n-1}} \\ &= ln \frac{g(d)^d \cdot g(n-d)^{n-d}}{g(n-1)^{n-1} \cdot g(1)} \\ &< ln 1 = 0. \end{aligned}$$

Hence, the theorem holds, and this completes the proof.  $\square$

In the remaining of this section, by utilizing the monotonicity and concavity of functions, we will give sufficient conditions for the star  $S_n$  being the minimal tree of  $T_{lnf}$ .

**Lemma 11.** Let  $T$  and  $T'$  be the trees in Transformation 2 (see Fig. 2). If  $f(x, y)$  meets the conditions  $\frac{\partial f}{\partial x} < 0$ , and  $\frac{\partial^2 f}{\partial x^2} \cdot f - (\frac{\partial f}{\partial x})^2 \leq 0$ , then  $T_{lnf}(T) > T_{lnf}(T')$ .

**Proof.** Denote  $N_1 = \{u_1, u_2, \dots, u_s\}$  and  $N_3 = \{v_1, v_2, \dots, v_t\}$ , where  $s \leq t$ . Similar to Lemma 4.1, we have  $d_T(x) = s + 1, d_T(z) = t + 1$ , and

$$\begin{aligned} T_{lnf}(T) - T_{lnf}(T') &= \sum_{i=1}^s \left( \gamma(s+1, d_T(u_i)) - \gamma(s+t+1, d_T(u_i)) \right) + \sum_{j=1}^t \left( \gamma(t+1, d_T(v_j)) - \gamma(s+t+1, d_T(v_j)) \right) \\ &\quad + \gamma(s+1, d_T(w)) + \gamma(t+1, d_T(w)) - \gamma(1, d_T(w)) - \gamma(s+t+1, d_T(w)). \end{aligned}$$

As  $\frac{\partial \gamma(x,y)}{\partial x} = (\ln f(x,y))' = \frac{f'(x,y)}{f(x,y)}$ , and  $\frac{\partial f}{\partial x} < 0$ ,  $\gamma(x,y)$  is a decreasing function with respect to  $x$ . Then, for  $i = 1, 2, \dots, s$ ,

$$\left( \gamma(s+1, d_T(u_i)) - \gamma(s+t+1, d_T(u_i)) \right) > 0,$$

and for  $j = 1, 2, \dots, t$ ,

$$\left( \gamma(t+1, d_T(v_j)) - \gamma(s+t+1, d_T(v_j)) \right).$$

Since  $\frac{\partial^2 \gamma(x,y)}{\partial x^2} = \frac{\partial \left( \frac{f'(x,y)}{f(x,y)} \right)}{\partial x} = \frac{f''_{xx}f - f_x'^2}{f^2} \leq 0$ , thus,  $\gamma(x,y)$  is concave down in respect to  $x$ . So,

$$\gamma(s+1, d_T(w)) + \gamma(t+1, d_T(w)) \geq \gamma(1, d_T(w)) + \gamma(s+t+1, d_T(w)).$$

Combining the above two equations, the lemma holds true.  $\square$

**Theorem 12.** Suppose  $f(x,y)$  meets the conditions  $\frac{\partial f}{\partial x} < 0$ ,  $f''_{xx}f - f_x'^2 < 0$ , and  $f(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d) > f(n-1,1)^{n-1}$ , then among all trees of order  $n$ , the minimum index  $T_{\ln f}$  is the star  $S_n$ .

**Proof.** Firstly, we prove the extremal tree with the minimum index of  $T_{\ln f}$  is  $S_n$  or  $S_{d,n-d}$ . Let  $|p(T)|$  be the number of pendent vertices of  $T$ . Then  $2 \leq |p(T)| \leq n-1$ . If  $|p(T)| = n-1$  or  $n-2$ , then  $T$  is the star  $S_n$  or double star  $S_{d,n-d}$ , where  $2 \leq d \leq \lfloor \frac{n}{2} \rfloor$ . So, assume  $|p(T)| \leq n-3$  for the rest of the proof.

Let  $T_0$  be the graph obtained by removing all pendant vertices from  $T$ . Then  $T_0$  is a subtree of  $T$  with  $n - |p(T)|$  vertices, where  $n - |p(T)| \geq 3$ , and  $d_T(v) \geq 2$  hold for all  $v \in V(T_0)$ . Take two adjacent edges in  $T_0$ , such as  $uw$  and  $wv$ , thus  $\{uw, wv\} \subseteq E(T)$ ,  $d_T(v) \geq 2$ , and  $d_T(u) \geq 2$ . Without loss of generality, let  $d_T(v) \geq d_T(u)$ . By Transformation 2, we obtain a new tree  $T'$  from the tree  $T$ , and have  $|p(T')| = |p(T)| + 1$ . According to Lemma 4.3,  $T_{\ln f}(T) < T_{\ln f}(T')$ .

If  $|p(T')| \neq n-2$ , then using Transformation 2 again for  $T'$ , we can finally obtain the double star  $S_{d,n-d}$ . Therefore, according to Lemma 4.3,  $T_{\ln f}(T) < T_{\ln f}(T')$ .

Secondly, we will prove that  $T_{\ln f}(S_n) < T_{\ln f}(S_{d,n-d})$ . Note that

$$\begin{aligned} T_{\ln f}(S_{d,n-d}) &= (d-1)\ln f(d,1) + (n-d-1)\ln f(n-d,1) + \ln f(d,n-d) \\ &= \ln f(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d). \\ T_{\ln f}(S_n) &= (n-1)\ln f(n-1,1) = \ln f(n-1,1)^{n-1}. \end{aligned}$$

By the condition  $f(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d) > f(n-1,1)^{n-1}$ , we obtain

$$\begin{aligned} T_{\ln f}(S_{d,n-d}) - T_{\ln f}(S_n) &= \ln f(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d) - \ln f(n-1,1)^{n-1} \\ &= \ln \frac{f(d,1)^{d-1} \cdot f(n-d,1)^{n-d-1} \cdot f(d,n-d)}{f(n-1,1)^{n-1}} \\ &> \ln 1 = 0. \end{aligned}$$

Therefore, the theorem holds, and this completes the proof.  $\square$

## 5. Applications

In this paper, the main contribution of the current work is to investigate the minimal and maximal trees for logarithmic VDB topological indices. Sufficient conditions for  $P_n$  being the minimal tree, sufficient conditions for  $S_n$  being the minimal and maximal tree are given in section 3 and 4.

Note that  $f(x, y) = \sqrt{xy}$ ,  $(xy)^\alpha$  ( $\alpha \geq 1$ ),  $x^2 + y^2$ ,  $\sqrt{x^2 + y^2}$ ,  $\sqrt{(x-1)^2 + (y-1)^2}$ ,  $(x+y)^\alpha$  ( $\alpha \geq 1$ ),  $x + y + xy$ ,  $(x + y + xy)^2$ ,  $(x + y)xy$ ,  $(x + y + xy)^2$ , and  $\sqrt{(x + y)xy}$ , then, the conditions of Theorem 8 are established. So, as an application of Theorem 8, we declare that the minimal tree is  $P_n$  for the logarithmic VDB indices labeled in Table 1.

Likewise, if  $f(x, y) = \sqrt{xy}$ , or  $(xy)^\alpha$  ( $\alpha \geq 1$ ), by Lemma 3, the conditions of Theorem 10 are satisfied. Thus, according to Theorem 10, the maximal tree is  $S_n$  for the logarithmic reciprocal Randić index and general second Zagreb index. Similarly, if  $f(x, y) = \frac{xy}{x+y}$ , then by Lemma 4, the conditions of Theorem 12 are satisfied. Thus, applying Theorem 12, the minimal tree is  $S_n$  for the logarithmic Inverse sum index. The relevant results are shown in Table 1, where  $n \geq 5$  in all cases.

**Table 1.** Extremal trees of  $T_{Inf}$ .

Indices	$f(x, y)$	Min	Max
Inverse sum index	$\frac{xy}{x+y}$	$S_n$	
reciprocal Randić index	$\sqrt{xy}$	$P_n$	$S_n$
general second Zagreb index	$(xy)^\alpha$ ( $\alpha \geq 1$ )	$P_n$	$S_n$
forgotten index	$x^2 + y^2$	$P_n$	
Sombor index	$\sqrt{x^2 + y^2}$	$P_n$	
reduced Sombor index	$\sqrt{(x-1)^2 + (y-1)^2}$	$P_n$	
general first Zagreb index	$(x + y)^\alpha$ ( $\alpha \geq 1$ )	$P_n$	
first Gourava index	$x + y + xy$	$P_n$	
first hyper-Gourava index	$(x + y + xy)^2$	$P_n$	
second Gourava index	$(x + y)xy$	$P_n$	
second hyper-Gourava index	$((x + y)xy)^2$	$P_n$	
product-connectivity Gourava index	$\sqrt{(x + y)xy}$	$P_n$	

**Data Availability Statement:** No underlying data were collected or produced in this study.

**Conflicts of Interest:** The authors declare that they have no conflicts of interest.

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