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Research Article

The Hyperbolic Sombor Index of Maximal Outerplanar Graphs

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Abstract

Let $G = (V(G), E(G))$ be a simple connected graph, where $V(G)$ is its vertex set and $E(G)$ is its edge set. The hyperbolic Sombor index of G is a vertex-degree-based topological index defined by

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)^2 + d(v)^2}}{\min\{d(u), d(v)\}},$$

where $d(u)$ and $d(v)$ are the degrees of the vertices u and v, respectively. In this paper, we determine the maximum and minimum values of this index among all maximal outerplanar graphs of a given order n, and characterize the corresponding extremal graphs.

Keywords: hyperbolic Sombor index; maximal outerplanar graph; extremal value.

2020 Mathematics Subject Classification: 05C07, 05C09.

1. Introduction

In this paper, we only consider finite, simple, undirected and connected graphs. Let $G = (V(G), E(G))$ be a graph, where $V(G)$ is its vertex set and $E(G)$ is its edge set. The order and size of G are denoted by $n = |V(G)|$ and $m = |E(G)|$, respectively. The neighborhood of a vertex v is denoted by $N_G(v)$ (or $N(v)$ for short), and its degree is denoted by $d_G(v)$ (or $d(v)$ for short). For terminology and notation not defined here, we refer to [4].

Gutman [8] proposed the Sombor index from the geometric interpretation of the vertex-degree pair $(d(u), d(v))$. Recently, Barman and Das [3] proposed the hyperbolic Sombor (HSO) index from the geometric background of the eccentricity of a hyperbola, which is defined as

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)^2 + d(v)^2}}{\min\{d(u), d(v)\}}.$$

Here, $d(u)$ and $d(v)$ are the degrees of the vertices u and v, respectively. Barman and Das [2] observed that the HSO index is a strong predictor of polarizability, π-electron energy, heavy atom count, and molar refractivity. The HSO index is not uniformly monotone under edge addition [1, 5]. For further mathematical studies of the HSO index, see [1, 5, 6, 11, 12].

A graph is planar if it can be drawn in the plane so that distinct edges intersect only at a common endvertex. Such a drawing is called a plane embedding. The connected regions of the plane determined by the embedding are its faces, and the unbounded region is the outer face.

A graph is outerplanar if it has a plane embedding in which every vertex lies on the boundary of the outer face. An outerplanar graph is maximal if no edge can be added between nonadjacent vertices while preserving outerplanarity.

For $n \geq 3$, a maximal outerplanar graph of order n is a triangulation of an n-sided polygon: its outer boundary is a Hamilton cycle, its bounded faces are triangular, and it has $n - 3$ chords and $2n - 3$ edges. It also has at least two vertices of degree 2.

Hou et al. [9] determined sharp bounds for the Zagreb indices of maximal outerplanar graphs; Li, Deng, and Tang [10] determined the extremal values and extremal graphs of the Sombor index for this graph class.

This paper investigates the extremal values of the HSO index for maximal outerplanar graphs. We determine the maximum and minimum values of this index among all maximal outerplanar graphs of a given order n, and characterize the corresponding extremal graphs.

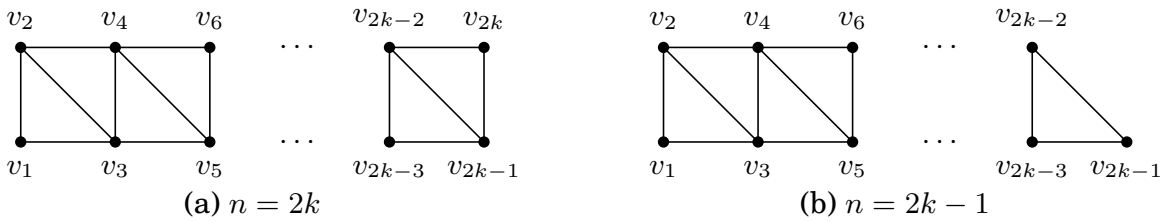
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2. Preliminaries

In this section, we give special graphs, low-order cases, structural lemmas of maximal outerplanar graphs, and the analytic lemmas needed later.

Let $\mathcal{H}_n$ denote the set of all maximal outerplanar graphs of order n.

Let $P_n = v_1v_2\cdots v_n$ be a path of order n. The *path square graph* P_n^2 is the graph obtained from P_n by adding an edge between every pair of vertices at distance 2 in P_n (see Figure 2.1).



(a) $n = 2k$ (b) $n = 2k - 1$

Figure 2.1 The graph P_n^2.

Let $F_n = K_1 \vee P_{n-1}$ denote the fan graph of order n, obtained by adding one vertex adjacent to every vertex of P_{n-1}.

If $n = 3, 4, 5$, the maximal outerplanar graph is unique up to isomorphism (see [4]), and

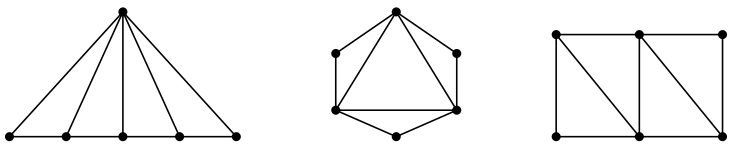
$$P_3^2 \cong F_3, \qquad P_4^2 \cong F_4, \qquad P_5^2 \cong F_5.$$

Direct calculation gives

$$HSO(P_3^2) = 3\sqrt{2}, \quad HSO(P_4^2) = 2\sqrt{13} + \sqrt{2}, \quad HSO(P_5^2) = \sqrt{13} + 2\sqrt{5} + \sqrt{2} + \frac{10}{3}.$$

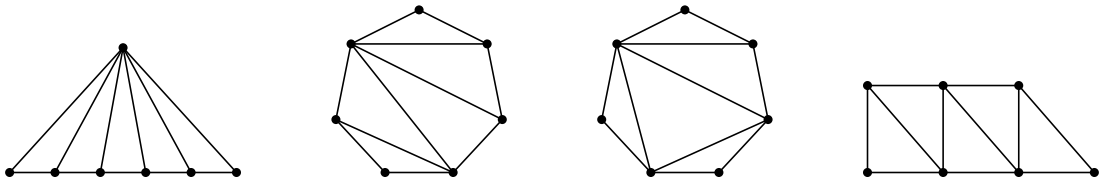
If $n = 6$, there are three non-isomorphic maximal outerplanar graphs, shown in Figure 2.2.

In particular, H_2 is obtained from a triangle by adding, for each of its three edges, one new vertex adjacent to both endvertices of that edge. Thus H_2 has three vertices of degree 4 and three vertices of degree 2, and $HSO(H_2) = 6\sqrt{5} + 3\sqrt{2}$.



(a) H_1 (b) H_2 (c) H_3

Figure 2.2 Non-isomorphic maximal outerplanar graphs of order 6.



(a) U_1 (b) U_2 (c) U_3 (d) U_4

Figure 2.3 Non-isomorphic maximal outerplanar graphs of order 7.

If $n = 7$, there are four non-isomorphic maximal outerplanar graphs, shown in Figure 2.3. The values of the HSO index for these graphs are listed in Table 2.1.

Table 2.1 Hyperbolic Sombor indices of the graphs.

Graph	H_1	H_2	H_3	U_1	U_2	U_3	U_4
HSO	17.650	17.659	16.159	23.117	20.713	22.122	18.987

Therefore, $HSO(H_3) < HSO(H_1) < HSO(H_2)$ and $HSO(U_4) < HSO(U_2) < HSO(U_3) < HSO(U_1)$. Let

$$h(x,y) = \frac{\sqrt{x^2+y^2}}{\min\{x,y\}}, \qquad x,y \geq 2.$$

Obviously, $h(x,y) = h(y,x)$.

Lemma 2.1. *For any $x, y \geq 2$, it holds that $h(x,y) \geq \sqrt{2}$, where the equality holds if and only if $x = y$.*

Proof. Without loss of generality, let $x \leq y$. Then

$$h(x,y) = \frac{\sqrt{x^2+y^2}}{x} = \sqrt{1+\left(\frac{y}{x}\right)^2} \geq \sqrt{2},$$

with equality if and only if $x = y$. □

Lemma 2.2 (see [6]). *Fix any real number $x \geq 3$ and define*

$$D_x(y) = h(x,y) - h(x-1,y), \qquad y \geq 2.$$

Then $D_x(y)$ is strictly decreasing in y on $[2,\infty)$. Moreover,

$$D_x(y) > 0 \quad (2 \leq y \leq x-1), \qquad D_x(y) < 0 \quad (y \geq x).$$

Lemma 2.3. *Let $3 \leq p \leq q$ and define $J(p,q) = h(p,q) - h(p-1,q-1)$. Then $J(p,q) \leq 0$, with equality if and only if $p = q$.*

Proof. If $p \leq q$, then

$$h(p,q) = \sqrt{1+\left(\frac{q}{p}\right)^2}, \qquad h(p-1,q-1) = \sqrt{1+\left(\frac{q-1}{p-1}\right)^2}.$$

Also, $\frac{q}{p} \leq \frac{q-1}{p-1}$ is equivalent to $p \leq q$. Hence the conclusion holds. □

Lemma 2.4. *Let $a \geq 2$ and define*

$$s_a(x) = \frac{\sqrt{x^2+a^2}}{a}, \qquad x \geq a.$$

Then s_a is strictly increasing and strictly convex on $[a,\infty)$.

Proof. If $x \geq a$, we have that

$$s_a'(x) = \frac{x}{a\sqrt{x^2+a^2}} > 0, \qquad s_a''(x) = \frac{a}{(x^2+a^2)^{3/2}} > 0.$$

Since $s_a'(x) > 0$ on the interval, $s_a(x)$ is strictly increasing. Since $s_a''(x) > 0$ on the interval, $s_a(x)$ is strictly convex. □

Lemma 2.5. *Let $x \geq 4$ and define $\Psi(x) = \sqrt{2} + 2\big[s_2(x) - s_2(x-1)\big] + s_3(x) + (x-3)\big[s_3(x) - s_3(x-1)\big]$. Then $\Psi(x+1) - \Psi(x) > 0$ for $x \geq 4$.*

Proof. Let $\Delta_a(x) = s_a(x) - s_a(x-1)$. Rewriting the expression for $\Psi(x)$, we have that

$$\Psi(x) = \sqrt{2} + 2\Delta_2(x) + s_3(x) + (x-3)\Delta_3(x).$$

By Lemma 2.4, $\Delta_a(x)$ is positive and strictly increasing in x for $a \in \{2,3\}$ and $x \geq 4$. Therefore,

$$\begin{aligned}\Psi(x+1) - \Psi(x) &= 2\big[\Delta_2(x+1) - \Delta_2(x)\big] + (x-1)\Delta_3(x+1) - (x-3)\Delta_3(x) \\ &= 2\big[\Delta_2(x+1) - \Delta_2(x)\big] + (x-1)[\Delta_3(x+1) - \Delta_3(x)] + 2\Delta_3(x) > 0.\end{aligned}$$

□

Lemma 2.6 (see [9]). *Let $G \in \mathcal{H}_n$ and v be a vertex of degree 2 with $N(v) = \{u,w\}$. Then $uw \in E(G)$.*

Lemma 2.7 (see [9]). *Let $G \in \mathcal{H}_n$ with $n \geq 4$ and v be a vertex of degree 2 with $N(v) = \{u,w\}$. Then $|N(u) \cap N(w)| = 2$.*

Lemma 2.8 (see [9]). *Let $G \in \mathcal{H}_n$ with $n \geq 5$ and v be a vertex of degree 2 with $N(v) = \{u,w\}$. Then*

$$7 \leq d(u) + d(w) \leq n+2.$$

Lemma 2.9 (see [7]). *Every outerplanar graph G of minimum degree 2 contains an edge uv with $d(v) = 2$ and $2 \le d(u) \le 3$ or a 3-path v, u, w with $d(v) = 2, d(u) = 4$ and $d(w) = 2$.*

The weight of an edge $uv \in E(G)$ is the sum of its endvertex degrees, denoted by $w(uv) = d_G(u) + d_G(v)$. The minimum edge weight of G is $w(G) = \min\{w(uv) : uv \in E(G)\}$.

By Lemma 2.9, we obtain the following result.

Lemma 2.10. *If $G \in \mathcal{H}_n$ with $n \ge 6$, then $5 \le w(G) \le 6$.*

Lemma 2.11 (see [7]). *Let G be a 2-connected outerplanar graph. If the minimum edge weight of G satisfies $w(G) \ge 6$, then G contains a subgraph isomorphic to*

$$A_4 = \big(\{x, y, z, t\}, \{xy, xz, xt, yz\}\big),$$

such that the degrees of its vertices in G satisfy

$$d_G(x) = 4, \qquad 4 \le d_G(y) \le 6, \qquad d_G(z) = d_G(t) = 2.$$

Moreover, the upper bound 6 for $d_G(y)$ is best possible.

Remark 2.1. *If $n \ge 4$, two degree-2 vertices are not adjacent, and any vertex is adjacent to at most two degree-2 vertices, because the outer boundary of a maximal outerplanar graph is a Hamilton cycle, and the two neighbors of a degree-2 vertex are exactly its predecessor and successor on this cycle. The weak dual graph $T(G)$ of a maximal outerplanar graph G has the bounded triangular faces of G as its vertices, with two vertices adjacent if the corresponding faces share a chord. It is well known that $T(G)$ is a tree, and the degree-2 vertices of G correspond one-to-one with the leaves of $T(G)$. Consequently, if G has exactly two degree-2 vertices, then $T(G)$ is a path.*

Direct calculation gives the formulas given in the following lemma.

Lemma 2.12. *For $n \ge 6$,*

$$HSO(P_n^2) = A_n := (2n - 11)\sqrt{2} + \sqrt{13} + 2\sqrt{5} + \frac{20}{3}.$$

For $n \ge 4$,

$$HSO(F_n) = B_n := \sqrt{(n-1)^2 + 4} + \frac{n-3}{3}\sqrt{(n-1)^2 + 9} + \sqrt{13} + (n-4)\sqrt{2},$$

and

$$A_n - A_{n-1} = 2\sqrt{2} \qquad (n \ge 7),$$
$$B_n - B_{n-1} = \Psi(n-1) \qquad (n \ge 5).$$

3. The Minimum Hyperbolic Sombor Index Among Maximal Outerplanar Graphs

In this section, we determine the minimum hyperbolic Sombor index over $\mathcal{H}_n$ and characterize the extremal graphs.

Lemma 3.1. *Let $G \in \mathcal{H}_n$ with $n \ge 6$, and suppose G has exactly two degree-2 vertices. Take an end face of the weak dual path, and let v be the corresponding ear vertex. Then there exist distinct vertices u, w, z such that vuw and uwz are two adjacent bounded triangles, and by appropriately swapping u, w we have*

$$d(v) = 2, \qquad d(u) = 3, \qquad d(w) = p \ge 4, \qquad d(z) = r \ge 3.$$

Furthermore:

(i) If $p = 4$, then $r \ge 4$;

(ii) Let $E_v = \{vu, vw, uw, uz\}$. Then

$$\sum_{xy \in E_v} h(d(x), d(y)) \ge h(2,3) + h(2,4) + 2h(3,4),$$

where equality holds if and only if $p = r = 4$;

(iii) The two four-edge sets E_v corresponding to the two end faces are pairwise disjoint.

Proof. Since G has exactly two ear vertices, the weak dual $T(G)$ is a path. Let the bounded faces of this path be $f_1, f_2, \ldots, f_{n-2}$ in order, where $f_1 = vuw$ and $f_2 = uwz$. The bounded faces incident with a boundary vertex form a contiguous subpath in the weak dual path. Since f_3 (if it exists) can only be adjacent to f_2 through one of the edges uz or wz, one of the vertices u, w no longer appears after f_2. This vertex is incident with exactly two bounded triangles, so its degree is 3. Without loss of generality, let $d(u) = 3$. Then the other vertex w appears in at least f_1, f_2, f_3, so $p = d(w) \geq 4$.

If $p = 4$, then w is incident with exactly three bounded faces f_1, f_2, f_3. Since $n \geq 6$, the weak dual has at least four vertices, so f_4 exists.

The edge shared by f_3 and f_4 no longer contains w, but must contain z. Therefore z is incident with at least three bounded faces f_2, f_3, f_4, and thus $r = d(z) \geq 4$. The total contribution of the four edges vu, vw, uw, uz is $h(2,3)+h(2,p)+h(3,p)+h(3,r)$.

If $p = 4$, by $r \geq 4$ and the strict monotonicity of $h(3, y)$ for $y \geq 3$, we have

$$h(2,3) + h(2,p) + h(3,p) + h(3,r) \geq h(2,3) + h(2,4) + 2h(3,4).$$

If $p \geq 5$, then

$$h(2,p) \geq h(2,5), \qquad h(3,p) \geq h(3,5), \qquad h(3,r) \geq h(3,3),$$

and

$$\big[h(2,5) + h(3,5) + h(3,3)\big] - \big[h(2,4) + 2h(3,4)\big] = \frac{\sqrt{29}}{2} + \frac{\sqrt{34}}{3} + \sqrt{2} - \sqrt{5} - \frac{10}{3} > 0.$$

Hence (ii) holds, and equality can only hold if $p = r = 4$.

Finally, the two four-edge sets at the two ends involve only the first two faces and the last two faces of the weak dual path, respectively. If $n > 6$, the two are obviously disjoint. If $n = 6$, the weak dual has four vertices in total; the left-end set specifically takes the outer edge uz corresponding to the degree-3 vertex u, rather than the common chord of f_2 and f_3, so it is still disjoint from the right-end four-edge set. □

Figure 3.1 illustrates the end structure of Lemma 3.1.

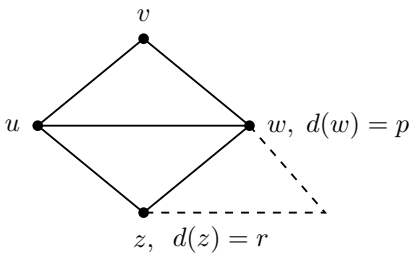


Figure 3.1 Local structure at one end of the weak dual path.

Theorem 3.1. *Let $G \in \mathcal{H}_n$ with $n \geq 6$. Then*

$$HSO(G) \geq (2n-11)\sqrt{2} + \sqrt{13} + 2\sqrt{5} + \frac{20}{3}, \tag{1}$$

with equality if and only if $G \cong P_n^2$.

Proof. Let t be the number of degree-2 vertices in G. By the basic properties of maximal outerplanar graphs, $t \geq 2$.

Case 1: $t \geq 3$. Let v be any degree-2 vertex and $N(v) = \{u, w\}$. By Remark 2.1 and Lemma 2.8, $d(u), d(w) \geq 3$ and $d(u) + d(w) \geq 7$. Since

$$h(2,x) = \frac{\sqrt{x^2+4}}{2}$$

is strictly increasing in x, we have

$$h(2,d(u)) + h(2,d(w)) \geq h(2,3) + h(2,4).$$

For every edge, we have $h \geq \sqrt{2}$. Comparing the two incident edges of each ear vertex with the benchmark contribution $2\sqrt{2}$, we obtain that each ear vertex produces at least the extra amount

$$c_0 = h(2,3) + h(2,4) - 2\sqrt{2} = \frac{\sqrt{13}}{2} + \sqrt{5} - 2\sqrt{2}.$$

By Remark 2.1, the two incident edges corresponding to different ear vertices do not coincide. Therefore

$$HSO(G) \geq (2n-3)\sqrt{2} + t\,c_0 \geq (2n-3)\sqrt{2} + 3c_0.$$

Subtracting A_n from this lower bound yields

$$\big[(2n-3)\sqrt{2}+3c_0\big]-A_n=2\sqrt{2}+\frac{\sqrt{13}}{2}+\sqrt{5}-\frac{20}{3}>0.$$

Hence,

$$HSO(G)\geq(2n-3)\sqrt{2}+3c_0>A_n.$$

Thus the lower bound equality cannot be attained if $t\geq 3$.

Case 2: $t=2$. Then the weak dual of G is a path. Applying Lemma 3.1 to the two end faces, we obtain two disjoint four-edge sets E_L, E_R, and

$$\sum_{xy\in E_L}h(d(x),d(y))\geq h(2,3)+h(2,4)+2h(3,4),$$

$$\sum_{xy\in E_R}h(d(x),d(y))\geq h(2,3)+h(2,4)+2h(3,4).$$

Besides these eight edges, G has $(2n-3)-8=2n-11$ more edges. By Lemma 2.1, each remaining edge contributes at least $\sqrt{2}$. Hence,

$$HSO(G)\geq 2\big[h(2,3)+h(2,4)+2h(3,4)\big]+(2n-11)\sqrt{2}=\sqrt{13}+2\sqrt{5}+\frac{20}{3}+(2n-11)\sqrt{2}.$$

Thus, inequality (1) holds.

Next, we characterize the equality case. Suppose equality holds in (1). Then $t=2$, and equality holds in Lemma 3.1 at both ends of the weak dual path.

Relabel the first two faces as $f_1=x_1x_2x_3$ and $f_2=x_2x_3x_4$, where $d(x_1)=2$, $d(x_2)=3$ and $d(x_3)=d(x_4)=4$.

Since $d(x_2)=3$, the common edge of f_2 and f_3 is x_3x_4. Thus $f_3=x_3x_4x_5$ for a new vertex x_5. Since $d(x_3)=4$, the vertex x_3 is incident with exactly the three bounded faces f_1,f_2,f_3. Consequently, the common edge of f_3 and f_4 is x_4x_5.

For $2\leq i\leq n-4$, the common edge of f_i and f_{i+1} lies outside the two end four-edge sets. Equality in (1) therefore forces the endvertices of each such edge to have equal degrees. Starting with $d(x_3)=d(x_4)=4$, this propagates degree 4 through the intermediate vertices. Each such vertex is incident with exactly three consecutive bounded faces, which forces the next shared edge. Continuing in this way gives

$$f_i=x_ix_{i+1}x_{i+2},\qquad 1\leq i\leq n-2,$$

with

$$d(x_j)=4,\qquad 3\leq j\leq n-2.$$

The final two vertices occur in two bounded faces and one bounded face, respectively, so $d(x_{n-1})=3$ and $d(x_n)=2$. The common edge of the last two faces belongs to the right-end four-edge set; no equality of its endvertex degrees is required.

Hence, $G\cong P_n^2$. Conversely, Lemma 2.12 shows that P_n^2 attains the lower bound. □

4. The Maximum Hyperbolic Sombor Index Among Maximal Outerplanar Graphs

In this section, we determine the maximum hyperbolic Sombor index over $\mathcal{H}_n$ and characterize the extremal graphs.

Lemma 4.1. *Let $G\in\mathcal{H}_n$ with $n\geq 6$. Then G has a degree-2 vertex v with $N(v)=\{u,w\}$, $d(u)\leq d(w)$, and $w(uv)=w(G)$ such that one of the following holds:*

(i) $d(u)=3$;

(ii) $d(u)=4$ *and* $4\leq d(w)\leq 6$, *and u is also adjacent to another degree-2 vertex.*

Proof. By Lemma 2.10, $w(G)=5$ or $w(G)=6$. Also, no two degree-2 vertices are adjacent, by Remark 2.1.

If $w(G)=5$, choose an edge of weight 5. Its endvertex degrees are 2 and 3, yielding case (i).

If $w(G)=6$, then G is a 2-connected outerplanar graph, so Lemma 2.11 guarantees a subgraph

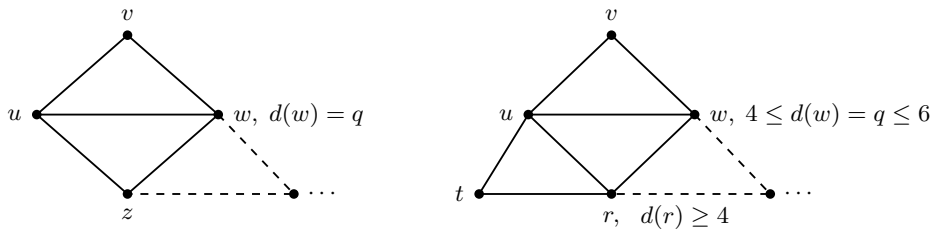
$$Q_4=(\{x,y,z,t\},\{xy,xz,xt,yz\}),$$

satisfying

$$d(x)=4,\qquad 4\leq d(y)\leq 6,\qquad d(z)=d(t)=2.$$

Taking $v = z$, $u = x$, $w = y$ gives case (ii). □

Figure 4.1 illustrates the two local structures. In case (ii) of Lemma 4.1, recall that t is the other degree-2 vertex adjacent to u. Let r be the common neighbor of u and w on the other side of triangle uvw. If $wt \in E(G)$, then $t = r$, and the chord uw is blocked on both sides by triangles uvw and uwt, allowing no further vertices, so $n = 4$, contradicting $n \geq 6$. Hence $wt \notin E(G)$, and the four neighbors of u along the outer cycle appear in the order v, w, r, t. Consequently, $tr \in E(G)$. Since the minimum edge weight in case (ii) is at least 6, applying this to tr yields $d(t) + d(r) \geq 6$. With $d(t) = 2$, we obtain $d(r) \geq 4$.



(a) Case (i) (b) Case (ii)

Figure 4.1 Two types of local structures in the upper bound induction.

Let $G \in \mathcal{H}_n$ with $n \geq 4$. Let v be a degree-2 vertex with $N_G(v) = \{u, w\}$. Furthermore, let $p = d_G(u)$, $q = d_G(w)$, $G' = G - v$ and $N_0(u) = N_G(u) \setminus \{v, w\}, N_0(w) = N_G(w) \setminus \{v, u\}$. Then by subtracting term by term, we have

$$HSO(G) - HSO(G') = h(2,p) + h(2,q) + \big[h(p,q) - h(p-1,q-1)\big] + \sum_{x \in N_0(u)} \big[h(p,d(x)) - h(p-1,d(x))\big] + \sum_{y \in N_0(w)} \big[h(q,d(y)) - h(q-1,d(y))\big]. \tag{2}$$

Equivalently, writing

$$J(p,q) = h(p,q) - h(p-1,q-1), \qquad D_x(y) = h(x,y) - h(x-1,y),$$

we obtain

$$HSO(G) - HSO(G') = h(2,p) + h(2,q) + J(p,q) + \sum_{x \in N_0(u)} D_p(d(x)) + \sum_{y \in N_0(w)} D_q(d(y)). \tag{3}$$

Lemma 4.2. *Let $G \in \mathcal{H}_n$ with $n \geq 5$ and $w(G) = 5$. There is a degree-2 vertex v such that $N(v) = \{u, w\}$ and $d(u) \leq d(w)$ and $w(uv) = 5$ in G. Let $d(w) = q$. Then*

$$HSO(G) - HSO(G - v) \leq \Psi(q).$$

Proof. By Lemma 2.7, besides v, the vertices u, w have exactly one common neighbor z. Since $d(u) = 3$, we have $N_0(u) = \{z\}$, and $d(z) \geq 3$, since $d(z) = 2$ would force $n = 4$. By Equation (3),

$$HSO(G) - HSO(G - v) = h(2,3) + h(2,q) + J(3,q) + D_3(d(z)) + \sum_{y \in N_0(w)} D_q(d(y)).$$

By Lemma 2.2, $D_3(d(z)) \leq D_3(3)$. Also, by Remark 2.1, besides v, w has at most one more degree-2 neighbor; all other neighbors have degree at least 3. Since $|N_0(w)| = q - 2$, we have

$$\sum_{y \in N_0(w)} D_q(d(y)) \leq D_q(2) + (q-3)D_q(3).$$

Therefore,

$$HSO(G) - HSO(G - v) \leq h(2,3) + h(2,q) + J(3,q) + D_3(3) + D_q(2) + (q-3)D_q(3).$$

Using

$$D_3(3) = h(3,3) - h(2,3) = \sqrt{2} - h(2,3), \qquad J(3,q) = h(3,q) - h(2,q-1),$$

we obtain $HSO(G) - HSO(G - v) \leq \Psi(q)$ after simplification. □

In case (ii) of Lemma 4.1, let r be as shown in Figure 4.1(b). Define

$$\Theta(q) = h(2,4) + h(2,q) + J(4,q) + D_4(2) + D_4(4) + D_q(2) + (q-4)D_q(3) + D_q(4), \qquad q \in \{4,5,6\}.$$

Lemma 4.3. *Let $G \in \mathcal{H}_n$ with $n \geq 6$ and $w(G) = 6$. There is a degree-2 vertex v such that $N(v) = \{u, w\}$ and $d(u) \leq d(w)$ and $w(uv) = 6$ in G. Let $d(w) = q$. Then*

$$HSO(G) - HSO(G - v) \leq \Theta(q), \qquad q = d(w) \in \{4, 5, 6\}.$$

Proof. By Lemma 4.1, the local structure in Figure 4.1(b) gives

$$N_0(u) = \{t, r\}, \qquad d(t) = 2, \qquad d(r) \geq 4.$$

Therefore, by Lemma 2.2,

$$D_4(d(t)) + D_4(d(r)) \leq D_4(2) + D_4(4).$$

On the other hand, $r \in N_0(w)$ and w has at most one more degree-2 neighbor besides v. Thus

$$\sum_{y \in N_0(w)} D_q(d(y)) \leq D_q(2) + (q-4)D_q(3) + D_q(4).$$

Substituting into Equation (3) yields the desired inequality. □

Theorem 4.1. *Let $G \in \mathcal{H}_n$.*

(1) If $n = 6$,

$$HSO(G) \leq 6\sqrt{5} + 3\sqrt{2}, \tag{4}$$

with equality if and only if $G \cong H_2$.

(2) If $4 \leq n \leq 5$ or $n \geq 7$,

$$HSO(G) \leq \sqrt{(n-1)^2 + 4} + \frac{n-3}{3}\sqrt{(n-1)^2 + 9} + \sqrt{13} + (n-4)\sqrt{2}, \tag{5}$$

with equality if and only if $G \cong K_1 \vee P_{n-1}$.

Proof. The conclusions for $4 \leq n \leq 5$ and $n = 6$ follow directly from Section 2.

We proceed by induction for $n \geq 7$. For $n = 7$, Section 2 shows that F_7 uniquely attains the maximum, establishing the base case.

Assume that for any $H \in \mathcal{H}_{n-1} (n \geq 8)$, $HSO(H) \leq B_{n-1}$, with equality if and only if $H \cong F_{n-1}$.

Take any $G \in \mathcal{H}_n$. By Lemma 2.10, $5 \leq w(G) \leq 6$. By Lemma 4.1, we can choose a degree-2 vertex v and label its neighbors so that $w(uv) = w(G)$ and

$$N(v) = \{u, w\}, \qquad p = d(u) \leq q = d(w),$$

such that either $p = 3$, or $p = 4$ and $4 \leq q \leq 6$. Let $G' = G - v$. Obviously $G' \in \mathcal{H}_{n-1}$.

Case 1: $p = 3$. By Lemma 4.2,

$$HSO(G) - HSO(G') \leq \Psi(q).$$

By Lemma 2.8, $q \geq 4$. Since $q \leq n - 1$, Lemma 2.5 gives

$$\Psi(q) \leq \Psi(n-1).$$

Combining the inductive hypothesis with $B_n - B_{n-1} = \Psi(n-1)$ from Lemma 2.12,

$$HSO(G) \leq B_{n-1} + \Psi(n-1) = B_n.$$

If equality holds, then we must have $q = n - 1$. Therefore w is adjacent to all other vertices of G. The graph G has $2n - 3$ edges, of which $n - 1$ are incident with w, so

$$|E(G - w)| = (2n-3) - (n-1) = n - 2.$$

Also, $G - w$ contains $n - 1$ vertices, and after removing w from the outer Hamilton cycle we still obtain a path passing through all remaining vertices. Therefore $G - w$ is a tree containing this Hamilton path, which can only be P_{n-1}. Thus,

$$G \cong K_1 \vee P_{n-1} = F_n.$$

Case 2: $p = 4$ and $4 \leq q \leq 6$. The numerical values of Ψ and Θ at the relevant points are listed in Table 4.1.

Table 4.1 Some values of the functions Θ and Ψ.

Symbol	$\Theta(4)$	$\Theta(5)$	$\Theta(6)$	$\Psi(7)$	$\Psi(8)$
Value	4.834	5.964	6.695	6.118	6.775

By direct comparison of a finite number of fixed radicals, we have

$$\Theta(q) \leq \Theta(6) \quad (q = 4, 5, 6), \qquad \Theta(6) < \Psi(8), \qquad \Theta(5) < \Psi(7).$$

First, we consider $n \geq 9$. By Lemma 4.3 and the comparisons above,

$$HSO(G) - HSO(G') \leq \Theta(q) \leq \Theta(6) < \Psi(8).$$

Since $n - 1 \geq 8$ and Ψ is strictly increasing, we have $\Psi(8) \leq \Psi(n-1)$. Hence

$$HSO(G) - HSO(G') < \Psi(n-1),$$

and combining this with the inductive hypothesis yields

$$HSO(G) < B_{n-1} + \Psi(n-1) = B_n.$$

Thus, Case 2 cannot attain equality if $n \geq 9$.

It remains to handle $n = 8$. For this case, define

$$C_7 := HSO(U_3) = 3\sqrt{5} + \sqrt{29} + \frac{\sqrt{41}}{2} + \frac{\sqrt{13}}{2} + \frac{5}{3} + \frac{\sqrt{34}}{3} + \sqrt{2}.$$

If $q = 4$ or 5, then by Lemma 4.3,

$$HSO(G) - HSO(G') \leq \Theta(q) \leq \Theta(5) < \Psi(7),$$

and thus,

$$HSO(G) < B_7 + \Psi(7) = B_8.$$

If $q = 6$, then after deleting v, the degree of w in G' becomes 5. But the degree sequence of F_7 is $\{6, 3, 3, 3, 3, 2, 2\}$, which has no vertex of degree 5, and hence $G' \ncong F_7$. From the $n = 7$ enumeration, the maximum HSO among graphs other than F_7 is C_7, so $HSO(G') \leq C_7$. Applying Lemma 4.3 again,

$$HSO(G) \leq C_7 + \Theta(6).$$

Direct comparison of fixed radicals gives

$$B_8 - C_7 - \Theta(6) = -7\sqrt{5} - 2\sqrt{10} - \frac{\sqrt{29}}{2} - \frac{\sqrt{41}}{4} + 2\sqrt{2} + \frac{2\sqrt{34}}{3} + \sqrt{53} + \frac{5\sqrt{58}}{3} \approx 0.418 > 0,$$

and hence $HSO(G) < B_8$. Therefore, equality cannot occur in Case 2 if $n = 8$ either.

In summary, if $n = 6$, the maximum is uniquely attained by H_2, as stated in (4), and if $n \geq 7$, the maximum is uniquely attained by $K_1 \vee P_{n-1}$, as stated in (5). For $4 \leq n \leq 5$, the conclusion follows from the uniqueness of the maximal outerplanar graph up to isomorphism. □

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