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Trees with Maximum Vertex–Degree–Based Topological Indices

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Abstract

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, and $d(v_i)$ be the degree of the vertex v_i. The definition of a vertex-degree-based topological index of G is as follows

$$\mathcal{T}_f = \mathcal{T}_f(G) = \sum_{v_iv_j \in E(G)} f(d(v_i), d(v_j)),$$

where $f(x, y) > 0$ is a symmetric real function with $x > 0$ and $y > 0$.

In this paper, we find the extremal trees with the maximum vertex-degree-based topological index $\mathcal{T}_f$ among all trees of order n when $f(x, y)$ is increasing and concave up in respect to variable x (to variable y too, of course).

1 Introduction

All graphs considered in this paper are finite, undirected and simple. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For $i = 1, 2, \ldots, n$, denote by $d_G(v_i)$ (or $d(v_i)$ for short) the degree of the vertex v_i in G, and $N(v_i)$ the set of neighbors of vertex v_i in G. We use S_n and P_n to denote the star and the path of order n, respectively, and $S_{d,n-d}$ to denote the double star of order n with the degrees of two centers being d and $n - d$, where $2 \leq d \leq \lfloor \frac{n}{2} \rfloor$.

In the mathematical and chemical literature, several dozens of vertex-degree-based graph invariants (usually referred to as vertex-degree-based (VDB for short) topological indices) have been introduced and extensively studied [1, 2].

The definition of a VDB topological index of G is as follows

$$\mathcal{T}_f = \mathcal{T}_f(G) = \sum_{v_i v_j \in E(G)} f(d(v_i), d(v_j)), \tag{1}$$

where $f(x, y) > 0$ is a symmetric real function with $x > 0$ and $y > 0$. Gutman [4] collected some important and well-studied VDB topological indices (see Table 1).

Table 1. The main VDB topological indices of the form (1)

$f(x,y)$	Name
$x+y$	First Zagreb index
xy	Second Zagreb index
$(x+y)^2$	First hyper-Zagreb index
$(xy)^2$	Second hyper-Zagreb index
$x^{-3}+y^{-3}$	Modified first Zagreb index
$\lvert x-y \rvert$	Albertson index
$\frac{1}{2}(\frac{x}{y}+\frac{y}{x})$	Extended index
$(x-y)^2$	Sigma index
$\frac{1}{\sqrt{xy}}$	Randić index
$\sqrt{xy}$	Reciprocal Randić index
$\frac{1}{\sqrt{x+y}}$	Sum-connectivity index
$\sqrt{x+y}$	Reciprocal sum-connectivity index
$\frac{2}{x+y}$	Harmonic index
$\sqrt{\frac{x+y-2}{xy}}$	ABC index
$\left(\frac{xy}{x+y-2}\right)^3$	Augmented Zagreb index
x^2+y^2	Forgotten index
$x^{-2}+y^{-2}$	Inverse degree
$\frac{2\sqrt{xy}}{x+y}$	Geometric-arithmetic index
$\frac{x+y}{2\sqrt{xy}}$	Arithmetic-geometric index
$\frac{xy}{x+y}$	Inverse sum index
$x+y+xy$	First Gourava index
$(x+y)xy$	Second Gourava index
$(x+y+xy)^2$	First hyper-Gourava index
$((x+y)xy)^2$	Second hyper-Gourava index
$\frac{1}{\sqrt{x+y+xy}}$	Sum-connectivity Gourava index
$\sqrt{(x+y)xy}$	Product-connectivity Gourava index
$\sqrt{x^2+y^2}$	Sombor index

In 2019, Rada introduced the following exponential VDB topological index of a graph [3]. Given a VDB topological index $\mathcal{T}_f$ defined as in (1), the exponential VDB topological index, denoted by $e^{\mathcal{T}_f}$, is defined as

$$e^{\mathcal{T}_f} = e^{\mathcal{T}_f}(G) = \sum_{v_iv_j \in E(G)} e^{f(d(v_i),d(v_j))}. \tag{2}$$

A very interesting question is to find the extremal values of a VDB topological index $\mathcal{T}_f$ or exponential VDB topological index $e^{\mathcal{T}_f}$ for some special graph classes. There are many papers to study the above problem among all trees of order n ([4]- [19]). Some of the known results are shown in Tables 2 and 3 below.

Table 2. Extremal trees for some indices $\mathcal{T}_f$.

$f(x,y)$	Name	Notation	Min	Max	Ref.
$x+y$	First Zagreb index	$\mathcal{M}_1$	P_n	S_n	[6]
xy	Second Zagreb index	$\mathcal{M}_2$	P_n	S_n	[7]
$\frac{1}{\sqrt{xy}}$	Randić index	χ	S_n	P_n	[8]
$\frac{2}{x+y}$	Harmonic index	$\mathcal{H}$	S_n	P_n	[9]
$\frac{2\sqrt{xy}}{x+y}$	Geometric-arithmetic index	$\mathcal{GA}$	S_n	P_n	[10]
$\frac{x+y}{2\sqrt{xy}}$	Arithmetic-geometric index	$\mathcal{AG}$	P_n	S_n	[11]
$\frac{1}{\sqrt{x+y}}$	Sum-connectivity index	$\mathcal{SC}$	S_n	P_n	[12]
$\sqrt{\frac{x+y-2}{xy}}$	Atom-bond-connectivity index	$\mathcal{ABC}$		S_n	[13]
$(\frac{xy}{x+y-2})^3$	Augmented Zagreb index	$\mathcal{AZ}$	S_n	$S_{\lfloor\frac{n-2}{2}\rfloor,\lceil\frac{n-2}{2}\rceil}$	[14, 15]
$(x+y)^2$	First hyper-Zagreb index	$\mathcal{HM}$	P_n	S_n	[16]
$\frac{xy}{x+y}$	Inverse sum index	$\mathcal{ISI}$	S_n		[17]
$\sqrt{x^2+y^2}$	Sombor index	$\mathcal{SO}$	P_n	S_n	[4]

In this paper, we find the extremal trees with the maximum VDB topological index $\mathcal{T}_f$ among all trees of order n when $f(x,y)$ is increasing and concave up in respect to variable x (to variable y too, of course). Here, we say that $f(x,y)$ is increasing and concave up (decreasing and concave down) in respect to variable x if $\frac{\partial f(x,y)}{\partial x} > 0$ and $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$ ($\frac{\partial f(x,y)}{\partial x} < 0$ and $\frac{\partial^2 f(x,y)}{\partial x^2} \leq 0$).

Table 3. Extremal trees for some indices $e^{\mathcal{T}_f}$.

$e^{f(x,y)}$	Name	Notation	Min	Max	Ref.
e^{x+y}	Exponential first Zagreb index	$e^{\mathcal{M}_1}$	P_n	S_n	[5]
e^{xy}	Exponential second Zagreb index	$e^{\mathcal{M}_2}$	P_n	$S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$	[5, 18]
$e^{\frac{1}{\sqrt{xy}}}$	Exponential Randić index	$e^{\mathcal{X}}$	S_n	P_n	[5, 19]
$e^{\frac{2}{x+y}}$	Exponential Harmonic index	$e^{\mathcal{H}}$	S_n	P_n	[5]
$e^{\frac{2\sqrt{xy}}{x+y}}$	Exponential Geometric-arithmetic index	$e^{\mathcal{GA}}$	S_n	P_n	[5]
$e^{\frac{1}{\sqrt{x+y}}}$	Exponential Sum-connectivity index	$e^{\mathcal{SC}}$	S_n	P_n	[5]
$e^{\sqrt{\frac{x+y-2}{xy}}}$	Exponential Atom-bond-connectivity index	$e^{\mathcal{ABC}}$		S_n	[5]
$e^{(\frac{xy}{x+y-2})^3}$	Exponential Augmented Zagreb index	$e^{\mathcal{AZ}}$	S_n		[5]

2 Main results

Firstly, we introduce a transformation which is very useful to prove our results.

Let T be a tree of order n, $\{uw, wv\} \subseteq E(T)$, and $d_T(v) \geq d_T(u) \geq 2$. Denote $N_1 = N(u) \setminus \{w\}$, $N_2 = N(w) \setminus \{u, v\}$, and $N_3 = N(v) \setminus \{w\}$. Let T' be a tree obtained from T by replacing the edge ux by a new edge vx for each vertex $x \in N_1$. We call that T' is obtained from T by **the edge-moving transformation on vertices** u **and** v (as depicted in Fig. 1).

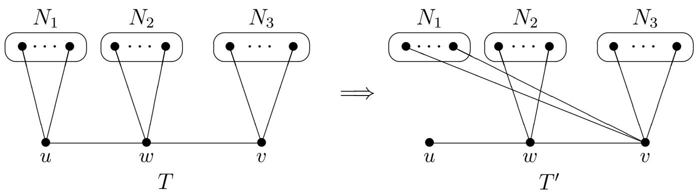

Figure 1. The edge-moving transformation on vertices u and v.

Lemma 1 *Let T' be obtained from T by the edge-moving transformation on vertices u and v (as depicted in Fig. 1). Let $f(x,y) > 0$ be a symmetric real function with $x > 0$ and $y > 0$.*

(1) If $f(x,y)$ is increasing and concave up in respect to x, then $\mathcal{T}_f(T) < \mathcal{T}_f(T')$.

(2) If $f(x,y)$ is decreasing and concave down in respect to x, then $\mathcal{T}_f(T) > \mathcal{T}_f(T')$.

Proof. Let T' be obtained from T by the edge-moving transformation on vertices u and v as depicted in Fig. 1. Denote $N_1 = \{u_1, \ldots, u_s\}$ and $N_3 = \{v_1, \ldots, v_t\}$. Then $d_T(u) = s+1$, $d_T(v) = t+1$, and

$$\begin{aligned}
&\mathcal{T}_f(T) - \mathcal{T}_f(T') \\
&= \sum_{i=1}^{s} f(d_T(u), d_T(u_i)) + \sum_{j=1}^{t} f(d_T(v), d_T(v_j)) + f(d_T(u), d_T(w)) + f(d_T(v), d_T(w)) \\
&\quad - \sum_{i=1}^{s} f(d_T(v)+s, d_T(u_i)) - \sum_{j=1}^{t} f(d_T(v)+s, d_T(v_j)) - f(1, d_T(w)) \\
&\quad - f(d_T(v)+s, d_T(w)) \\
&= \sum_{i=1}^{s} f(s+1, d_T(u_i)) + \sum_{j=1}^{t} f(t+1, d_T(v_j)) + f(s+1, d_T(w)) + f(t+1, d_T(w)) \\
&\quad - \sum_{i=1}^{s} f(s+t+1, d_T(u_i)) - \sum_{j=1}^{t} f(s+t+1, d_T(v_j)) - f(1, d_T(w)) \\
&\quad - f(s+t+1, d_T(w)) \\
&= \sum_{i=1}^{s} (f(s+1, d_T(u_i)) - f(s+t+1, d_T(u_i))) \\
&\quad + \sum_{j=1}^{t} (f(t+1, d_T(v_j)) - f(s+t+1, d_T(v_j))) \\
&\quad + f(s+1, d_T(w)) + f(t+1, d_T(w)) - f(1, d_T(w)) - f(s+t+1, d_T(w)).
\end{aligned}$$

Note that $t \geq s \geq 1$. Then for $i = 1, \ldots, s$,

$$f(s+1, d_T(u_i)) - f(s+t+1, d_T(u_i)) \begin{cases} < 0, & \text{if } f(x,y) \text{ is increasing in respect to } x, \\ > 0, & \text{if } f(x,y) \text{ is decreasing in respect to } x, \end{cases}$$

for $j = 1, \ldots, t$,

$$f(t+1, d_T(v_j)) - f(s+t+1, d_T(v_j)) \begin{cases} < 0, & \text{if } f(x,y) \text{ is increasing in respect to } x, \\ > 0, & \text{if } f(x,y) \text{ is decreasing in respect to } x, \end{cases}$$

and

$$\begin{aligned}
&f(s+1, d_T(w)) + f(t+1, d_T(w)) - f(1, d_T(w)) - f(s+t+1, d_T(w)) \\
&\quad \begin{cases} \leq 0, & \text{if } f(x,y) \text{ is concave up in respect to } x, \\ \geq 0, & \text{if } f(x,y) \text{ is concave down in respect to } x. \end{cases}
\end{aligned}$$

Then the lemma follows. ∎

Theorem 2 *Assume that $f(x, y) > 0$ is a symmetric real function with $x > 0$ and $y > 0$. If $f(x, y)$ is increasing and concave up in respect to x (to variable y too, of course), then among all trees of order n, the extremal tree with the maximum index $\mathcal{T}_f$ is the star S_n or a double star $S_{d,n-d}$ with $2 \le d \le \lfloor \frac{n}{2} \rfloor$.*

Proof. Let T be a tree of order n, and $p(T)$ be the number of pendant vertices of T. Then $2 \le p(T) \le n - 1$. If $p(T) = n - 1$ or $n - 2$, then T is the star S_n or a double star $S_{d,n-d}$. So we now may assume $p(T) \le n - 3$.

Let T_0 be the graph obtained from T by deleting all pendant vertices of T. Then T_0 is a subtree of T with $n - p(T)$ vertices, where $n - p(T) \ge 3$, and $d_T(v) \ge 2$ for all $v \in V(T_0)$. Take two adjacent edges in T_0, such as uw and wv. In this case, $\{uw, wv\} \subseteq E(T)$, $d_T(v) \ge 2$ and $d_T(u) \ge 2$. Without losing its generality, assume that $d_T(v) \ge d_T(u)$. By the edge-moving transformation on vertices u and v for T (see Fig. 1), we obtain a new tree of order n, denoted by T', with $p(T') = p(T) + 1$. By Lemma 1, $\mathcal{T}_f(T) < \mathcal{T}_f(T')$.

If $p(T') \ne n - 2$ (that is, $T' \ne S_{d,n-d}$), then performs above process for T' again. Finally, the process will end up with a double star $S_{d,n-d}$. By Lemma 1, the theorem holds. ■

Remark 3 *The following indices satisfy the conditions of Theorem 2. Then for each of those VDB topological indices, the extremal tree with the maximum index $\mathcal{T}_f$ is the star S_n or a double star $S_{d,n-d}$ with $2 \le d \le \lfloor \frac{n}{2} \rfloor$ among all trees of order n (the VDB topological indices considered here are shown in Table 1.*

- *First Zagreb index: $f(x, y) = x + y$;*
- *Second Zagreb index: $f(x, y) = xy$;*
- *First hyper-Zagreb index: $f(x, y) = (x + y)^2$;*
- *Second hyper-Zagreb index: $f(x, y) = (xy)^2$;*
- *Forgotten index: $f(x, y) = x^2 + y^2$;*
- *First Gourava index: $f(x, y) = x + y + xy$;*
- *Second Gourava index: $f(x, y) = (x + y)xy$;*
- *First hyper-Gourava index: $f(x, y) = (x + y + xy)^2$;*

- *Second hyper-Gourava index:* $f(x,y) = ((x+y)xy)^2$*;*

- *Sombor index:* $f(x,y) = \sqrt{x^2+y^2}$*.*

Thus for each of these indices, in order to determine the extremal tree with the maximum index, we only need to compare the values of $\mathcal{T}_f(S_n)$ *and* $\mathcal{T}_f(S_{d,n-d})$ *with* $2 \le d \le \lfloor \frac{n}{2} \rfloor$*. In the next section, we will do it.*

Corollary 4 *If* $f(x,y)$ *satisfies the conditions of Theorem 2, then among all trees of order* n*, the extremal tree with the maximum index* $e^{\mathcal{T}_f}$ *is* S_n *or a double star* $S_{d,n-d}$ *with* $2 \le d \le \lfloor \frac{n}{2} \rfloor$*.*

Proof. Note that if $f(x,y)$ satisfies the conditions of Theorem 2, then $e^{f(x,y)}$ satisfies the conditions of Theorem 2, too. So the result holds. ■

Theorem 5 *Let* $f(x,y) > 0$ *be a symmetric polynomial with nonnegative coefficients. Then among all trees of order* n*, the extremal tree with the maximum index* $\mathcal{T}_f$ *is* S_n *or a double star* $S_{d,n-d}$ *with* $2 \le d \le \lfloor \frac{n}{2} \rfloor$*, and the extremal tree with the maximum index* $e^{\mathcal{T}_f}$ *is also* S_n *or a double star* $S_{d,n-d}$ *with* $2 \le d \le \lfloor \frac{n}{2} \rfloor$*.*

Proof. It is easy to see that $f(x,y)$ satisfies the conditions of Theorem 2. By Theorem 2 and Corollary 4, the theorem is clear. ■

Theorem 6 *Assume that* $f(x,y) > 0$ *is a symmetric real function with* $x > 0$ *and* $y > 0$*. If* $\frac{\partial f}{\partial x} > 0$ *and* $\left(\frac{\partial f}{\partial x}\right)^2 + \frac{\partial^2 f}{\partial x^2} \ge 0$*, then among all trees of order* n*, the extremal tree with the maximum index* $e^{\mathcal{T}_f}$ *is the star* S_n *or a double star* $S_{d,n-d}$ *with* $2 \le d \le \lfloor \frac{n}{2} \rfloor$*.*

Proof. Note that

$$\frac{\partial}{\partial x} e^{f(x,y)} = e^{f(x,y)} \frac{\partial f(x,y)}{\partial x},$$

$$\frac{\partial^2}{\partial x^2} e^{f(x,y)} = e^{f(x,y)} \left(\frac{\partial f(x,y)}{\partial x}\right)^2 + e^{f(x,y)} \frac{\partial^2 f(x,y)}{\partial x^2}.$$

If $\frac{\partial f}{\partial x} > 0$ and $\left(\frac{\partial f}{\partial x}\right)^2 + \frac{\partial^2 f}{\partial x^2} \ge 0$, then $e^{f(x,y)}$ satisfies the conditions of Theorem 2. By Theorem 2, the result holds. ■

Remark 7 *The following VDB topological indices don't satisfy the conditions of Theorem 2, but they satisfy the conditions of Theorem 6.*

- *Reciprocal Randić index:* $f(x,y)=\sqrt{xy}$;
- *Reciprocal sum-connectivity index:* $f(x,y)=\sqrt{x+y}$;
- *Product-connectivity Gourava index:* $f(x,y)=\sqrt{(x+y)xy}$.

Thus for each of those indices, the extremal tree with the maximum index $e^{\mathcal{T}_f}$ *is the star* S_n *or a double star* $S_{d,n-d}$ *with* $2\le d\le\lfloor\frac{n}{2}\rfloor$ *among all trees of order* n.

Lemma 8 (Geometric–Arithmetic inequality) *Let* $x_i>0$ *for* $i=1,2,\ldots,n$. *Then*

$$\frac{x_1+\cdots+x_n}{n}\ge\sqrt[n]{x_1x_2\ldots x_n},$$

the equality is attained if and only if $x_1=x_2=\cdots=x_n$.

Lemma 9 *Let* $2\le d\le\lfloor\frac{n}{2}\rfloor$. *If* $\mathcal{T}_f(S_{d,n-d})>\mathcal{T}_f(S_n)$, *then* $e^{\mathcal{T}_f}(S_{d,n-d})>e^{\mathcal{T}_f}(S_n)$.

Proof. Note that

$$\begin{aligned}
&\mathcal{T}_f(S_n)=(n-1)f(n-1,1),\\
&\mathcal{T}_f(S_{d,n-d})=(d-1)f(d,1)+(n-d-1)f(n-d,1)+f(d,n-d),\\
&e^{\mathcal{T}_f}(S_n)=(n-1)e^{f(n-1,1)},\\
&e^{\mathcal{T}_f}(S_{d,n-d})=(d-1)e^{f(d,1)}+(n-d-1)e^{f(n-d,1)}+e^{f(d,n-d)}.
\end{aligned}$$

If $\mathcal{T}_f(S_{d,n-d})>\mathcal{T}_f(S_n)$, then

$$(d-1)f(d,1)+(n-d-1)f(n-d,1)+f(d,n-d)>(n-1)f(n-1,1).$$

By Lemma 8,

$$\begin{aligned}
e^{\mathcal{T}_f}(S_{d,n-d})&=(d-1)e^{f(d,1)}+(n-d-1)e^{f(n-d,1)}+e^{f(d,n-d)}\\
&\ge(n-1)\sqrt[n-1]{\left(e^{f(d,1)}\right)^{d-1}\cdot\left(e^{f(n-d,1)}\right)^{n-d-1}\cdot e^{f(d,n-d)}}\\
&=(n-1)\sqrt[n-1]{e^{(d-1)f(d,1)+(n-d-1)f(n-d,1)+f(d,n-d)}}\\
&=(n-1)e^{\frac{(d-1)f(d,1)+(n-d-1)f(n-d,1)+f(d,n-d)}{n-1}}\\
&>(n-1)e^{\frac{(n-1)f(n-1,1)}{n-1}}\\
&=(n-1)e^{f(n-1,1)}=e^{\mathcal{T}_f}(S_n).
\end{aligned}$$

The lemma holds. ■

Theorem 10 *Assume that $f(x,y)$ satisfies the conditions of Theorem 2. Among all trees of order n, if the double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique extremal tree with maximum index $\mathcal{T}_f$, then the double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is also the unique extremal tree with maximum index $e^{\mathcal{T}_f}$.*

Proof. By Theorem 2, Corollary 4, and Lemma 9, the theorem is clear. ■

It is worth noting that for a VDB topological index $\mathcal{T}_f$ which satisfies the conditions of Theorem 2, even if the star S_n is the extremal tree with maximum index $\mathcal{T}_f$ among all trees of order n, it may not be the extremal tree with maximum index $e^{\mathcal{T}_f}$ among all trees of order n.

For example, we consider the Second Zagreb index, that is, $f(x,y) = xy$. This index satisfies the conditions of Theorem 2. From [7, 18] (see Tables 2 and 3), we know that among all trees of order n, the star S_n is the unique extremal tree with maximum Second Zagreb index, and the double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique extremal tree with maximum Exponential second Zagreb index.

Theorem 11 *Let $\alpha > 0$. Assume that $g(x) > 0$ is increasing and concave up in respect to $x > 0$, and $f(x,y) = (g(x) + g(y))^{\alpha}$. Then among all trees of order n, the star S_n is the extremal tree with the maximum index $\mathcal{T}_f$, and S_n is also the extremal tree with the maximum index $e^{\mathcal{T}_f}$.*

Proof. Let T be a tree of order n. For any edge $e = v_iv_j \in E(T)$, without loss of generality, assume that $d(v_i) \leq d(v_j)$. Since $d(v_i) + d(v_j) \leq n$, we have that $1 \leq d(v_i) \leq \lfloor \frac{n}{2} \rfloor$, and $d(v_j) \leq n - d(v_i)$. Note that $g(x)$ is increasing and concave up in respect to x. Then

$$\begin{aligned} f(d(v_i), d(v_j)) &= (g(d(v_i)) + g(d(v_j)))^{\alpha} \\ &\leq (g(d(v_i)) + g(n - d(v_i)))^{\alpha} \\ &\leq (g(1) + g(n-1))^{\alpha} = f(1, n-1). \end{aligned}$$

Thus

$$\mathcal{T}_f(T) = \sum_{v_iv_j \in E(G)} f(d(v_i), d(v_j)) \leq (n-1) f(1, n-1) = \mathcal{T}_f(S_n),$$

and

$$e^{\mathcal{T}_f}(T) = \sum_{v_iv_j \in E(G)} e^{f(d(v_i), d(v_j))} \leq (n-1) e^{f(1,n-1)} = e^{\mathcal{T}_f}(S_n).$$

The theorem follows. ■

At the end of this section, we give the following result for the minimum index $\mathcal{T}_f$. Its proof is similar to the proof of Theorem 2, and we omit it.

Theorem 12 *Assume that $f(x,y) > 0$ is a symmetric real function with $x > 0$ and $y > 0$. If $f(x,y)$ is decreasing and concave down in respect to variable x (to variable y too, of course), then the extremal tree with the minimum index $\mathcal{T}_f$ is S_n or a double star $S_{d,n-d}$ with $2 \le d \le \lfloor \frac{n}{2} \rfloor$ among all trees of order n.*

It is worth pointing out that we haven't found any well-known VDB topological index $\mathcal{T}_f$ that satisfies Theorem 12.

3 Application

In this section, we will determine the extremal tree with the maximum index $\mathcal{T}_f$ among all trees of order n for each VDB topological index $\mathcal{T}_f$ in Remark 3. Note that for $n \le 3$, there is only one tree of order n. So we assume $n \ge 4$.

Please keep in mind that

$$\begin{aligned}&\mathcal{T}_f(S_{d,n-d}) - \mathcal{T}_f(S_n)\\=&(d-1)f(d,1) + (n-d-1)f(n-d,1) + f(d,n-d) - (n-1)f(n-1,1).\end{aligned}$$

(1) First Zagreb index: $f(x,y) = x + y$.

Note that for $2 \le d \le \lfloor \frac{n}{2} \rfloor$, $1 + d < n$. So

$$\begin{aligned}&\mathcal{T}_f(S_{d,n-d}) - \mathcal{T}_f(S_n)\\=&(d-1)(d+1) + (n-d-1)(n-d+1) + n - n(n-1)\\=&-2(d-1)(n-d-1) < 0.\end{aligned}$$

Then by Theorem 2, the unique tree with maximum First Zagreb index is the star S_n (this result is also shown in [6]).

(2) Second Zagreb index: $f(x,y) = xy$.

Note that for $2 \le d \le \lfloor \frac{n}{2} \rfloor$, $1 + d < n$. So

$$\begin{aligned}&\mathcal{T}_f(S_{d,n-d}) - \mathcal{T}_f(S_n)\\=&(d-1)d + (n-d-1)(n-d) + d(n-d) - (n-1)^2\\=&-(d-1)(n-d-1) < 0.\end{aligned}$$

Then by Theorem 2, the unique tree with maximum Second Zagreb index is the star S_n (this result is also shown in [7]).

(3) First hyper-Zagreb index: $f(x,y)=(x+y)^2$.

Note that for $2 \le d \le \lfloor \frac{n}{2} \rfloor$, $1+d<n$. So

$$\begin{aligned}&\mathcal{T}_f(S_{d,n-d})-\mathcal{T}_f(S_n)\\ =&(d-1)(d+1)^2+(n-d-1)(n-d+1)^2+(d+n-d)^2-(n-1)n^2\\ =&-(d-1)(n-d-1)(3n+2)<0.\end{aligned}$$

Then by Theorem 2, the unique tree with maximum First hyper-Zagreb index is the star S_n (this result is also shown in [16]).

(4) Second hyper-Zagreb index: $f(x,y)=(xy)^2$.

Note that

$$\begin{aligned}&\mathcal{T}_f(S_n)=(n-1)f(n-1,1)=(n-1)^3,\\ &\mathcal{T}_f(S_{d,n-d})=(d-1)d^2+(n-d-1)(n-d)^2+d^2(n-d)^2,\\ &\mathcal{T}_f(S_{d,n-d})-\mathcal{T}_f(S_n)=d^4-2nd^3+(n^2+3n-2)d^2-(3n^2-2n)d+2n^2-3n+1.\end{aligned}$$

Case 1. $n \le 7$.

Then $d=2$ or 3. If $d=2$, then $\mathcal{T}_f(S_{d,n-d})-\mathcal{T}_f(S_n)=9-3n<0$. If $d=3$, then $n \ge 2d=6$, and $\mathcal{T}_f(S_{d,n-d})-\mathcal{T}_f(S_n)=2((n-6)^2-4)<0$. So in this case, $\mathcal{T}_f(S_{d,n-d})<\mathcal{T}_f(S_n)$.

Case 2. $n \ge 8$.

Note that for $n \ge 8$, and $2 \le d \le \lfloor \frac{n}{2} \rfloor$,

$$\begin{aligned}\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}&=4d^3-6nd^2+2(n^2+3n-2)d-3n^2+2n,\\ \frac{\partial^2 \mathcal{T}_f(S_{d,n-d})}{\partial d^2}&=12d^2-12nd+2n^2+6n-4,\\ \frac{\partial^3 \mathcal{T}_f(S_{d,n-d})}{\partial d^3}&=24d-12n\le 0.\end{aligned}$$

Thus $\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}$ is concave down in respect to d, and

$$\begin{aligned}\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}&\ge \min\left\{\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\Big|_{d=2}, \frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\Big|_{d=\lfloor \frac{n}{2}\rfloor}\right\}\\ &=\begin{cases}\min\{n^2-10n+24,0\}\ge 0, & \text{if } n \text{ is even},\\ \min\{n^2-10n+24,\frac{1}{2}(n^2-6n+3)\}>0, & \text{if } n \text{ is odd}.\end{cases}\end{aligned}$$

So $\mathcal{T}_f(S_{d,n-d})$ is increasing in respect to d. Then

$$\begin{aligned}
&\max_{2\le d\le\lfloor\frac{n}{2}\rfloor}\mathcal{T}_f(S_{d,n-d})=\mathcal{T}_f(S_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil})\\
=&\begin{cases}\mathcal{T}_f(S_{d,n-d})\Big|_{d=\frac{n}{2}}=\frac{1}{16}n^2\left(n^2+4n-8\right), & \text{if } n \text{ is even,}\\ \mathcal{T}_f(S_{d,n-d})\Big|_{d=\frac{n-1}{2}}=\frac{1}{16}\left(n^4+4n^3-10n^2+12n-7\right), & \text{if } n \text{ is odd.}\end{cases}
\end{aligned}$$

If $n\ge 8$ is even, then

$$\begin{aligned}
\mathcal{T}_f(S_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil})-\mathcal{T}_f(S_n)&=\frac{1}{16}n^2\left(n^2+4n-8\right)-(n-1)^3\\
&=\frac{1}{16}(n-2)^2\left(n^2-8n+4\right)>0.
\end{aligned}$$

If $n\ge 9$ is odd, then

$$\begin{aligned}
\mathcal{T}_f(S_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil})-\mathcal{T}_f(S_n)&=\frac{1}{16}\left(n^4+4n^3-10n^2+12n-7\right)-(n-1)^3\\
&=\frac{1}{16}(n-1)(n-3)(n^2-8n+3)>0.
\end{aligned}$$

It implies that for $n\ge 8$,

$$\max_{2\le d\le\lfloor\frac{n}{2}\rfloor}\mathcal{T}_f(S_{d,n-d})=\mathcal{T}_f(S_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil})>\mathcal{T}_f(S_n).$$

Based on the above discussions, by Theorem 2, we have that if $n\le 7$, then the unique extremal tree with maximum Second hyper-Zagreb index is the star S_n; and if $n\ge 8$, then the unique extremal tree with maximum Second hyper-Zagreb index is the double star $S_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$.

(5) Forgotten index: $f(x,y)=x^2+y^2$.

Note that for $2\le d\le\lfloor\frac{n}{2}\rfloor$, $1+d<n$. So

$$\begin{aligned}
&\mathcal{T}_f(S_{d,n-d})-\mathcal{T}_f(S_n)\\
=&(d-1)(d^2+1)+(n-d-1)((n-d)^2+1)+(d^2+(n-d)^2)-(n-1)((n-1)^2+1)\\
=&-3n(d-1)(n-d-1)<0.
\end{aligned}$$

Then by Theorem 2, the unique tree with maximum Forgotten index is the star S_n.

(6) First Gourava index: $f(x,y)=x+y+xy$.

Note that for $2\le d\le\lfloor\frac{n}{2}\rfloor$, $1+d<n$. So

$$\begin{aligned}
&\mathcal{T}_f(S_{d,n-d})-\mathcal{T}_f(S_n)\\
&=(d-1)(2d+1)+(n-d-1)(2n-2d+1)+n+d(n-d)-(n-1)(2n-1)\\
&=-3(d-1)(n-d-1)<0.
\end{aligned}$$

Then by Theorem 2, the unique tree with maximum First Gourava index is the star S_n.

(7) Second Gourava index: $f(x,y) = (x+y)xy$.

Note that for $2 \le d \le \lfloor \frac{n}{2} \rfloor$, $1+d < n$. So

$$\begin{aligned}
&\mathcal{T}_f(S_{d,n-d}) - \mathcal{T}_f(S_n)\\
&= (d-1)(d+1)d + (n-d-1)(n-d+1)(n-d) + nd(n-d) - (n-1)n(n-1)\\
&= -2n(d-1)(n-d-1) < 0.
\end{aligned}$$

Then by Theorem 2, the unique tree with maximum Second Gourava index is the star S_n.

(8) First hyper-Gourava index: $f(x,y) = (x+y+xy)^2$.

Note that

$$\begin{aligned}
\mathcal{T}_f(S_n) &= (n-1)f(n-1,1) = (n-1)(2n-1)^2,\\
\mathcal{T}_f(S_{d,n-d}) &= (d-1)(2d+1)^2 + (n-d-1)(2n-2d+1)^2 + (n+d(n-d))^2\\
&= d^4 - 2nd^3 + (n^2+10n)d^2 - 10n^2 d + 4n^3 + n^2 - 3n - 2,\\
\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d} &= 4d^3 - 6nd^2 + 2(n^2+10n)d - 10n^2.
\end{aligned}$$

If $n \le 20$, noting that

$$\frac{\partial^2 \mathcal{T}_f(S_{d,n-d})}{\partial d^2} = 12d^2 - 12nd + 2(n^2+10n) = 3(n-2d)^2 - n(n-20) \ge 0,$$

then $\mathcal{T}_f(S_{d,n-d})$ is concave up in respect to d, and so

$$\max_{2 \le d \le \lfloor \frac{n}{2} \rfloor} \mathcal{T}_f(S_{d,n-d}) = \max\left\{ \mathcal{T}_f(S_{d,n-d})\Big|_{d=2}, \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} \right\}.$$

If $n \ge 21$, noting that

$$\frac{\partial^3 \mathcal{T}_f(S_{d,n-d})}{\partial d^3} = 12(2d-n) \le 0,$$

then $\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}$ is concave down in respect to d. Note that

$$\begin{aligned}
\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\Big|_{d=2} &= -6n^2 + 16n + 32 < 0,\\
\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\Big|_{d=\lfloor \frac{n}{2} \rfloor - 1} &= \begin{cases} n^2 - 20n - 4 > 0, & \text{if } n \text{ is even},\\ \frac{3}{2}\left(n^2 - 20n - 9\right) > 0, & \text{if } n \text{ is odd}, \end{cases}\\
\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\Big|_{d=\lfloor \frac{n}{2} \rfloor} &= \begin{cases} 0, & \text{if } n \text{ is even},\\ \frac{1}{2}\left(n^2 - 20n - 1\right) > 0, & \text{if } n \text{ is odd}. \end{cases}
\end{aligned}$$

It implies that there is $2 < d_0 < \lfloor \frac{n}{2} \rfloor$ such that $\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d} \leq 0$ for $2 \leq d \leq d_0$, and $\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d} \geq 0$ for $d_0 \leq d \leq \lfloor \frac{n}{2} \rfloor$. Thus

$$\max_{2\leq d\leq \lfloor \frac{n}{2} \rfloor} \mathcal{T}_f(S_{d,n-d}) = \max\left\{ \mathcal{T}_f(S_{d,n-d})\Big|_{d=2}, \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} \right\}.$$

Note that

$$\mathcal{T}_f(S_{d,n-d})\Big|_{d=2} = 4n^3 - 15n^2 + 21n + 14,$$

$$\mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} = \begin{cases} \frac{1}{16}\left(n^4 + 24n^3 + 16n^2 - 48n - 32\right), & \text{if } n \text{ is even,} \\ \frac{1}{16}\left(n^4 + 24n^3 + 14n^2 - 8n - 31\right), & \text{if } n \text{ is odd.} \end{cases}$$

Then

$$\mathcal{T}_f(S_{d,n-d})\Big|_{d=2} - \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} = \begin{cases} -\frac{1}{16}(n-4)^2(n^2 - 32n - 16), & \text{if } n \text{ is even,} \\ -\frac{1}{16}(n-5)(n-3)(n^2 - 32n - 17), & \text{if } n \text{ is odd.} \end{cases}$$

It implies that if $n \leq 32$ then $\mathcal{T}_f(S_{d,n-d})\Big|_{d=2} > \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor}$, and if $n \geq 33$ then $\mathcal{T}_f(S_{d,n-d})\Big|_{d=2} < \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor}$. So

$$\begin{aligned} \max_{2\leq d\leq \lfloor \frac{n}{2} \rfloor} \mathcal{T}_f(S_{d,n-d}) &= \max\left\{ \mathcal{T}_f(S_{d,n-d})\Big|_{d=2}, \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} \right\} \\ &= \begin{cases} \mathcal{T}_f(S_{d,n-d})\Big|_{d=2}, & \text{if } n \leq 32, \\ \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor}, & \text{if } n \geq 33. \end{cases} \end{aligned}$$

Note that

$$\mathcal{T}_f(S_{d,n-d})\Big|_{d=2} - \mathcal{T}_f(S_n) = -(n-3)(7n+5),$$

$$\mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} - \mathcal{T}_f(S_n) = \begin{cases} \frac{1}{16}(n-2)^2(n^2 - 36n - 4), & \text{if } n \text{ is even,} \\ \frac{1}{16}(n-3)(n-1)(n^2 - 36n - 5), & \text{if } n \text{ is odd.} \end{cases}$$

It implies that $\mathcal{T}_f(S_{d,n-d})\Big|_{d=2} < \mathcal{T}_f(S_n)$, if $n \leq 36$ then $\mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} < \mathcal{T}_f(S_n)$; and if $n \geq 37$ then $\mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} > \mathcal{T}_f(S_n)$.

Based on the above discussions, by Theorem 2, we get that if $n \leq 36$, then the unique extremal tree with maximum First hyper-Gourava index is the star S_n; if $n \geq 37$, then the unique extremal tree with maximum First hyper-Gourava index is the double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

(9) Second hyper-Gourava index: $f(x, y) = ((x + y)xy)^2$;

Note that

$$\mathcal{T}_f(S_n) = (n-1)f(n-1,1) = (n-1)(n(n-1))^2,$$

$$\begin{aligned}\mathcal{T}_f(S_{d,n-d}) &= (d-1)((d+1)d)^2 + (n-d-1)((n-d+1)(n-d))^2 + (nd(n-d))^2\\ &= \left(n^2+5n+2\right)d^4 - 2\left(n^3+5n^2+2n\right)d^3 + \left(n^4+10n^3+6n^2-3n-2\right)d^2\\ &\quad - \left(5n^4+4n^3-3n^2-2n\right)d + n^5+n^4-n^3-n^2\end{aligned}$$

Case 1. $n \le 7$.

In this case, $2 \le d \le 3$. Note that

$$\mathcal{T}_f(S_{d,n-d}) - \mathcal{T}_f(S_n) = \begin{cases} -2(n^4-6n^3+17n^2-20n-12) < 0, & \text{if } d=2,\ 4\le n\le 7,\\ -2(n^4-10n^3+63n^2-138n-72) < 0, & \text{if } d=3,\ 6\le n\le 7.\end{cases}$$

Then $\mathcal{T}_f(S_{d,n-d}) < \mathcal{T}_f(S_n)$.

Case 2. $n \ge 8$.

Note that

$$\begin{aligned}\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d} =&4\left(n^2+5n+2\right)d^3 - 6n\left(n^2+5n+2\right)d^2 + 2\left(n^4+10n^3+6n^2-3n-2\right)d\\ &- \left(5n^4+4n^3-3n^2-2n\right),\\ \frac{\partial^2 \mathcal{T}_f(S_{d,n-d})}{\partial d^2} =&12\left(n^2+5n+2\right)d^2 - 12n\left(n^2+5n+2\right)d + 2\left(n^4+10n^3+6n^2-3n-2\right),\\ \frac{\partial^3 \mathcal{T}_f(S_{d,n-d})}{\partial d^3} =&24\left(n^2+5n+2\right)d - 12n\left(n^2+5n+2\right) = -12(n^2+5n+2)(n-2d) \le 0.\end{aligned}$$

Then $\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}$ is concave down in respect to d. Note that

$$\left.\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\right|_{d=2} = -n^4+12n^3-61n^2+102n+56 < 0,$$

$$\left.\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\right|_{d=\lfloor\frac{n}{2}\rfloor-1} = \begin{cases} n^4-5n^3-10n^2-14n-4 > 0, & \text{if } n \text{ is even},\\ \frac{3}{2}\left(n^4-5n^3-15n^2-39n-14\right) > 0, & \text{if } n \text{ is odd},\end{cases}$$

$$\left.\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d}\right|_{d=\lfloor\frac{n}{2}\rfloor} = \begin{cases} 0, & \text{if } n \text{ is even},\\ \frac{1}{2}\left(n^4-5n^3-7n^2+n+2\right) > 0, & \text{if } n \text{ is odd}.\end{cases}$$

It implies that there is $2 < d_0 < \lfloor\frac{n}{2}\rfloor$ such that $\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d} \le 0$ for $2 \le d \le d_0$, and $\frac{\partial \mathcal{T}_f(S_{d,n-d})}{\partial d} \ge 0$ for $d_0 \le d \le \lfloor\frac{n}{2}\rfloor$. That is, $\mathcal{T}_f(S_{d,n-d})$ is concave up in respect to d. Thus

$$\max_{2\le d\le\lfloor\frac{n}{2}\rfloor} \mathcal{T}_f(S_{d,n-d}) = \max\left\{\left.\mathcal{T}_f(S_{d,n-d})\right|_{d=2}, \left.\mathcal{T}_f(S_{d,n-d})\right|_{d=\lfloor\frac{n}{2}\rfloor}\right\},$$

where

$$\left.\mathcal{T}_f(S_{d,n-d})\right|_{d=2} = n^5-5n^4+15n^3-35n^2+40n+24,$$

$$\left.\mathcal{T}_f(S_{d,n-d})\right|_{d=\lfloor\frac{n}{2}\rfloor} = \begin{cases} \frac{1}{16}\left(n^6+n^5+2n^4-4n^3-8n^2\right), & \text{if } n \text{ is even},\\ \frac{1}{16}\left(n^6+n^5+6n^3+5n^2-7n-6\right), & \text{if } n \text{ is odd}.\end{cases}$$

Since

$$\mathcal{T}_f(S_{d,n-d})\Big|_{d=2} - \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor}$$
$$= \begin{cases} -\frac{1}{16}(n-4)^2\left((n-7)n^3 + 2(n-6)(5n+4) + 24\right) < 0, & \text{if } n \text{ is even}, \\ -\frac{1}{16}(n-3)(n-5)\left((n-7)n^3 + 3(n-7)(3n+2) + 16\right) < 0, & \text{if } n \text{ is odd}, \end{cases}$$

we have

$$\max_{2\le d\le \lfloor \frac{n}{2} \rfloor} \mathcal{T}_f(S_{d,n-d}) = \max\left\{\mathcal{T}_f(S_{d,n-d})\Big|_{d=2}, \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor}\right\} = \mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor}.$$

Note that

$$\mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} - \mathcal{T}_f(S_n)$$
$$= \begin{cases} \frac{1}{16}n^2(n-2)^2(n^2-11n+2), & \text{if } n \text{ is even}, \\ \frac{1}{16}(n-3)(n-1)\left(n\left(n^3-11n^2+n-5\right)-2\right), & \text{if } n \text{ is odd}. \end{cases}$$

It is easy to see that if $8 \le n \le 10$, then $\mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} - \mathcal{T}_f(S_n) < 0$; and if $n \ge 11$, then $\mathcal{T}_f(S_{d,n-d})\Big|_{d=\lfloor \frac{n}{2} \rfloor} - \mathcal{T}_f(S_n) > 0$.

Based on the above discussions, by Theorem 2, we get that if $n \le 10$, then the unique extremal tree with maximum Second hyper-Gourava index is the star S_n; and if $n \ge 11$, then the unique extremal tree with maximum Second hyper-Gourava index is the double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

(10) Sombor index: $f(x, y) = \sqrt{x^2 + y^2}$.
Note that for $2 \le d \le \lfloor \frac{n}{2} \rfloor$, $1 + d < n$. So $d^2 + (n-d)^2 < (n-1)^2 + 1$ and

$$\begin{aligned} &\mathcal{T}_f(S_{d,n-d}) - \mathcal{T}_f(S_n) \\ &= (d-1)\sqrt{d^2+1} + (n-d-1)\sqrt{(n-d)^2+1} + \sqrt{d^2+(n-d)^2} - (n-1)\sqrt{(n-1)^2+1} \\ &< (d-n)\sqrt{(n-1)^2+1} + (n-d-1)\sqrt{(n-d)^2+d^2} + \sqrt{d^2+(n-d)^2} \\ &= (n-d)(\sqrt{d^2+(n-d)^2} - \sqrt{(n-1)^2+1}) < 0. \end{aligned}$$

Then by Theorem 2, the unique tree with maximum Sombor index is the star S_n (this result is also shown in [4]).

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