Extremal Polygonal Cacti for General Sombor Index

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Abstract

The Sombor index of a graph $G$ was recently introduced by Gutman from the geometric point of view, defined as $SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}$, where $d(u)$ is the degree of a vertex $u$. For two real numbers $\alpha$ and $\beta$, the $\alpha$-Sombor index and general Sombor index of $G$ are two generalized forms of the Sombor index defined as $SO_\alpha(G) = \sum_{uv \in E(G)} (d(u)^\alpha + d(v)^\alpha)^{1/\alpha}$ and $SO_\alpha(G; \beta) = \sum_{uv \in E(G)} (d(u)^\alpha + d(v)^\alpha)^\beta$, respectively. A $k$-polygonal cactus is a connected graph in which every block is a cycle of length $k$. In this paper, we establish a lower bound on $\alpha$-Sombor index for $k$-polygonal cacti and show that the bound is attained only by chemical $k$-polygonal cacti. The extremal $k$-polygonal cacti for $SO_\alpha(G; \beta)$ with some particular $\alpha$ and $\beta$ are also considered.

Keywords: general Sombor index, polygonal cactus, extremal problem

Mathematics Subject Classification: 05C07, 05C09, 05C90

1 Introduction

We consider only connected simple graphs. For a graph $G$, we denote by $V(G)$ and $E(G)$ the vertex set and edge set of $G$, respectively. For a vertex $v \in V(G)$, we denote by $d_G(v)$, or $d(v)$ if no confusion can occur, the degree of $v$. A vertex $v$ is called a cut vertex of $G$ if $G - v$ is not connected.

In mathematical chemistry, particularly in QSPR/QSAR investigation, a large number of topological indices were introduced in an attempt to characterize the physical-chemical
properties of molecules. Among these indices, the vertex-degree-based indices play important roles [4, 7, 8]. Probably the most studied are, for examples, the Randić connectivity index $R(G)$ [18], the first and second Zagreb indices $M_1(G)$ and $M_2(G)$ [9], which were introduced for the total $\pi$-energy of alternant hydrocarbons.

A vertex-degree-based index of a graph $G$ can be generally represented as the sum of a real function $f(d(u), d(v))$ associated with the edges of $G$ [10], i.e.,

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

where $f(s, t) = f(t, s)$. In the literature, $I_f(G)$ is also called the connectivity function [22] or bond incident degree index [1, 21, 23].

Recently, Gutman [10] introduced an idea to view an edge $e = uv$ as a geometric point, namely the degree-point, that is, to view the ordered pair $(d(u), d(v))$ as the coordinate of $e$. Therefore, it is interesting to consider the function $f(s, t)$ from the geometric point of view. A natural considering is to define $f(s, t)$ as a geometric distance from the degree-point $(s, t)$ to the origin. In this sense, the first Zagreb index, i.e., $M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)) = \sum_{uv \in E(G)} (|d(u)| + |d(v)|)$, is exactly the index defined on the Manhattan distance. Along this direction, a more natural considering would be to define $f(s, t)$ as the Euclidean distance, i.e., $f(s, t) = \sqrt{s^2 + t^2}$. Indeed, based on this idea, Gutman [10] introduced the Somber index defined by

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}$$

and further determined the extremal trees for the index. In [3], Das et al. established some bounds on the Sombor index and some relations between Sombor index and the Zagreb indices and, in [19], Redžpović studied chemical applicability of the Sombor index. Further, Cruz et al. [2] characterized the extremal chemical graphs and hexagonal systems for the Sombor index.

More recently, for positive real number $\alpha$, Réti et al. [20] defined the $\alpha$-Sombor index as

$$SO_\alpha(G) = \sum_{uv \in E(G)} (d(u)^\alpha + d(v)^\alpha)^{1/\alpha},$$

which could be viewed as the one based on Minkowski distance. In the same paper, they also characterized the extremal graphs with few cycles for $\alpha$-Sombor index.
In this paper we consider a more generalized form of Sombor index defined as

\[ SO_\alpha(G; \beta) = \sum_{uv \in E(G)} (d(u)\alpha + d(v)\alpha)^\beta, \]

where \( \alpha, \beta \) are real numbers. We note that this form is a natural generalization of the Sombor index, which was also introduced elsewhere, e.g., the first \((\alpha, \beta) – KA\) index in [12] and the general Sombor index in [11]. In addition to the first Zagreb, Sombor and the \( \alpha \)-Sombor index listed above, the general Sombor index also includes many other known indices, e.g., the modified first Zagreb index \((\alpha = -3, \beta = 1)\) [17], forgotten index \((\alpha = 2, \beta = 1)\) [9], inverse degree index \((\alpha = -2, \beta = 1)\) [5], modified Sombor index \((\alpha = 2, \beta = -1/2)\) [13], first Banhatti-Sombor index \((\alpha = -2, \beta = 1/2)\) [15] and general sum-connectivity index \((\alpha = 1, \beta \in \mathbb{R})\) [24].

A block in a graph is a cut edge or a maximal 2-connected component. A cactus is a connected graph in which every block is a cut edge or a cycle. Equivalently, a cactus has no edge lies in more than one cycle. In the following, we call a \( k \)-cycle (a cycle of length \( k \)) a \( k \)-polygon. If each block of a cactus \( G \) is a \( k \)-polygon, then \( G \) is called a \( k \)-polygonal cactus or polygonal cactus with no confusion.

In this paper, we consider the extremal \( k \)-polygonal cacti for \( SO_\alpha(G; \beta) \). In the following section we establish a lower bound on \( \alpha \)-Sombor index for \( k \)-polygonal cacti and show that the bound is attained only by chemical \( k \)-polygonal cacti. In the third section we characterize the extremal polygonal cactus with maximum \( SO_\alpha(G; \beta) \) for (i) \( \alpha > 1 \) and \( \beta \geq 1 \); and (ii) \( 1/2 \leq \alpha < 1 \) and \( \beta = 2 \), respectively. In the fourth section, we characterize the extremal polygonal cacti with minimum \( SO_\alpha(G; \beta) \) for \( \alpha > 1 \) and \( \beta \geq 1 \).

2 Polygonal cacti with minimum \( \alpha \)-Sombor index

For convenience, in what follows we denote \( r_\alpha(s, t; \beta) = (s^\alpha + t^\alpha)^\beta \), \( r_\alpha(s, t) = (s^\alpha + t^\alpha)^{1/\alpha} \) and \( r(s, t) = \sqrt{s^2 + t^2} \), where \( s > 0, t > 0, \alpha, \beta \in \mathbb{R} \) and \( \alpha \neq 0 \). For integers \( n \) with \( n \geq 1 \) and \( k \) with \( k \geq 3 \), we denote by \( \mathcal{G}_{n,k} \) the class of \( k \)-polygonal cacti with \( n \) polygons.

In this section we consider the \( \alpha \)-Sombor index \( SO_\alpha(G) \), i.e., \( SO_\alpha(G; 1/\alpha) \). For \( G \in \mathcal{G}_{n,k} \), it is clear that \(|V(G)| = nk - n + 1, |E(G)| = nk \) and every vertex of \( G \) has even degree no more than \( 2n \). Further, it is clear that \( v \) is a cut vertex of \( G \) if and only if \( v \) has degree...
no less than 4, i.e., \( d_G(v) \geq 4 \). A polygon is called a *pendent polygon* if it contains exactly one cut-vertex of \( G \). For \( 2 \leq s \leq t \leq 2n \), we denote by \( n_{s,t} = n_{s,t}(G) \) the number of edges in \( G \) that join two vertices of degrees \( s \) and \( t \). Let \( X = \{(s,t) : s, t \in \{2, 4, \ldots, 2n\}, s \leq t \} \) and \( Y = X \setminus \{(2, 2), (2, 4), (4, 4)\} \).

**Definition 2.1.** \[16\] Let \( \pi = (w_1, w_2, \ldots, w_n) \) and \( \pi' = (w'_1, w'_2, \ldots, w'_n) \) be two non-increasing sequences of nonnegative real numbers. We write \( \pi < \pi' \) if and only if \( \pi \neq \pi' \), \( \sum_{i=1}^n w_i = \sum_{i=1}^n w'_i \), and \( \sum_{i=1}^j w_i \leq \sum_{i=1}^j w'_i \) for all \( j = 1, 2, \ldots, n \).

A function \( \zeta(x) \) defined on a convex set \( X \) is called *strictly convex* if

\[
\zeta(\mu x_1 + (1-\mu)x_2) < \mu \zeta(x_1) + (1-\mu)\zeta(x_2)
\]

for any \( 0 < \mu < 1 \) and \( x_1, x_2 \in X \) with \( x_1 \neq x_2 \).

**Lemma 2.1.** \[16\] Let \( \pi = (w_1, w_2, \ldots, w_n) \) and \( \pi' = (w'_1, w'_2, \ldots, w'_n) \) be two non-increasing sequences of nonnegative real numbers. If \( \pi < \pi' \), then for any strictly convex function \( \zeta(x) \), we have \( \sum_{i=1}^n \zeta(w_i) < \sum_{i=1}^n \zeta(w'_i) \).

**Lemma 2.2.** Let \( \alpha > 1 \) and \( n \geq 3 \). Then

(i). \( r_\alpha(2n, 2) - r_\alpha(2n - 2, 4) > 0 \);

(ii). \( r_\alpha(6, 2) + r_\alpha(2, 2) - 2r_\alpha(4, 2) > 0 \).

**Proof.** Since \( \alpha > 1 \) and \( n \geq 3 \), then by Lemma 2.1 we have \( (2n)^\alpha + 2^\alpha > (2n - 2)^\alpha + 4^\alpha \). Hence (i) holds clearly. Let \( g(x) = r_\alpha(x, 2) = (x^\alpha + 2^\alpha)^{1/\alpha} \), where \( x > 0 \) and \( \alpha > 1 \). Since \( g''(x) = \frac{(\alpha-1)2^{\alpha}x^{\alpha-2}}{(x^\alpha + 2^\alpha)^{2(1/\alpha)}} > 0 \), then \( g(x) \) is strictly convex. Then by Lemma 2.1 \( g(6) + g(2) > 2g(4) \). Hence (ii) also holds.

**Lemma 2.3.** Let \( \alpha \neq 0 \) and \( G \in \mathcal{G}_{n,k} \), where \( n \geq 1 \) and \( k \geq 3 \). Then

\[
SO_\alpha(G) = (4n - 4)(2^\alpha + 4^\alpha)^{1/\alpha} + 2(nk - 4n + 4)^{2/\alpha}
+ (6 \times 2^{1/\alpha} - 2(2^\alpha + 4^\alpha)^{1/\alpha})n_{4,4} + \sum_{(s,t) \in Y} \eta(s, t; \alpha)n_{s,t},
\]

where \( \eta(s, t; \alpha) = (s^\alpha + t^\alpha)^{1/\alpha} - 2 \left( \frac{1}{s} + \frac{1}{t} \right) 2^{1/\alpha} \).

**Proof.** By the definition of \( n_{s,t} \), it is not difficult to see that

\[
\left\{
\begin{array}{c}
k n - n + 1 = \sum_{(s,t) \in X} \left( \frac{1}{s} + \frac{1}{t} \right) n_{s,t}, \\
k n = \sum_{(s,t) \in X} n_{s,t}
\end{array}
\right.
\]

\[2\]
Lemma 2.4. If \( s, t > 0 \),

\[
\begin{align*}
4n_{2,2} + 3n_{2,4} &= 4(nk - n + 1) - 2n_{4,4} - 4 \sum_{(s,t) \in Y} \left( \frac{1}{s} + \frac{1}{t} \right) n_{s,t}, \\
n_{2,2} + n_{2,4} &= nk - n_{4,4} - \sum_{(s,t) \in Y} \left( \frac{1}{s} + \frac{1}{t} \right) n_{s,t}.
\end{align*}
\]

Therefore,

\[
\begin{align*}
\begin{cases}
4n_{2,4} &= 4n - 4 - 2n_{4,4}, \\
n_{2,2} &= nk - 4n + 4 + n_{4,4} - \sum_{(s,t) \in Y} \left( \frac{1}{s} + \frac{1}{t} \right) n_{s,t}.
\end{cases}
\end{align*}
\]

Consequently, by (3) we have

\[
SO_\alpha(G) = (4^\alpha + 4^\alpha)^{1/\alpha} n_{4,4} + (2^\alpha + 4^\alpha)^{1/\alpha} n_{2,4} + (2^\alpha + 2^\alpha)^{1/\alpha} n_{2,2} + \sum_{(s,t) \in Y} (s^\alpha + t^\alpha)^{1/\alpha} n_{s,t}.
\]

For \( \alpha \neq 0 \) and positive integer \( p \), let \( \delta_{\alpha,p}(s,t) = ((s+p)^\alpha + t^\alpha)^{1/\alpha} - (s^\alpha + t^\alpha)^{1/\alpha} \), where \( s, t > 0 \).

**Lemma 2.4.** If \( s, t > 0 \) and \( p \) is an arbitrary positive integer, then

(i). \( r_\alpha(s,t; \beta) \) strictly increases in \( s \) for fixed \( t \), and in \( t \) for fixed \( s \) when \( \alpha, \beta > 0 \);

(ii). \( \delta_{\alpha,p}(s,t) > 0 \) and \( \delta_{\alpha,p}(s,t) \) strictly decreases in \( t \) for fixed \( s \) when \( \alpha > 1 \);

(iii). \( \delta_{\alpha,p}(s,t) \) strictly increases in \( s \) for fixed \( t \) when \( \alpha > 1 \).

**Proof.** (i) follows directly since \( \alpha, \beta > 0 \).

Since \(-1 < 1/\alpha - 1 < 0 \) when \( \alpha > 1 \),

\[
\frac{\partial \delta_{\alpha,1}(s,t)}{\partial t} = t^{\alpha-1} \left( ((s + 1)^\alpha + t^\alpha)^{1/\alpha-1} - (s^\alpha + t^\alpha)^{1/\alpha-1} \right) < 0.
\]

We also note that \( \delta_{\alpha,1}(s,t) > 0 \), hence (ii) follows as \( \delta_{\alpha,p}(s,t) = \sum_{i=0}^{p-1} \delta_{\alpha,1}(s+i,t) \).

Finally, since \(-1 - 1/\alpha > 0 \) when \( \alpha > 1 \),

\[
\frac{\partial \delta_{\alpha,1}(s,t)}{\partial s} = \frac{((s + 1)^\alpha s^\alpha + (s + 1)^\alpha t^\alpha)^{1-1/\alpha} - ((s + 1)^\alpha s^\alpha + s^\alpha t^\alpha)^{1-1/\alpha}}{(((s + 1)^\alpha + t^\alpha)(s^\alpha + t^\alpha))^{1-1/\alpha}} > 0.
\]
Hence (iii) follows as $\delta_{\alpha,p}(s,t) = \sum_{i=0}^{p-1} \delta_{\alpha,1}(s+i,t)$. \hfill \Box

The distance $d_G(u,v)$ between two vertices $u$ and $v$ of a connected graph $G$ is defined as usual as the length of a shortest path that connects $u$ and $v$. In general, for two subgraphs $G_1$ and $G_2$ of $G$, we define the distance between $G_1$ and $G_2$ by $d_G(G_1,G_2) = \min\{d_G(u,v) : u \in V(G_1), v \in V(G_2)\}$. For $n \geq 2$, a star-like cactus $S_{n,k}$ is defined intuitively as a $k$-polygonal cactus such that all polygons have a vertex in common. It is clear that $S_{n,k}$ is unique and contains exactly one vertex of degree $2n$ while all other vertices have degree two.

**Lemma 2.5.** Let $\alpha > 1$ and $G \in \mathcal{G}_{n,k}$, where $n \geq 3$ and $k \geq 3$. If $G$ contains a vertex of degree at least 6, then $SO_\alpha(G)$ is not minimum in $\mathcal{G}_{n,k}$.

**Proof.** Suppose to the contrary that $G$ contains $q$ ($q \geq 1$) vertices of degree at least 6 and $SO_\alpha(G)$ is minimum in $\mathcal{G}_{n,k}$.

**Case 1.** $q \geq 2$.

Let $u_1$ and $w$ be two vertices of degree at least 6 such that $d_G(u_1,w)$ is maximum and let $P$ be a shortest path connecting $u_1$ and $w$. Since $d_G(u_1) \geq 6$, $u_1$ is contained in at least three polygons, exactly one of which, say $C$, has at least two common vertices with $P$. Let $C_1 = u_1u_2\cdots u_ku_1$ and $C_2 = u_1z_2\cdots z_ku_1$ be two polygons other than $C$ that contain $u_1$ as a common vertex. Since $d_G(u_1,w)$ is maximum, we have $d_G(v) \leq 4$ for every $v \in \{u_2, u_k, z_2, z_k\}$. Let $C_3 = v_1v_2\cdots v_kv_1$ be a pendant polygon that lies in the same component with $w$ in $G - u_1$ and the distance $d_G(u_1,C_3)$ is as large as possible, where $d_G(v_1) = 2a \geq 4$ and $d_G(v_2) = d_G(v_3) = 2$.

Without loss of generality, assume $d_G(u_1) = 2b \geq d_G(w) \geq 6$. Let $G' = G - u_1u_2 - u_1u_k + v_2u_2 + v_2u_k$. Then by Lemma 2.4, we have
which contradicts the minimality of $G$.

**Case 2.** $q = 1$.

If $G \not\cong S_{n,k}$, then the discussion for this case is similar to that for Case 1 by choosing $u_1$ to be the vertex with degree at least 6 and $C_3 = v_1v_2\cdots v_kv_1$ to be a pendent polygon such that $d_G(u_1, C_3)$ is maximum. Otherwise, $G \cong S_{n,k}$. Let $u_1$ be the vertex with degree $2n \geq 6$, $C_1 = u_1u_2\cdots u_ku_1$ and $C_2 = u_2z_2\cdots z_ku_1$ be two pendent polygons. Let $G' = G - u_1u_2 - u_1u_k + z_2u_2 + z_2u_k$. Then by Lemma 2.4 and Lemma 2.2, we have

\[
SO_\alpha(G) - SO_\alpha(G') = (2n \times r_\alpha(2n, 2) + (nk - 2n) \times r_\alpha(2, 2)) \\
- ((2n - 3) \times r_\alpha(2n - 2, 2) + r_\alpha(2n - 2, 4)) \\
+ 3r_\alpha(4, 2) + (nk - 2n - 1)r_\alpha(2, 2)
\]

\[
= 2n \times r_\alpha(2n, 2) + r_\alpha(2, 2) - (2n - 3) \times r_\alpha(2n - 2, 2) \\
- r_\alpha(2n - 2, 4) - 3r_\alpha(4, 2)
\]

\[
> 3r_\alpha(2n, 2) + r_\alpha(2, 2) - r_\alpha(2n - 2, 4) - 3r_\alpha(4, 2)
\]

\[
> 2r_\alpha(2n, 2) + r_\alpha(2, 2) - 3r_\alpha(4, 2)
\]

\[
> r_\alpha(6, 2) + r_\alpha(2, 2) - 2r_\alpha(4, 2)
\]

\[
> 0,
\]

which contradicts the minimality of $G$. 

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Recall that a graph is called a chemical graph if it has no vertex of degree more than 4. For $G \in \mathcal{G}_{n,k}$, we call $G$ a chemical $(n,k)$-cactus, or chemical cactus for short, if $G$ has no vertex of degree greater than 4. It is clear that every cut vertex in a chemical cactus has degree 4, which connects exactly two polygons. The following corollary follows directly from Lemma 2.3 and Lemma 2.5, which shows that the minimum value of $SO_\alpha(G)$ among all cacti in $\mathcal{G}_{n,k}$ is attained only by chemical cacti.

**Corollary 2.1.** For $\alpha > 1$, $n \geq 3$, $k \geq 3$ and $G \in \mathcal{G}_{n,k}$, if $G$ attains the minimum value of $SO_\alpha(G)$, then $G$ is a chemical cactus and

$$SO_\alpha(G) = (4n - 4)(2^\alpha + 4^\alpha)^{1/\alpha} + 2(nk - 4n + 4)2^{1/\alpha} + (6 \times 2^{1/\alpha} - 2(2^\alpha + 4^\alpha)^{1/\alpha}) n_{4,4}(G).$$

In the following we will determine the minimum value of $SO_\alpha(G)$ among all chemical cacti. By Corollary 2.1, this is equivalent to determine the maximum value of $n_{4,4}(G)$ as $6 \times 2^{1/\alpha} - 2(2^\alpha + 4^\alpha)^{1/\alpha} < 6 \times 2^{1/\alpha} - 2 \times 3^\alpha)^{1/\alpha} = 0$ by Lemma 2.1. For a chemical cactus $H$, we call a polygon $C$ in $H$ a saturated polygon if every vertex on $C$ is a cut vertex, i.e., a vertex of degree 4. Further, we call a chemical cactus $H$ nice-saturated if the following two conditions hold:

1). $H$ has as many as possible saturated polygons;  
2). the cut vertices on each polygon of $H$ are successively arranged.

For a chemical cactus $H$, let $T(H)$ be the tree whose vertices are the polygons in $H$ and two vertices are adjacent provided their corresponding polygons has a common vertex. It is clear that $T(H)$ is a tree with maximum vertex degree no more than $k$. Let $p$ be the number of the vertices of degree $k$ in $T(H)$, and let $d_1, d_2, \ldots, d_s$ be the degrees of all the vertices in $H$ that are neither of degree 1 nor of degree $k$, i.e., $1 < d_i < k$ for each $i \in \{1,2,\ldots,s\}$. Since $T(H)$ is a tree, we have

$$kp + d_1 + d_2 + \cdots + d_s + (n - p - s) = 2n - 2$$

and every saturated polygon in $H$ corresponds to a vertex of degree $k$ in $T(H)$. Further, $T(H)$ has as many as possible vertices of degree $k$ if and only if $d_1 + d_2 + \cdots + d_s - s < k - 1$. This implies that

$$\frac{n - 2}{k - 1} - 1 < p = \frac{n - 2 - (d_1 + d_2 + \cdots + d_s - s)}{k - 1} \leq \frac{n - 2}{k - 1}. \quad (6)$$
That is, if $\tilde{H}$ is nice-saturated then $\tilde{H}$ has exactly $\lfloor \frac{n-2}{k-1} \rfloor$ saturated cycles. As an example, a chemical $(6,4)$-cactus with $p < \lfloor \frac{n-2}{k-1} \rfloor = 1$, a chemical $(6,4)$-cactus in which the cut vertices on some polygon are not successively arranged, and a nice-saturated $(6,4)$-cactus are illustrated as (a), (b) and (c), respectively, in Figure 1.

Figure 1: (a). $p = 0$; (b). The cut vertices on the $k$-cycle $C$ are not successively arranged; (c). A nice-saturated $(6,4)$-cactus.

**Lemma 2.6.** A chemical cactus $H$ attains the maximum value of $n_{4,4}(H)$ if and only if $H$ is nice-saturated.

**Proof.** Let $p$ and $d_1, d_2, \ldots, d_s$ be defined as above. By a simple calculation, we have

\[
n_{4,4}(H) \leq kp + \sum_{v \in V(G), d(v) < k} (d(v) - 1) = kp + (d_1 - 1) + (d_2 - 1) + \cdots + (d_s - 1) \quad (7)
\]

and the equality holds if and only if the cut vertices on each polygon of $H$ are successively arranged.

Suppose $p < \lfloor \frac{n-2}{k-1} \rfloor$. Then by the previous analysis, we have $d_1 + d_2 + \cdots + d_s - s \geq k - 1$. Let $d'_1, d'_2, \ldots, d'_s$ be a sequence satisfying $d'_1 = k, 1 \leq d'_i \leq d_i$ for $i \in \{2, 3, \ldots, s\}$ and $\sum_{i=1}^s d'_i = \sum_{i=1}^s d_i$. Let $S$ be the sequence obtained from the degree sequence of $T(H)$ by replacing $d_1, d_2, \ldots, d_s$ by $d'_1, d'_2, \ldots, d'_s$, respectively. It is clear that $S$ is still a degree sequence of a tree with maximum degree not greater than $k$. Let $H'$ be a cactus such that $T(H')$ has degree sequence $S$ and the cut vertices on each polygon of $H'$ are successively arranged. Then by (7) and a direct calculation, we have $n_{4,4}(H') = n_{4,4}(H) + 1$. That is, $H$ does not attain the maximum value of $n_{4,4}(H)$, which completes our proof. \qed

**Theorem 2.1.** Let $G \in \mathcal{G}_{n,k}$, where $n \geq 3$ and $k \geq 3$. Then

\[
SO_\alpha(G) \geq (4n - 4)(2^\alpha + 4^\alpha)^{1/\alpha} + 2(nk - 4n + 4)^{2^{1/\alpha}}
\]
\[ + (6 \times 2^{1/\alpha} - 2(2^\alpha + 4^\alpha)^{1/\alpha}) \left( n - 2 + \left\lceil \frac{n - 2}{k - 1} \right\rceil \right), \]

and the equality holds if and only if \( G \) is a nice-saturated chemical cactus.

**Proof.** By (7), (5) and (6), if \( G \) is minimum, then

\[ n_{4,4}(G) = kp + (d_1 - 1) + (d_2 - 1) + \cdots + (d_s - 1) = n - 2 + p = n - 2 + \left\lceil \frac{n - 2}{k - 1} \right\rceil. \]

Hence, the theorem follows directly from Corollary 2.1 and Lemma 2.6. \( \square \)

### 3 Polygonal cactus with maximum general Sombor index

In this section we will characterize the polygonal cactus with maximum general Sombor index for the two cases \( \alpha \geq 1, \beta > 1; \) and \( \alpha = 2, 1/2 \leq \beta < 1, \) respectively.

**Lemma 3.1.** Let \( \Delta ABM \) be a triangle in Euclidean space and \( O \) the midpoint of the triangle side \( AB \). Then \( |MA|^{2\beta} + |MB|^{2\beta} > 2|MO|^{2\beta} \) for any real number \( \beta \geq \frac{1}{2} \), where \( |MA| \) is the length of the side \( MA \).

**Proof.** Let \( |MA| = a, |MB| = b \) and \( |MO| = d \). When \( a = b \), the lemma follows directly. Without loss of generality, we now assume \( a > b > 0 \). By the triangle inequality, \( d < \frac{a+b}{2} < a \) and so \((a,b) \triangleright (\frac{a+b}{2}, \frac{a+b}{2})\). Hence, by Lemma 2.1 \( a^{2\beta} + b^{2\beta} > 2 \left( \frac{a+b}{2} \right)^{2\beta} > 2d^{2\beta} \) when \( \beta \geq \frac{1}{2} \). \( \square \)

**Lemma 3.2.** Let \( s > 2 \) and \( t > 2 \). Then

(i). \( r_\alpha(s + 2, 2; \beta) - r_\alpha(s - 2, 2; \beta) > 0 \) for any \( \alpha > 0 \) and \( \beta > 0 \);

(ii). \( r_\alpha(s + 2, t; \beta) + r_\alpha(s - 2, t; \beta) > 2r_\alpha(s, t; \beta) \) for any \( \alpha \geq 1 \) and \( \beta > 1 \);

(iii). \( r_\alpha(s + 2, t - 2; \beta) + r_\alpha(s - 2, t + 2; \beta) \geq 2r_\alpha(s, t; \beta) \) for any \( \alpha \geq 1 \) and \( \beta > 1 \).

**Proof.** (i) follows directly.

For (ii), by Lemma 2.1 and the monotonicity of \( r_\alpha(s, t; \beta) \), we have

\[
\begin{align*}
 r_\alpha(s + 2, t; \beta) + r_\alpha(s - 2, t; \beta) &= ((s + 2)^\alpha + t^\alpha)^\beta + ((s - 2)^\alpha + t^\alpha)^\beta \\
 &\geq 2 \left( \frac{(s + 2)^\alpha + (s - 2)^\alpha}{2} + t^\alpha \right)^\beta \\
 &\geq 2(s^\alpha + t^\alpha)^\beta \\
 &= 2r_\alpha(s, t; \beta).
\end{align*}
\]
Theorem 3.1. Let $n \geq 3, k \geq 3$ and $G \in G_{n,k}$. If $\alpha \geq 1$ and $\beta > 1$; or $\alpha = 2$ and $\frac{1}{2} \leq \beta < 1$, then

$$SO_{\alpha}(G; \beta) \leq 2n((2n)^{\alpha} + 2^{\alpha})^{\beta} + n(k - 2)(2^{\alpha+1})^{\beta}$$

and the equality holds if and only if $G \cong S_{n,k}$.

Proof. We first assume that $\alpha \geq 1$ and $\beta > 1$.

Let $G$ be such that $SO_{\alpha}(G; \beta)$ is as large as possible. Further, let $C_1 = z_1 z_2 \cdots z_k z_1$ and $C_2 = v_1 v_2 \cdots v_l v_1$ be two pendent polygons such that $d_G(C_1, C_2)$ is as large as possible, where $z_1$ and $v_1$ are the cut-vertices of $C_1$ and $C_2$, respectively.

If $G \cong S_{n,k}$, then the theorem follows directly. We now assume $G \not\cong S_{n,k}$. Then, $z_1 \neq v_1$. Let $G_1 = G - v_1 v_2 - v_1 v_k + z_1 v_2 + z_1 v_k$ and $G_2 = G - z_1 z_2 - z_1 z_k + v_1 z_2 + v_1 z_k$. We consider the following two cases:

Case 1. $z_1$ and $v_1$ are adjacent in $G$.

In this case, we have

$$SO_{\alpha}(G_1; \beta) - SO_{\alpha}(G; \beta) =
\sum_{v \in N_G(v_1) \setminus \{z_1\}} \left( r_\alpha(d_G(v_1) - 2, d_G(v); \beta) - r_\alpha(d_G(v_1), d_G(v); \beta) \right)
+ \sum_{z \in N_G(z_1) \setminus \{v_1\}} \left( r_\alpha(d_G(z_1) + 2, d_G(z); \beta) - r_\alpha(d_G(z_1), d_G(z); \beta) \right)
+ 2r_\alpha(d_G(z_1) + 2, 2; \beta) - 2r_\alpha(d_G(v_1) - 2, 2; \beta)
+ r_\alpha(d_G(v_1) - 2, d_G(z_1) + 2; \beta) - r_\alpha(d_G(v_1), d_G(z_1); \beta),$$

and

$$SO_{\alpha}(G_2; \beta) - SO_{\alpha}(G; \beta) =
\sum_{v \in N_G(v_1) \setminus \{z_1\}} \left( r_\alpha(d_G(v_1) + 2, d_G(v); \beta) - r_\alpha(d_G(v_1), d_G(v); \beta) \right)
+ \sum_{z \in N_G(z_1) \setminus \{v_1\}} \left( r_\alpha(d_G(z_1) - 2, d_G(z); \beta) - r_\alpha(d_G(z_1), d_G(z); \beta) \right)
+ 2r_\alpha(d_G(v_1) + 2, 2; \beta) - 2r_\alpha(d_G(z_1) - 2, 2; \beta)
+ r_\alpha(d_G(v_1) + 2, d_G(z_1) - 2; \beta) - r_\alpha(d_G(v_1), d_G(z_1); \beta).$$
Recall that $z_1$ and $v_1$ are the cut-vertices of $C_1$ and $C_2$, respectively. Therefore, $d_G(z_1) \geq 4$ and $d_G(v_1) \geq 4$. Combining with Lemma 3.2, we have

\[
\begin{align*}
&\quad r_\alpha(d_G(v_1) + 2, d_G(v); \beta) + r_\alpha(d_G(v_1) - 2, d_G(v); \beta) > 2r_\alpha(d_G(v_1), d_G(v); \beta), \\
&\quad r_\alpha(d_G(z_1) + 2, d_G(z); \beta) + r_\alpha(d_G(z_1) - 2, d_G(z); \beta) > 2r_\alpha(d_G(z_1), d_G(z); \beta), \\
&\quad r_\alpha(d_G(v_1) + 2, d_G(z_1) - 2; \beta) + r_\alpha(d_G(v_1) - 2, d_G(z_1) + 2; \beta) > 2r_\alpha(d_G(v_1), d_G(z_1); \beta), \\
&\quad r_\alpha(d_G(z_1) + 2; \beta) - r_\alpha(d_G(z_1) - 2, 2; \beta) > 0, \quad \text{and} \\
&\quad r_\alpha(d_G(v_1) + 2, 2; \beta) - r_\alpha(d_G(v_1) - 2, 2; \beta) > 0.
\end{align*}
\]

This means that $SO_\alpha(G_1; \beta) > SO_\alpha(G; \beta)$ or $SO_\alpha(G_2; \beta) > SO_\alpha(G; \beta)$, a contradiction.

**Case 2.** $z_1$ and $v_1$ are not adjacent in $G$.

In this case, we have

\[
\begin{align*}
SO_\alpha(G_1; \beta) - SO_\alpha(G; \beta) &= \sum_{v \in N_G(z_1)} (r_\alpha(d_G(v_1) - 2, d_G(v); \beta) - r_\alpha(d_G(v_1), d_G(v); \beta)) \\
&\quad + \sum_{z \in N_G(z_1)} (r_\alpha(d_G(z_1) + 2, d_G(z); \beta) - r_\alpha(d_G(z_1), d_G(z); \beta)) \\
&\quad + 2r_\alpha(d_G(z_1) + 2, 2; \beta) - 2r_\alpha(d_G(v_1) - 2, 2; \beta), \\
SO_\alpha(G_2; \beta) - SO_\alpha(G; \beta) &= \sum_{v \in N_G(v_1)} (r_\alpha(d_G(v_1) + 2, d_G(v); \beta) - r_\alpha(d_G(v_1), d_G(v); \beta)) \\
&\quad + \sum_{z \in N_G(z_1)} (r_\alpha(d_G(z_1) - 2, d_G(z); \beta) - r_\alpha(d_G(z_1), d_G(z); \beta)) \\
&\quad + 2r_\alpha(d_G(v_1) + 2, 2; \beta) - 2r_\alpha(d_G(z_1) - 2, 2; \beta).
\end{align*}
\]

Recall that $d_G(z_1) \geq 4$ and $d_G(v_1) \geq 4$. Similar to Case 1, by Lemma 3.2, we have

\[
\begin{align*}
&\quad r_\alpha(d_G(v_1) + 2, d_G(v); \beta) + r_\alpha(d_G(v_1) - 2, d_G(v); \beta) > 2r_\alpha(d_G(v_1), d_G(v); \beta), \\
&\quad r_\alpha(d_G(z_1) + 2, d_G(z); \beta) + r_\alpha(d_G(z_1) - 2, d_G(z); \beta) > 2r_\alpha(d_G(z_1), d_G(z); \beta), \\
&\quad r_\alpha(d_G(z_1) + 2, 2; \beta) - r_\alpha(d_G(z_1) - 2, 2; \beta) > 0, \quad \text{and} \\
&\quad r_\alpha(d_G(v_1) + 2, 2; \beta) - r_\alpha(d_G(v_1) - 2, 2; \beta) > 0,
\end{align*}
\]

which means that $SO_\alpha(G_1; \beta) > SO_\alpha(G; \beta)$ or $SO_\alpha(G_2; \beta) > SO_\alpha(G; \beta)$, a contradiction.

Therefore, $S_n,k$ is the unique maximal polygonal cactus. Further, we have

\[
SO_\alpha(S_n,k; \beta) = 2nr_\alpha(2n, 2; \beta) + n(k - 2)r_\alpha(2, 2; \beta) = 2n((2n)^\alpha + 2^\alpha)\beta + n(k - 2)(2^{\alpha+1})\beta.
\]
The discussion for the case that \( \alpha = 2 \) and \( \frac{1}{2} \leq \beta < 1 \) is analogous by Lemma 3.2 (i) and Lemma 3.1.

4 Polygonal cacti with minimum general Sombor index

A symmetric function \( \varphi(s, t) \) defined on positive real numbers is called escalating if

\[
\varphi(s_1, s_2) + \varphi(t_1, t_2) \geq \varphi(s_2, t_1) + \varphi(s_1, t_2)
\]

for any \( s_1 \geq t_1 > 0 \) and \( s_2 \geq t_2 > 0 \), and the inequality holds if \( s_1 > t_1 > 0 \) and \( s_2 > t_2 > 0 \). Further, an escalating function \( \varphi(s, t) \) is called special escalating if

\[
4\varphi(2l, 2) - \varphi(2l - 2, 4) - \varphi(2l - 2, 2) - \varphi(4, 2) - \varphi(4, 4) \geq 0
\]

for \( l \geq 3 \) and

\[
\varphi(s_1, s_2) - \varphi(t_1, t_2) \geq 0
\]

for any \( s_1 \geq t_1 \geq 2 \) and \( s_2 \geq t_2 \geq 2 \).

**Lemma 4.1.** If \( s, t > 0 \), then \( r_\alpha(s, t; \beta) = (s^\alpha + t^\alpha)^\beta \) is special escalating for \( \alpha \geq 1 \) and \( \beta > 1 \).

**Proof.** Set \( \varphi(s, t) = (s^\alpha + t^\alpha)^\beta \). Since \( \alpha \geq 1 \) and \( \beta > 1 \), we have \( (s_1^\alpha + s_2^\alpha, t_1^\alpha + t_2^\alpha) \triangleright (s_2^\alpha + t_1^\alpha, s_1^\alpha + t_2^\alpha) \) when \( s_1 > t_1 > 0 \) and \( s_2 > t_2 > 0 \). Then by Lemma 2.1, the inequality in (8) strictly holds. Further, it is clear that the equality in (8) holds when \( s_1 = t_1 > 0 \) or \( s_2 = t_2 > 0 \). This means that \((s^\alpha + t^\alpha)^\beta\) is escalating.

In addition, by Lemma 2.1 and the monotonicity of \((s^\alpha + t^\alpha)^\beta\), if \( l \geq 3 \) and \( \alpha \geq 1 \) then \((2l)^\alpha + 2^\alpha \geq (2l - 2)^\alpha + 4^\alpha > (2l - 2)^\alpha + 2^\alpha \), \((2l)^\alpha + 2^\alpha > 4^\alpha + 2^\alpha \) and \((2l)^\alpha + 2^\alpha \geq 6^\alpha + 2^\alpha \geq 4^\alpha + 4^\alpha \). Hence, (9) follows directly as \( \beta > 1 \).

Finally, it is easy to see that (10) holds when \( \alpha \geq 1 \) and \( \beta > 1 \) by the monotonicity of \((s^\alpha + t^\alpha)^\beta\). Therefore, \((s^\alpha + t^\alpha)^\beta\) is special escalating.

A \( k \)-polygonal cactus \( G \) is called a cactus chain if each polygon in \( G \) has at most two cut-vertices and each cut-vertex is the common vertex of exactly two polygons. It is clear...
that each cactus chain has exactly \( n - 2 \) non-pendent polygons and two pendent polygons for \( n \geq 2 \). We denote by \( A_{n,k} \) the class consisting of those cactus chains such that each pair of cut-vertices that lies in the same polygon of \( G \) are adjacent. In contrast, we denote by \( B_{n,k} \) the class consisting of those cactus chains such that each pair of cut-vertices that lies in the same polygon of \( G \) are not adjacent. It can be seen that \( A_{n,k} \) is unique for \( k \geq 3 \) and \( B_{n,3} = \emptyset \).

**Theorem 4.1.** [23] Let \( f(s, t) \) be a special escalating function and \( G \) be a cactus of \( G_{n,k} \), where \( n \geq 3 \) and \( k \geq 3 \).

(i). If \( k = 3 \), then

\[
I_f(G) \geq 2f(2, 2) + 2nf(4, 2) + (n - 2)f(4, 4)
\]

with equality holding if and only if \( G \in A_{n,3} \).

(ii). If \( k \geq 4 \), then

\[
I_f(G) \geq (kn - 4n + 4)f(2, 2) + (4n - 4)f(4, 2),
\]

where the equality holds if \( G \in B_{n,k} \). Furthermore, if \( k \in \{4, 5\} \), then the equality holds if and only if \( G \in B_{n,k} \).

**Corollary 4.1.** Let \( n \geq 3, k \geq 3, \alpha \geq 1, \beta > 1 \) and \( G \in G_{n,k} \).

(i). If \( k = 3 \), then \( SO_{\alpha}(G; \beta) \geq 2(2^{n+1})^\beta + 2n(4^\alpha + 2^\alpha)\beta + (n - 2)(2 \cdot 4^\alpha)\beta \), where the equality holds if and only if \( G \in A_{n,3} \).

(ii). If \( k \geq 4 \), then \( SO_{\alpha}(G; \beta) \geq (kn - 4n + 4)(2^{n+1})^\beta + (4n - 4)(4^\alpha + 2^\alpha)\beta \), where the equality holds if \( G \in B_{n,k} \). Furthermore, if \( k \in \{4, 5\} \), then the equality holds if and only if \( G \in B_{n,k} \).

**Proof.** In Theorem [4.1] set \( f(s, t) = r_{\alpha}(s, t; \beta) \). Then the corollary follows immediately by Lemma [4.1] and a simple calculation. \( \square \)

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