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On extremal Sombor index of bipartite graphs with given order and diameter

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Abstract. We consider the extremal value of the Sombor index in the class of bipartite graphs of a given order n and diameter d. Using a layered perspective on bipartite graphs, we first derive structural lemmas and an exact formula for the Sombor index $SO(G)$ in terms of the vertex partition sizes at successive distances from a fixed vertex. This framework allows us to transform the problem into a constrained optimization, which we solve by applying concavity and convexity arguments. As a main result, we prove a comprehensive characterization of the graphs that maximize $SO(G)$ for each fixed n and d. In particular, our results show that for $d = 3$ the unique extremal graph has one vertex in each of the distance-0 and distance-3 partitions and splits the remaining $n - 2$ vertices as evenly as possible between the distance-1 and distance-2 partitions. For any $d \geq 4$, the graph with maximum Sombor index is obtained by placing a single vertex in each outer distance partition while distributing the other $n - (d + 1)$ vertices between two inner partitions (one of which receives $\lceil (n - d + 1)/2 \rceil$ vertices and the other $\lfloor (n - d + 1)/2 \rfloor$). These findings contribute further insights in the extremal graph theory of the Sombor index under diameter constraints, extending the known case of unconstrained bipartite graphs (attaining their maximum SO at $d = 2$) to arbitrary prescribed diameters.

1. Introduction

Topological indices are graph invariants widely used in mathematical chemistry to quantify molecular structure. One of the newest degree-based indices is the *Sombor index*, introduced by Gutman in 2021 [1]. For a graph $G = (V(G), E(G))$, where $V(G)$ is the set of vertices and $E(G)$ denotes the set of graph edges, the Sombor index is defined as

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

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where $d_G(u)$ is the degree of a vertex $u \in V(G)$. Gutman's foundational paper on this index established its basic properties and provided a clear geometric interpretation.

Soon after its introduction, numerous researchers began investigating the Sombor index from various perspectives. Das *et al.* [2] presented initial bounds for $SO(G)$ in terms of other graph parameters and discussed relations with well-known indices. Liu *et al.* studied applications of the Sombor index in modeling physicochemical properties of molecular graphs [4], while other authors examined a *reduced* Sombor index variant and its mathematical properties [5]. The Sombor index has also been compared with other degree-based descriptors; for instance, Wang *et al.* derived analytical relations between the Sombor index and several classical indices [8]. Connections to spectral graph theory have been explored as well: Rejaa and Nayeem introduced the notion of Sombor energy and investigated how the Sombor index relates to graph energy [7].

Beyond general bounds and correlations, a major trend in recent research is to determine extremal values of the Sombor index under various graph constraints. A fundamental result by Gutman [1] and independently by Das *et al.* [2] characterized the bipartite graphs of a given order with maximum Sombor index. They showed that for a fixed number of vertices n, the largest $SO(G)$ among all n-vertex bipartite graphs is attained by a complete bipartite graph, which necessarily has diameter 2. This observation naturally raised the question of how additional constraints influence extremal values of the Sombor index. In particular, one may ask which graphs maximize the Sombor index within prescribed graph classes.

Over the past two years, numerous extremal problems of this type have been studied. Li, Wang and Zhang [6] investigated trees with a given diameter. Zhou, Lin and Miao considered extremal Sombor indices under different parameters: in one work they studied trees and unicyclic graphs with a given matching number [11], while in another they examined graphs with a prescribed maximum degree [12]. Zhang, Meng and Wang [10] extended such analyses to several graph families; in particular, they derived sharp upper bounds for $SO(G)$ among connected bipartite graphs with a fixed matching number. Very recently, Das [13] determined the maximum Sombor index of n-vertex trees with a prescribed independence number. In addition, Wang, Gao, Zhao and Liu [14] established a sharp upper bound on the Sombor index of bipartite graphs with a given diameter and proposed an algorithmic approach for identifying extremal configurations. This rapid development of extremal results highlights the central role of various graph invariants (such as matching number, degree, and independence number) in shaping the possible range of the Sombor index.

It is also worth noting that analogous extremal questions have been investigated for other graph invariants, providing further insight into the behavior of the Sombor index. For example, Zhai, Liu and Shu [9] examined the spectral radius of bipartite graphs with a given diameter. They characterized the n-vertex bipartite graphs of diameter d that maximize the spectral radius and identified the graph with the second-largest spectral radius. Although the spectral radius is primarily related to eigenvalues, while the Sombor index reflects structural graph features, both quantities are strongly influenced by degree distribution and connectivity. Restricting the diameter imposes constraints on the degree distribution and the number of edges of the graph, thereby bounding the attainable Sombor index.

Motivated by these developments, the present paper focuses on bipartite graphs with a prescribed diameter and investigates extremal values of the Sombor index within this class. In contrast to the above-mentioned approaches, our analysis relies on a layered structural description of extremal graphs combined with convexity-based optimization arguments. Let $\mathcal{B}(n, d)$ denote the class of all bipartite graphs of order n and diameter d ($d \geq 2$). Our goal is to characterize the graphs in $\mathcal{B}(n, d)$ that maximize $SO(G)$ for each n and d, thereby providing further insight into extremal behavior under diameter constraints.

The rest of the paper is organized as follows. Section 2 provides the necessary preliminary results and structural properties of bipartite graphs with a given diameter. Section 3 presents the main results, including complete characterizations of extremal graphs for prescribed order and diameter, with a detailed analysis of small diameters and the general case. Section 4 concludes the paper and outlines directions for future research.

2. Preliminary results

Let $G \in \mathcal{B}(n, d)$ be a graph with the maximal Sombor index. Then, there is a vertex $v \in V(G)$ and a partition $V_0, V_1, \ldots, V_d$ of the vertex set $V(G)$, i.e. $V(G) = V_0 \sqcup V_1 \sqcup \cdots \sqcup V_d$, where $\sqcup$ stands for the disjoint union, such that $V_0 = \{v\}$ and $d(v, u) = i$, for each vertex $u \in V_i$, and $i = 1, 2, \ldots, d$. Here, as usual, $d(u, v)$ stands for the distance between vertices u and v in G, i.e. the length of the shortest path between them. Each set V_i is called a *partition set*, and we will suppose that $|V_i| = m_i$, where $i = 0, 1, 2, \ldots, d$. In accordance with this, G can be denoted as $G = [V_0, V_1, \ldots, V_d]$, that is $G = [m_0, m_1, \ldots, m_d]$.

The following two statements has been proved in [2]:

Lemma 2.1. *[2] Let $G = (V(G), E(G))$ be a connected graph. Then,*

1. *if $uv \in E(G)$, then $SO(G) > SO(G - uv)$;*
2. *if $uv \notin E(G)$, then $SO(G + uv) > SO(G)$.*

Regarding the nature of $G \in \mathcal{B}(n, d)$, the subsequent lemma is obvious:

Lemma 2.2. *Let $G \in \mathcal{B}(n, d)$ be a graph with the maximal Sombor index. The induced subgraph $G[V_i]$, for each $i = 0, 1, \ldots, d$, has no edges.*

Lemma 2.3. *Let $G \in \mathcal{B}(n, d)$ be a graph with the maximal Sombor index. Then, $G[V_{i-1} \cup V_i]$, for $i = 1, 2, \ldots, d$, induces a complete bipartite subgraph. Furthermore, if $d \geq 3$, then $|V_d| = 1$.*

Proof. The first part of the statement is obvious, since G has maximal Sombor index in $\mathcal{B}(n, d)$.

For the second part of the statement, let us assume that $d \geq 3$. Let $x \in V_d$ and $y \in V_{d-3}$. If $|V_d| \geq 2$, then $G + xy \in \mathcal{B}(n, d)$, and $V_0 \sqcup V_1 \sqcup \cdots \sqcup V_{d-3} \sqcup (V_{d-2} \cup \{x\}) \sqcup V_{d-1} \sqcup (V_d \setminus \{x\})$ is a partition of the vertex set of the graph $G + xy$. By Lemma 2.1, we have $SO(G + xy) > SO(x)$, which is a contradiction with the assumption. Thus, $|V_d| = 1$. □

We make use of the following three lemmas in the next section.

Lemma 2.4. *Let $f : [a, b] \to \mathbb{R}$ be a strictly concave function. Let*

$$m := \frac{a + b}{2}$$

be the midpoint of the interval $[a, b]$. Assume f is symmetric about m, i.e.

$$f(m + t) = f(m - t), \text{ for every real } t \geq 0 \text{ with } m \pm t \in [a, b].$$

Then f attains its (unique) maximum at m.

Proof. By strict concavity we mean: for any distinct $x, y \in [a, b]$ and any $\lambda \in (0, 1)$,

$$f\Big(\lambda x + (1 - \lambda)y\Big) > \lambda f(x) + (1 - \lambda) f(y).$$

Take an arbitrary point $x \in [a, b]$. Then, $x = m \pm t$, for the unique real $t \geq 0$ with $m \pm t \in [a, b]$.
If $t \neq 0$, $m + t \neq m - t$, so strict concavity with $\lambda = \frac{1}{2}$ yields

$$f(m) = f\Big(\tfrac{1}{2}(m + t) + \tfrac{1}{2}(m - t)\Big) > \tfrac{1}{2} f(m + t) + \tfrac{1}{2} f(m - t). \tag{1}$$

Using the symmetry $f(m + t) = f(m - t)$, the right-hand side of (1) simplifies to $f(m + t)$. Therefore, for every $t \neq 0$ (equivalently, for every $x \neq m$)

$$f(m) > f(m + t) = f(x).$$

If $t = 0$ (i.e. $x = m$) the previous inequality is an equality $f(m) = f(x)$. Thus $f(m) \geq f(x)$, for all $x \in [a, b]$, and the inequality is strict for all $x \neq m$. Hence f attains its maximum at m, and that maximum is unique. □

Lemma 2.5. *Let $g : [1, S - 1] \to \mathbb{R}$ be a strictly convex function. Then the maximum of g in the interval $[1, S - 1]$ is attained only at the endpoints of the interval, i.e.*

$$\max_{x\in[1,S-1]} g(x) \in \{g(1), g(S-1)\}.$$

Proof. Suppose, for the sake of contradiction, that the maximum occurs at some interior point $x_0 \in (1, S-1)$, i.e.,

$$g(x_0) = \max_{x\in[1,S-1]} g(x).$$

Choose any points $t \in (1, x_0)$ and $s \in (x_0, S - 1)$. There exists $\lambda \in (0, 1)$ such that

$$x_0 = \lambda t + (1 - \lambda)s.$$

By strict convexity of g, we have

$$g(x_0) = g(\lambda t + (1 - \lambda)s) < \lambda g(t) + (1 - \lambda)g(s).$$

However, by maximality of x_0, we also have $g(t) \le g(x_0)$ and $g(s) \le g(x_0)$. Therefore,

$$\lambda g(t) + (1 - \lambda)g(s) \le \lambda g(x_0) + (1 - \lambda)g(x_0) = g(x_0),$$

which gives a contradiction, i.e.

$$g(x_0) < \lambda g(t) + (1 - \lambda)g(s) \le g(x_0).$$

□

Lemma 2.6. *Let $\alpha > 0$, $A > 0$, $B > 0$, and $S > 1$. Define canonical functions*

$$h_{\alpha,A,B}(x) := \alpha x \sqrt{A + (x + B)^2},$$
$$k_{\alpha,A,B}(x) := \alpha \sqrt{A + (x + B)^2},$$
$$l_{\alpha,A,B,S}(x) := \alpha(S - x) \sqrt{A + (S - x + B)^2},$$
$$s_{\alpha,A,B,S}(x) := \alpha \sqrt{(x + A)^2 + (S - x + B)^2}.$$

Each of the functions $h_{\alpha,A,B}$, $k_{\alpha,A,B}$, $l_{\alpha,A,B,S}$ and $s_{\alpha,A,B,S}(x)$ is strictly convex in the interval $[1, S - 1]$.

Proof. Compute and estimate the second derivatives for $h_{\alpha,A,B}(x), k_{\alpha,A,B}(x)$ and $l_{\alpha,A,B,S}(x)$:

$$h''_{\alpha,A,B}(x) = \alpha \frac{2(x + B)(A + (x + B)^2) + xA}{(A + (x + B)^2)^{3/2}} > 0,$$

$$k''_{\alpha,A,B}(x) = \frac{\alpha A}{(A + (x + B)^2)^{3/2}} > 0,$$

$$l''_{\alpha,A,B,S}(x) = h''_{\alpha,A,B}(S - x) > 0.$$

Set

$$Q(x) := (x + A)^2 + (B + S - x)^2 = 2x^2 + 2(A - B - S)\, x + \left(A^2 + (B + S)^2\right).$$

Thus $s(x) = \alpha \sqrt{Q(x)}$. For a quadratic $Q(x) = ax^2 + bx + c$ with $a > 0$ and $Q(x) > 0$, one has

$$\frac{d^2}{dx^2} \sqrt{Q(x)} = \frac{ac - \frac{b^2}{4}}{(ax^2 + bx + c)^{3/2}}.$$

Here $a = 2$, $b = 2(A - B - S)$, and $c = A^2 + (B + S)^2$, so

$$ac - \frac{b^2}{4} = 2\Big(A^2 + (B + S)^2\Big) - \Big(A - B - S\Big)^2 = \Big(B + A + S\Big)^2 \; > \; 0.$$

Since $Q(x) > 0$ for all x (it is a sum of squares), we get

$$s''(x) = \alpha \, \frac{(B + A + S)^2}{\Big(Q(x)\Big)^{3/2}} \; > \; 0,$$

which proves that s is strictly convex in x.

Hence all four functions are strictly convex on $[1, S - 1]$. □

3. Main results

According to Lemma 2.3, we conclude that the induced subgraph $G[V_i \cup V_{i+1}]$, for $0 \leq i \leq d - 1$, in a bipartite graph with diameter d is itself a complete bipartite graph. Consequently, every vertex $v \in V_i$ has degree $m_{i-1} + m_{i+1}$ for $1 \leq i \leq d - 1$, while for $i = 0$ or $i = d$, the degrees of the vertices are m_1 and m_{d-1}, respectively.

It follows that each edge of $G[V_i \cup V_{i+1}]$ contributes to the total Sombor index with the value

$$\sqrt{(m_{i-1} + m_{i+1})^2 + (m_i + m_{i+2})^2}.$$

Since there are $m_i m_{i+1}$ such edges, the total contribution of all edges from $G[V_i \cup V_{i+1}]$ to the Sombor index is

$$m_i m_{i+1} \sqrt{(m_{i-1} + m_{i+1})^2 + (m_i + m_{i+2})^2}.$$

Therefore, we define

$$E_d(m_0, \ldots, m_d) = \sum_{k=1}^{d} T_k, \tag{2}$$

where

$$\begin{aligned} T_1 &= m_0 m_1 \sqrt{(m_0 + m_2)^2 + m_1^2}, \\ T_k &= m_{k-1} m_k \sqrt{(m_{k-2} + m_k)^2 + (m_{k-1} + m_{k+1})^2}, \quad 2 \leq k \leq d - 1, \\ T_d &= m_{d-1} m_d \sqrt{(m_{d-2} + m_d)^2 + m_{d-1}^2}. \end{aligned}$$

Our objective is to maximize E_d subject to the constraint

$$\sum_{i=0}^{d} m_i = n,$$

where d denotes the fixed diameter of the graph, and n represents its order. Additionally, the boundary conditions $m_0 = m_d = 1$ hold, as established in Lemma 2.3.

3.1. Bipartite Graphs of Prescribed Order and Small Diameter

3.1.1.

Bipartite graphs with diameter $d = 3$

For $d = 3$ put $(m_0, m_1, m_2, m_3) = (1, x, S - x, 1)$ with $S = n - 2$, and define

$$F(x) := E_3(1, x, S - x, 1), \qquad x \in [2, S - 2].$$

Theorem 3.1. *Let*

$$F(x) = \sqrt{f_1(x)} + \sqrt{f_2(x)} + \sqrt{f_3(x)},$$

where

$$f_1(x) = x^2\Big((n - x - 1)^2 + x^2\Big), \qquad f_2(x) = x^2(n - x - 2)^2\Big((n - x - 1)^2 + (x + 1)^2\Big),$$

$$f_3(x) = (n - x - 2)^2\Big((x + 1)^2 + (n - 2 - x)^2\Big).$$

For $n \geq 6$ and $x \in [2, n - 3]$, the function F attains its maximum at

$$x = c := \frac{n - 2}{2}.$$

Proof. **Step 1.** By Cauchy–Schwarz it holds that

$$\sqrt{f_1(x)} + \sqrt{f_3(x)} \leq \sqrt{2}\,\sqrt{f_1(x) + f_3(x)}.$$

Define

$$f(x) = 2\Big(f_1(x) + f_3(x)\Big), \qquad g(x) = f_2(x).$$

Since the square root function is concave, it follows that for any $y \geq 0$ and $y_0 > 0$ the following inequality holds:

$$\sqrt{y} \leq \sqrt{y_0} + \frac{y - y_0}{2\sqrt{y_0}}.$$

Applying this to $y = f(x)$ at $x = c$ and to $y = g(x)$ at $x = c$, set

$$T(x) := \sqrt{f(c)} + \sqrt{g(c)} + \frac{f(x) - f(c)}{2\sqrt{f(c)}} + \frac{g(x) - g(c)}{2\sqrt{g(c)}}.$$

Then

$$F(x) \leq \sqrt{f(x)} + \sqrt{g(x)} \leq T(x) \qquad (\forall x),$$

and equalities hold at $x = c$ (because $f_1(c) = f_3(c)$ and the tangents touch at $f(c), g(c)$). Hence

$$F(c) = \sqrt{f(c)} + \sqrt{g(c)} = T(c).$$

Step 2. Differentiate $T(x)$ and write $x = c + y$:

$$T'(x) = \frac{f'(x)}{2\sqrt{f(c)}} + \frac{g'(x)}{2\sqrt{g(c)}}, \qquad f'(c + y) = 8y\Big(n^2 - 5n + 4y^2 + 7\Big),$$

$$g'(c + y) = \frac{y}{4}\Big(4y^2 - (n - 2)^2\Big)\Big(n^2 + 4n + 12y^2 - 4\Big).$$

Thus

$$T'(c + y) = y\,\varphi_n(y), \qquad \varphi_n(y) = \Phi_n(z), \quad z = y^2,$$

with

$$\Phi_n(z) = A_f\,(n^2 - 5n + 7 + 4z) + A_g\,(4z - (n-2)^2)\,(n^2 + 4n - 4 + 12z),$$

and

$$A_f = \frac{8}{(n-2)\sqrt{n^2 + (n-2)^2}}, \qquad A_g = \frac{1}{\sqrt{2}\,n\,(n-2)^2}.$$

On $x \in [2, n-4]$ we have $y \in \left[\frac{6-n}{2}, \frac{n-6}{2}\right]$, hence

$$z = y^2 \in \left[0,\ z_{\max}\right], \qquad z_{\max} = \left(\frac{n-6}{2}\right)^2.$$

Note that Φ_n is a upward-opening quadratic in z (its z^2 coefficient is $48A_g > 0$), hence convex.

Step 3. According to Lemma 2.5, convexity implies that $\max_{z\in[0,z_{\max}]} \Phi_n(z)$ is attained at an endpoint. It therefore suffices to show

$$\Phi_n(0) \le 0 \qquad \text{and} \qquad \Phi_n(z_{\max}) \le 0.$$

(i) The value at $z = 0$. Using $\sqrt{n^2 + (n-2)^2} \ge \sqrt{2}\,(n-1)$,

$$\Phi_n(0) = A_f\,(n^2 - 5n + 7) - A_g\,(n-2)^2(n^2 + 4n - 4) \le \frac{4\sqrt{2}}{(n-2)(n-1)}(n^2 - 5n + 7) - \frac{1}{\sqrt{2}n}(n^2 + 4n - 4).$$

This upper bound equals

$$-\frac{1}{\sqrt{2}\,n(n-2)(n-1)}\,P_0(n), \qquad P_0(n) = n^4 - 7n^3 + 26n^2 - 36n - 8.$$

We observe that $P_0(4) = 72 > 0$. Furthermore, since $P_0'(n) = 4n^3 - 21n^2 + 52n - 36 > 0$ for all $n \ge 2$, it follows that $P_0(n)$ is strictly increasing for $n \ge 2$. Consequently, $P_0(n) > 0$ holds for all $n \ge 4$. Consequently $\Phi_n(0) \le 0$ for $n \ge 4$.

(ii) The value at $z = z_{\max}$. Let $t = \sqrt{n^2 - 2n + 2} \in (n-1, n)$. A direct simplification gives

$$\Phi_n(z_{\max}) = \frac{\sqrt{2}}{n\big(n^4 - 6n^3 + 14n^2 - 16n + 8\big)}\big(C_1(n)\,t + C_0(n)\big),$$

where

$$C_1(n) = 8n^4 - 84n^3 + 308n^2 - 344n, \qquad C_0(n) = -16n^5 + 224n^4 - 1344n^3 + 3904n^2 - 5184n + 3328.$$

Since $t \le n$ and $C_1(n) > 0$ for $n \ge 6$, we obtain the upper bound

$$\Phi_n(z_{\max}) \le \frac{\sqrt{2}}{n\big(n^4 - 6n^3 + 14n^2 - 16n + 8\big)}\big(C_1(n)\,n + C_0(n)\big),$$

and

$$C_1(n)\,n + C_0(n) = -4\,S(n), \qquad S(n) = 2n^5 - 35n^4 + 259n^3 - 890n^2 + 1296n - 832.$$

We have $S(6) = 1040 > 0$ and $S'(n) = 10n^4 - 140n^3 + 777n^2 - 1780n + 1296$ has positive second derivative for all n; hence $S'(n)$ is increasing, $S'(6) > 0$, and $S(n)$ is increasing on $[6, \infty)$, whence $S(n) > 0$ for all $n \ge 6$. Therefore $\Phi_n(z_{\max}) \le 0$ for $n \ge 6$.

Step 4. From Step 3, $\Phi_n(z) \le 0$ for every $z \in [0, z_{\max}]$. Hence for $y \in \left[\frac{6-n}{2}, \frac{n-6}{2}\right]$,

$$T'(c+y) = y\,\Phi_n(y^2)\begin{cases} > 0, & y < 0,\\ = 0, & y = 0,\\ < 0, & y > 0,\end{cases}$$

i.e., T is strictly increasing on $[2, c]$ and strictly decreasing on $[c, n-3]$. Together with Step 1,

$$F(x) \leq T(x) \leq T(c) = F(c) \qquad (x \in [2, n-3]),$$

so F attains its maximum at $x = c = \frac{n-2}{2}$. □

Corollary 3.2. *Let $G = [V_0, V_1, V_2, V_3] \in \mathcal{B}(n, 3)$ be the connected graph with the maximal Sombor index. Then $|V_0| = |V_3| = 1$, $|V_1| = \lceil \frac{n-2}{2} \rceil$ and $|V_2| = \lfloor \frac{n-2}{2} \rfloor$, i.e. $G = [1, \lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor, 1]$.*

Proof. According to the remarks given in the previous section, and Theorem 3.1, it holds $|V_0| = |V_3| = 1$. Let us suppose $|V_1| = x$ and $|V_2| = y$, where $x + y = n - 2$. Then the Sombor index $SO(G)$ of the graph G can be considered as the function $F(x)$ given by Theorem 3.1.From Theorem 3.1, it follows that if the order n of the graph G is even, then $|V_1| = |V_2| = \frac{n-2}{2}$. If n is odd, then $|V_1| = \frac{n-3}{2}$ and $|V_2| = \frac{n-1}{2}$. This conclusion holds because the function $F(x)$ is increasing up to $x = \frac{n-2}{2}$ and decreasing thereafter, and moreover, $F(\frac{n-3}{2}) = F(\frac{n-1}{2})$. Note that F is symmetric with respect to $x = \frac{n-2}{2}$, a property used in the proof of Theorem 3.1. This completes the proof. □

3.1.2.

Bipartite graphs with diameter $d = 4$

For $d = 4$ put $(m_0, m_1, m_2, m_3, m_4) = (1, S - t, t, 1, 1)$ with $S = n - 3$, and define

$$E_4(t) := E_4(1, S - t, t, 1, 1), \qquad t \in [2, S - 2].$$

Lemma 3.3. *Let*

$$N_1(t) = -4t^2 + (5n - 18)t - 2n^2 + 13n - 22.$$

Then $N_1(t) \leq 0$ for all real t. In particular,

$$\max_{t \in \mathbb{R}} N_1(t) = -\tfrac{7}{16}(n-2)^2 \leq 0,$$

and the maximum is attained at

$$t_{\max} = \frac{5n - 18}{8}.$$

Proof. The polynomial $N_1(t)$ is quadratic in t with leading coefficient $-4 < 0$, hence concave. Its maximum occurs at

$$t_{\max} = -\frac{b}{2a} = \frac{5n - 18}{8},$$

where $a = -4$ and $b = 5n - 18$. Substituting this into $N_1(t)$ yields

$$N_1(t_{\max}) = -\frac{7}{16}(n-2)^2 \leq 0.$$

Since the parabola opens downwards, this value is the global maximum, so $N_1(t) \leq 0$ for all $t \in \mathbb{R}$. □

Lemma 3.4. *Let*

$$N_2(t) = -6t^3 + (9n - 23)t^2 + (-5n^2 + 23n - 28)t + n^3 - 6n^2 + 13n - 10,$$

and assume $n \geq 7$. Then $N_2(t)$ is strictly decreasing for all real t. Moreover,

$$N_2\Big(\frac{n-3}{2}\Big) = \frac{n^2 - 2n + 1}{2} = \frac{(n-1)^2}{2} > 0, \qquad N_2\Big(\frac{n-3}{2} + 1\Big) = -n - 1 < 0.$$

Consequently, for all real t,

$$t \leq \frac{n-3}{2} \implies N_2(t) > 0, \qquad t \geq \frac{n-3}{2} + 1 \implies N_2(t) < 0.$$

Proof. Differentiate $N_2(t)$ to obtain

$$N_2'(t) = -18t^2 + (18n-46)t + (-5n^2+23n-28).$$

The discriminant of this quadratic is

$$\Delta = (18n-46)^2 - 4(-18)(-5n^2+23n-28) = (18n-46)^2 - 72(5n^2-23n+28).$$

A straightforward expansion and cancellation yields

$$\Delta = 100 - 36n^2 < 0,$$

hence $N_2'(t)$ has no real zeros, for $n \geq 2$. Since the leading coefficient of $N_2'(t)$ equals $-18 < 0$, we conclude $N_2'(t) < 0$ for all real t; i.e. N_2 is strictly decreasing on $\mathbb{R}$.

It remains to evaluate N_2 at the two points $\frac{n-3}{2}$ and $\frac{n-3}{2}+1$. First substitute $t = \dfrac{n-3}{2}$:

$$N_2\Big(\frac{n-3}{2}\Big) = -6\Big(\frac{n-3}{2}\Big)^3 + (9n-23)\Big(\frac{n-3}{2}\Big)^2 + (-5n^2+23n-28)\Big(\frac{n-3}{2}\Big) + n^3 - 6n^2 + 13n - 10.$$

After simplification (expand, collect terms and divide by 4) one obtains

$$N_2\Big(\frac{n-3}{2}\Big) = \frac{n^2-2n+1}{2} = \frac{(n-1)^2}{2} > 0.$$

Next substitute $t = \dfrac{n-3}{2} + 1 = \dfrac{n-1}{2}$. A direct substitution and simplification gives

$$N_2\Big(\frac{n-3}{2}+1\Big) = -n-1 < 0, \qquad \text{for } n \geq 0.$$

Since N_2 is strictly decreasing, the positivity at $t = (n-3)/2$ and negativity at the next integer imply the stated sign pattern: for every $t \leq (n-3)/2$ we have $N_2(t) \geq N_2\big((n-3)/2\big) > 0$, and for every $t \geq (n-3)/2+1$ we have $N_2(t) \leq N_2\big((n-3)/2+1\big) < 0$. This completes the proof. □

Lemma 3.5. *For $n \geq 7$ and $2 \leq t \leq \frac{n-3}{2}$,*

$$\frac{D_2(t)}{D_1(t)} < \frac{6}{5}, \qquad D_1(t) = \sqrt{(t+1)^2 + (n-3-t)^2}, \quad D_2(t) = \sqrt{(t+1)^2 + (n-2-t)^2}.$$

Proof. Put

$$a := t+1, \quad b := n-3-t, \quad S := a+b = n-2.$$

Then $a \in [3, \frac{S+1}{2}]$, $b \in [\frac{S-1}{2}, S-3]$, and

$$\Big(\frac{D_2}{D_1}\Big)^2 = 1 + \frac{2b+1}{a^2+b^2} \leq 1 + \frac{2b+1}{9+b^2} =: 1 + f(b).$$

$$\text{For } b \geq 3, \quad f'(b) = \frac{(9+b^2)\cdot 2 - (2b+1)\cdot 2b}{(9+b^2)^2} = \frac{18-2b-2b^2}{(9+b^2)^2} < 0,$$

so f is decreasing on $[3, \infty)$.

Case $S \geq 7$ **(**$n \geq 9$**).** Since $a \geq 3$ and $b \geq \frac{S-1}{2} \geq 3$ (because $S = n - 2 \geq 7$), the maximum of $f(b)$ on the admissible b occurs at $b_{\min} = \frac{S-1}{2}$. Thus,

$$\Big(\frac{D_2}{D_1}\Big)^2 \leq 1 + \frac{2b+1}{9+b^2} \leq 1 + \frac{2 \cdot \frac{S-1}{2} + 1}{9 + \left(\frac{S-1}{2}\right)^2} = 1 + \frac{4S}{(S-1)^2 + 36}.$$

We want to prove that the last expression is less than $\frac{36}{25}$. This is equivalent to

$$\frac{4S}{(S-1)^2+36} < \frac{11}{25} \iff 100S < 11\big((S-1)^2 + 36\big) \iff 11S^2 - 122S + 407 > 0,$$

which holds for all real S (discriminant < 0). Hence $D_2/D_1 < 6/5$ for $n \geq 9$.

Cases $S = 5, 6$ **(**$n = 7, 8$**).** Here $t \in [2, \frac{n-3}{2}]$ gives $a \in [3, \frac{S+1}{2}]$ and $b = S - a \in [\frac{S-1}{2}, S-3]$.

- If $S = 5$ ($n = 7$), then $t = 2$ only, so $(a, b) = (3, 2)$ and

$$\Big(\frac{D_2}{D_1}\Big)^2 = \frac{3^2+3^2}{3^2+2^2} = \frac{18}{13} < \frac{36}{25}.$$

- If $S = 6$ ($n = 8$), then $a \in [3, \frac{7}{2}]$, $b \in [\frac{5}{2}, 3]$ and

$$\frac{\partial}{\partial a}\left(\frac{a^2+(b+1)^2}{a^2+b^2}\right) = -\frac{2a(2b+1)}{(a^2+b^2)^2} < 0 \quad \Rightarrow \quad \text{maximum at } a = 3,\ b = 3,$$

hence

$$\Big(\frac{D_2}{D_1}\Big)^2 = \frac{3^2+4^2}{3^2+3^2} = \frac{25}{18} < \frac{36}{25}.$$

Therefore, for all $n \geq 7$ and $2 \leq t \leq \frac{n-3}{2}$ we have $D_2/D_1 < 6/5$. □

Lemma 3.6. *Let*

$$\begin{aligned} N_1(t) &= -4t^2 + (5n-18)t - 2n^2 + 13n - 22, \\ N_2(t) &= -6t^3 + (9n-23)t^2 + (-5n^2 + 23n - 28)t + n^3 - 6n^2 + 13n - 10, \\ P(t) &:= 6N_1(t) + 5N_2(t). \end{aligned}$$

For $n \geq 9$ *and* $2 \leq t \leq \frac{n-3}{2} - 1 = \frac{n-5}{2}$*, one has* $P(t) > 0$.

Proof. Expand:

$$P(t) = -30t^3 + (45n - 139)t^2 + (-25n^2 + 145n - 248)t + (5n^3 - 42n^2 + 143n - 182).$$

Derivatives:

$$P'(t) = -90t^2 + (90n - 278)t + (-25n^2 + 145n - 248), \qquad P''(t) = 90n - 180t - 278.$$

For $2 \leq t \leq \frac{n-5}{2}$ and $n \geq 9$,

$$P''(t) \ \geq\ P''\Big(\frac{n-5}{2}\Big) = 90n - 90(n-5) - 278 = 172 > 0,$$

so P is strictly convex and its minimum on the interval is at an endpoint. According to Lemma 1.5, the maximum is achieved at the endpoints of the closed interval.

Endpoint values:

$$P(2) = 5n^3 - 92n^2 + 613n - 1474, \qquad P\Big(\frac{n-5}{2}\Big) = 2n^2 + 4n + 38.$$

Clearly $P\left(\frac{n-5}{2}\right) > 0$ for all n. Moreover

$$\frac{d}{dn}P(2) = 15n^2 - 184n + 613 > 0 \quad \text{(discriminant } < 0),$$

hence $P(2)$ is increasing in n; at $n = 9$, $P(2) = 236 > 0$. Therefore $P(2) > 0$ for all $n \geq 9$.

Since both endpoints are positive and P is convex on the interval, $P(t) > 0$ for all $2 \leq t \leq \frac{n-5}{2}$. □

Remark. For $n = 7, 8$ the interval $[2, \frac{n-5}{2}]$ is empty, so the statement is vacuously true. □

Lemma 3.7. *Let $n \geq 7$ and define*

$$T_1(t) = (n-3-t)\sqrt{(t+1)^2 + (n-3-t)^2},$$
$$T_2(t) = (n-2-t)\,t\sqrt{(t+1)^2 + (n-2-t)^2},$$
$$T_3(t) = \sqrt{(t+1)^2 + 1}, \qquad E_4(t) = T_1(t) + T_2(t) + T_3(t).$$

With $a = \frac{n-3}{2}$, we have

$$E_4(a) > E_4(a-1) \qquad \textit{and} \qquad E_4(a) > E_4(a+1).$$

Proof. Throughout assume $a = \frac{n-3}{2} \geq 2$ (since $n \geq 7$).

We first prove that $E_4(a) - E_4(a-1) > 0$.

Compute termwise at $t = a$ and $t = a - 1$:

$$\begin{aligned}
T_1(a) &= a\sqrt{a^2 + (a+1)^2}, \\
T_1(a-1) &= (a+1)\sqrt{a^2 + (a+1)^2}, \\
T_2(a) &= a(a+1)\sqrt{(a+1)^2 + (a+1)^2} = a(a+1)^2\sqrt{2}, \\
T_2(a-1) &= (a-1)(a+2)\sqrt{a^2 + (a+2)^2} = (a-1)(a+2)\sqrt{2(a+1)^2 + 2}, \\
T_3(a) &= \sqrt{(a+1)^2 + 1}, \\
T_3(a-1) &= \sqrt{a^2 + 1}.
\end{aligned}$$

Thus

$$E_4(a) - E_4(a-1) = \underbrace{\left(T_2(a) - T_2(a-1)\right)}_{S_2} - \underbrace{\left(T_1(a-1) - T_1(a)\right)}_{S_1} + \underbrace{\left(T_3(a) - T_3(a-1)\right)}_{S_3}.$$

Note the exact simplification

$$S_1 = T_1(a-1) - T_1(a) = \sqrt{a^2 + (a+1)^2} = \sqrt{2a^2 + 2a + 1} \leq \sqrt{2}(a+1).$$

For S_2, rationalize the square-root increment:

$$\sqrt{2(a+1)^2 + 2} - \sqrt{2(a+1)^2} = \frac{2}{\sqrt{2(a+1)^2 + 2} + \sqrt{2(a+1)^2}} \leq \frac{1}{\sqrt{2}\,(a+1)}.$$

Hence

$$\begin{aligned}
S_2 &= a(a+1)^2\sqrt{2} - (a-1)(a+2)\sqrt{2(a+1)^2 + 2} \\
&= [a(a+1)^2\sqrt{2} - (a-1)(a+2)\sqrt{2}(a+1)] \\
&+ [(a-1)(a+2)\sqrt{2}(a+1) - (a-1)(a+2)\sqrt{2(a+1)^2 + 2}] = \\
&\geq \sqrt{2}(a+1)[a(a+1) - (a-1)(a+2)] - \frac{(a-1)(a+2)}{\sqrt{2}(a+1)}.
\end{aligned}$$

Since $a(a+1)-(a-1)(a+2)=2$ and $(a-1)(a+2)=a^2+a-2$, we get

$$S_2 \geq 2\sqrt{2}(a+1) - \frac{a^2+a-2}{\sqrt{2}(a+1)}.$$

Therefore

$$\begin{aligned} S_2 - S_1 &\geq \Big(2\sqrt{2}(a+1) - \frac{a^2+a-2}{\sqrt{2}(a+1)}\Big) - \sqrt{2}(a+1) = \sqrt{2}(a+1) - \frac{a^2+a-2}{\sqrt{2}(a+1)} \\ &= \frac{1}{\sqrt{2}} \cdot \frac{2(a+1)^2-(a^2+a-2)}{a+1} = \frac{1}{\sqrt{2}} \cdot \frac{a^2+3a+4}{a+1} = \frac{1}{\sqrt{2}}\Big(a+2+\frac{2}{a+1}\Big) > 0. \end{aligned}$$

Finally, $S_3 = T_3(a) - T_3(a-1) > 0$ because T_3 is increasing. Hence, we finally obtain that $E_4(a) - E_4(a-1) > 0$. Now, we prove that $E_4(a) - E_4(a+1) > 0$.

Observe that

$$\begin{aligned} &T_1(a) = a\sqrt{a^2+(a+1)^2}, && T_1(a+1) = (a-1)\sqrt{(a-1)^2+(a+2)^2}, \\ &T_2(a) = a(a+1)^2\sqrt{2}, && T_2(a+1) = a(a+1)\sqrt{a^2+(a+2)^2} = a(a+1)\sqrt{2(a+1)^2+2}, \\ &T_3(a) = \sqrt{(a+1)^2+1}, && T_3(a+1) = \sqrt{(a+2)^2+1}. \end{aligned}$$

Thus

$$E_4(a) - E_4(a+1) = \underbrace{\Big(T_1(a) - T_1(a+1)\Big)}_{R_1} - \underbrace{\Big(T_2(a+1) - T_2(a)\Big)}_{R_2} - \underbrace{\Big(T_3(a+1) - T_3(a)\Big)}_{R_3}.$$

Put $X = 2a^2 + 2a + 3$. Then

$$T_1(a) = a\sqrt{X-2}, \qquad T_1(a+1) = (a-1)\sqrt{X+2}.$$

By rationalizing the linear combination, we obtain the following expression:

$$\begin{aligned} R_1 &= a\sqrt{X-2} - (a-1)\sqrt{X+2} = \frac{a^2(X-2)-(a-1)^2(X+2)}{a\sqrt{X-2}+(a-1)\sqrt{X+2}} \\ &= \frac{(a^2-(a-1)^2)X - 2\Big(a^2+(a-1)^2\Big)}{a\sqrt{X-2}+(a-1)\sqrt{X+2}} \\ &= \frac{(2a-1)X-2(2a^2-2a+1)}{a\sqrt{X-2}+(a-1)\sqrt{X+2}} = \frac{4a^3-2a^2+8a-5}{a\sqrt{X-2}+(a-1)\sqrt{X+2}}. \end{aligned}$$

Since $a\sqrt{X-2}+(a-1)\sqrt{X+2} \leq (2a-1)\sqrt{X+2}$, we obtain the lower bound

$$R_1 \;\geq\; \frac{4a^3-2a^2+8a-5}{(2a-1)\sqrt{X+2}} = \frac{4a^3-2a^2+8a-5}{(2a-1)\sqrt{2a^2+2a+5}}.$$

Using the same rationalization as above we get

$$\sqrt{2(a+1)^2+2} - \sqrt{2(a+1)^2} = \frac{2}{\sqrt{2(a+1)^2+2}+\sqrt{2}(a+1)} \leq \frac{1}{\sqrt{2}(a+1)}.$$

Hence

$$R_2 = a(a+1)\Big(\sqrt{2(a+1)^2+2} - \sqrt{2(a+1)^2}\Big) \leq \frac{a}{\sqrt{2}}.$$

For R_3,

$$\sqrt{(a+2)^2+1}-\sqrt{(a+1)^2+1}=\frac{(a+2)^2-(a+1)^2}{\sqrt{(a+2)^2+1}+\sqrt{(a+1)^2+1}}=\frac{2a+3}{\sqrt{(a+2)^2+1}+\sqrt{(a+1)^2+1}}\le\frac{2a+3}{2\sqrt{(a+1)^2+1}}\le 1,$$

so $R_3 \le 1$.

In order to prove the stated inequality, it suffices to show

$$R_1 > R_2 + R_3.$$

Using the explicit bounds above, a sufficient condition is

$$\frac{4a^3-2a^2+8a-5}{(2a-1)\sqrt{2a^2+2a+5}} \;>\; \frac{a}{\sqrt{2}}+1.$$

The left-hand side is increasing for $a \ge 2$ (the numerator grows like $2a^2$ after normalization by the denominator), while the right-hand side is linear in a. A direct check at the endpoint $a = 2$ gives

$$\frac{4\cdot 8-2\cdot 4+16-5}{(4-1)\sqrt{13}}=\frac{35}{3\sqrt{13}}\approx 3.231 \;>\; \frac{2}{\sqrt{2}}+1\approx 2.414,$$

so the inequality holds at $a = 2$, hence for all $a \ge 2$. Therefore $E_4(a) - E_4(a+1) > 0$.

□

Lemma 3.8. *Let $n \ge 7$ and define*

$$T_1(t) = (n-3-t)\sqrt{(t+1)^2+(n-3-t)^2},$$

$$T_2(t) = (n-2-t)\,t\sqrt{(t+1)^2+(n-2-t)^2},$$

$$T_3(t) = \sqrt{(t+1)^2+1}, \qquad E_4(t) = T_1(t)+T_2(t)+T_3(t).$$

Set $b = \frac{n-2}{2}$ (so $b \ge \frac{5}{2}$). Then

$$E_4(b) > E_4(b-1) \quad \textit{and} \quad E_4(b) > E_4(b+1).$$

$$E_4(b) > E_4(b-2) \quad \textit{and} \quad E_4(b) > E_4(b+2).$$

Proof. First, we prove $E_4(b) > E_4(b-1)$.

At $t = b$ we have $n-3-b = b-1$ and $n-2-b = b$, so

$$\begin{aligned}
T_1(b) &= (b-1)\sqrt{(b+1)^2+(b-1)^2} = (b-1)\sqrt{2b^2+2},\\
T_1(b-1) &= b\sqrt{b^2+b^2} = b^2\sqrt{2},\\
T_2(b) &= b^2\sqrt{(b+1)^2+b^2} = b^2\sqrt{2b^2+2b+1},\\
T_2(b-1) &= (b^2-1)\sqrt{b^2+(b+1)^2} = (b^2-1)\sqrt{2b^2+2b+1},\\
T_3(b) &= \sqrt{(b+1)^2+1}, \qquad T_3(b-1) = \sqrt{b^2+1}.
\end{aligned}$$

Then

$$E_4(b)-E_4(b-1) = \underbrace{\Big[T_2(b)-T_2(b-1)\Big]}_{=\sqrt{2b^2+2b+1}} + \underbrace{\Big[T_1(b)-T_1(b-1)\Big]}_{:=\Delta_1} + \Big[T_3(b)-T_3(b-1)\Big].$$

We have the exact identity

$$T_2(b) - T_2(b-1) = \sqrt{2b^2 + 2b + 1},$$

and the bound

$$\Delta_1 = (b-1)\sqrt{2b^2+2} - b^2\sqrt{2} = \sqrt{2}\Big((b-1)\sqrt{b^2+1} - b^2\Big) \geq -\sqrt{2}\,b,$$

while $T_3(b) - T_3(b-1) > 0$. Thus

$$E_4(b) - E_4(b-1) \ \geq \ \sqrt{2b^2+2b+1} - \sqrt{2}\,b > 0,$$

because $\sqrt{2b^2+2b+1} > \sqrt{2}b$ for all $b > 0$.

We now establish the inequality $E_4(b) > E_4(b+1)$.
At $t = b+1$ we have $n-3-(b+1) = b-2$ and $n-2-(b+1) = b-1$, so

$$T_1(b+1) = (b-2)\sqrt{(b+2)^2 + (b-2)^2} = (b-2)\sqrt{2b^2+8},$$
$$T_2(b+1) = (b^2-1)\sqrt{(b+2)^2 + (b-1)^2} = (b^2-1)\sqrt{2b^2+2b+5},$$
$$T_3(b+1) = \sqrt{(b+2)^2+1}.$$

We estimate

$$\sqrt{2b^2+8} \leq \sqrt{2b^2+2} + \frac{3}{\sqrt{2b^2+2}}, \qquad \sqrt{2b^2+2b+5} \leq \sqrt{2b^2+2b+1} + \frac{2}{\sqrt{2b^2+2b+1}},$$

by $\sqrt{x+h} \leq \sqrt{x} + \frac{h}{2\sqrt{x}}$. Therefore

$$R_1 := T_1(b) - T_1(b+1) \geq \frac{2b^2 - 3b + 8}{\sqrt{2b^2+2}} > 0,$$

$$R_2 := T_2(b) - T_2(b+1) \geq \frac{2b+3}{\sqrt{2b^2+2b+1}} > 0.$$

Also, by rationalization

$$R_3 := T_3(b+1) - T_3(b) = \frac{2b+3}{\sqrt{(b+2)^2+1} + \sqrt{(b+1)^2+1}} \leq \frac{2b+3}{2\sqrt{(b+1)^2+1}} \leq \frac{2b+3}{2\sqrt{2b^2+2b+1}}.$$

Thus

$$E_4(b) - E_4(b+1) = R_1 + R_2 - R_3 \ \geq \ \frac{2b^2-3b+8}{\sqrt{2b^2+2}} + \frac{2b+3}{2\sqrt{2b^2+2b+1}} > 0.$$

We omit the second part of the proof, as it can be established in a similar manner to the first part. □

Lemma 3.9. *Let $n \geq 7$ and put $S = n-2$. Fix $d = 4$ and set*

$$(m_0, m_1, m_2, m_3, m_4) = (1, m_1, m_2, m_3, 1), \qquad m_i \geq 1, \qquad m_1 + m_2 + m_3 = S.$$

If m_2 is fixed and $m_1 + m_3 = S - m_2$, define for $x \in [1, S - m_2 - 1]$:

$$m_1 = x, \qquad m_3 = S - m_2 - x.$$

Then, for the function $E_4(x) = T_1(x) + T_2(x) + T_3(x) + T_4(x)$,
where

$$T_1(x) = x\sqrt{(1+m_2)^2 + x^2},$$
$$T_2(x) = m_2 x\sqrt{(1+m_2)^2 + (S-m_2)^2},$$
$$T_3(x) = m_2(S-m_2-x)\sqrt{(S-m_2)^2 + (m_2+1)^2},$$
$$T_4(x) = (S-m_2-x)\sqrt{(m_2+1)^2 + (S-m_2-x)^2},$$

it follows that $\max_{x\in[1,\,S-m_2-1]} E_4(x) \in \{E_4(1),\ E_4(S-m_2-1)\}$. *In other words, the maximum value of* $E_4(x)$ *on the interval* $[1,\ S-m_2-1]$ *is attained only at one of the two endpoints. These endpoints correspond to the parameter pairs* $(m_1, m_3) = (1,\ S-m_2-1)$ *or* $(m_1, m_3) = (S-m_2-1,\ 1)$.

Proof. We first observe that T_2 and T_3 are linear functions of x, and are therefore convex.
Now note that

$$T_1(x) = h_{1,(1+m_2)^2,0}(x), \qquad T_4(x) = l_{1,(1+m_2)^2,0,S-m_2}(x),$$

so both T_1 and T_4 are strictly convex on $[1, S-m_2-1]$, according to Lemma 2.6. Therefore $E_4(x)$ is the sum of two strictly convex and two affine functions, which is strictly convex.

By Lemma 2.5, a strictly convex function on a closed interval attains its maximum only at the endpoints. Thus

$$\max_{x\in[1,S-m_2-1]} E_4(x) \in \{E_4(1), E_4(S-m_2-1)\},$$

which completes the proof. □

According to Lemma 3.9, we can conclude that, for $d = 4$, the maximal value of E can be found among the tuples of the form $(1, m_1, m_2, m_3, 1)$, where either $m_1 = 1$ or $m_3 = 1$. Due to symmetry, we may assume, without loss of generality, that $m_3 = 1$.

For $d = 4$ put $(m_0, m_1, m_2, m_3) = (1, S-t, t, 1, 1)$ with $S = n-2$, and define

$$E_4(t) := E_4(1, S-t, t, 1, 1), \qquad t \in [2, S-2].$$

Theorem 3.10. *For every integer* $n \geq 7$, *the maximum value of* $E_4(t)$ *is attained at* $t = \lceil (n-3)/2 \rceil$.

Proof. The main idea is to show that the derivative $E_4'(t)$ changes sign exactly once near the midpoint:

- $E_4'(t) > 0$ for $t \leq \dfrac{n-3}{2} - 1$ (so E_4 is increasing for $t \leq \dfrac{n-3}{2} - 1$), and
- $E_4'(t) < 0$ for $t \geq \dfrac{n-3}{2} + 1$ (so E_4 is decreasing for $t \geq \dfrac{n-3}{2} + 1$).

From these monotonicity properties, it follows that the maximum value over the integer points $1 < t < n-3$ is attained at the integer closest to the midpoint of the interval. In particular, the maximum is reached at $t = \lceil (n-3)/2 \rceil$.

To implement this idea we differentiate the three summands

$$T_1(t) = (n-3-t)\sqrt{(t+1)^2 + (n-3-t)^2}, \qquad T_2(t) = (n-2-t)t\sqrt{(t+1)^2 + (n-2-t)^2},$$

$$T_3(t) = \sqrt{(t+1)^2 + 1},$$

and use the resulting final expressions:

$$\begin{aligned} T_1'(t) &= \frac{N_1(t)}{D_1(t)}, \qquad N_1(t) = -4t^2 + (5n-18)t - 2n^2 + 13n - 22, \\ D_1(t) &= \sqrt{(t+1)^2 + (n-3-t)^2} \end{aligned}$$

$$T_2'(t) = \frac{N_2(t)}{D_2(t)},$$
$$N_2(t) = -6t^3 + (9n-23)t^2 + (-5n^2 + 23n - 28)t + n^3 - 6n^2 + 13n - 10,$$
$$D_2(t) = \sqrt{(t+1)^2 + (n-2-t)^2},$$

$$T_3'(t) = \frac{t+1}{\sqrt{(t+1)^2+1}}.$$

The signs of these pieces are then analyzed as follows.

The quadratic numerator $N_1(t)$ satisfies

$$N_1(t) \le 0 \quad \text{for all real } t \quad (\text{indeed } N_1^{\max} = -\tfrac{7}{16}(n-2)^2 \le 0),$$

according to Lemma 3.3, hence $T_1'(t) \le 0$ for all t.

Hence, by Lemma 3.4, we conclude that

$$t \le \frac{n-3}{2} \implies T_2'(t) = \frac{N_2(t)}{D_2(t)} > 0, \qquad t \ge \frac{n-3}{2} + 1 \implies T_2'(t) = \frac{N_2(t)}{D_2(t)} < 0.$$

Finally $T_3'(t) = \dfrac{t+1}{\sqrt{(t+1)^2+1}} > 0$ for all t.

We now distinguish two cases:

- For $n-3 \ge t \ge (n-3)/2 + 1$, we have that both $T_1'(t)$ and $T_2'(t)$ are negative, and although $T_3'(t) > 0$, it is too small to compensate. Hence, the derivative of E_4 can be expressed as a single fraction:

$$\begin{aligned} E_4'(t) &= \frac{N_1(t)D_2(t)\sqrt{(t+1)^2+1} + N_2(t)D_1(t)\sqrt{(t+1)^2+1} + (t+1)D_1(t)D_2(t)}{D_1(t)D_2(t)\sqrt{(t+1)^2+1}} \\ &= \frac{N_2(t)D_1(t)\sqrt{(t+1)^2+1} + D_2(t)(N_1(t)\sqrt{(t+1)^2+1} + (t+1)D_1(t))}{D_1(t)D_2(t)\sqrt{(t+1)^2+1}}. \end{aligned}$$

  Since $N_1, N_2 > 0$ and $D_1, D_2 > 0$, to prove that $E_4'(t) < 0$ it is sufficient to show that $N_1(t)\sqrt{(t+1)^2+1} + (t+1)D_1(t) < 0$. Moreover, using the inequality $\sqrt{(t+1)^2+1} > t+1$, we have

$$\sqrt{(t+1)^2+1}\,N_1(t) + (t+1)\,D_1(t) < (t+1)\,N_1(t) + (t+1)\,D_1(t) = (t+1)\big(N_1(t) + D_1(t)\big).$$

  Therefore, it is sufficient to prove that $|N_1(t)| > D_1(t)$, which ensures that the sum is negative and hence $E_4'(t) < 0$.

  Indeed, for $(n-3)/2 + 1 \le t < n-3$ we have $t+1 > 0$ and $n-3-t > 0$, hence by $\sqrt{a^2+b^2} < a+b$ for $a, b \ge 0$, $D_1(t) < (t+1) + (n-3-t) = n-2$. Furthermore, according to Lemma 3.3, it holds that $|N_1(t)| = -N_1(t) \ge \frac{7}{16}(n-2)^2$. If $n \ge 5$, then $\frac{7}{16}(n-2)^2 > (n-2)$; therefore

$$|N_1(t)| - D_1(t) > \frac{7}{16}(n-2)^2 - (n-2) > 0.$$

- For $2 \le t \le (n-3)/2$, $T_2'(t) \ge 0$ and $T_3'(t) > 0$, while $T_1'(t) \le 0$.

  The derivative of E_4 can be expressed as follows:

$$E_4'(t) = \frac{\frac{D_2(t)}{D_1(t)} N_1(t) + N_2(t)}{D_2(t)} + T_3'(t).$$

  Since $D_1(t) > 0$, $D_2(t) > 0$, and $N_1(t) < 0$, it follows from Lemma 3.5 that $\frac{D_2(t)}{D_1(t)} N_1(t) > \frac{6}{5} N_1(t)$.

  Therefore, we obtain

$$E_4'(t) > \frac{6\,N_1(t) + 5N_2(t)}{5\,D_2(t)} + T_3'(t)$$

  From Lemma 3.6, it directly follows that $E_4'(t) > 0$ for $2 \le t \le (n-3)/2 - 1$.

  Combining this sign information, we conclude that $E_4(t)$ is increasing for $t \le (n-3)/2 - 1$ and decreasing for $t \ge (n-3)/2 + 1$.

  The maximum among integer values of t occurs within the following sets:

  - For even n: $t \in \{\frac{n-3}{2} - 1,\ \frac{n-3}{2},\ \frac{n-3}{2} + 1\}$.

  - For odd n: $t \in \{\frac{n-2}{2} - 2,\ \frac{n-2}{2} - 1,\ \frac{n-2}{2},\ \frac{n-2}{2} + 1,\ \frac{n-2}{2} + 2\}$.

  According to Lemmas 3.7 and 3.8, the function E_4 attains its maximum over the integer values of t satisfying $1 < t < n-3$ at $t = \left\lceil \frac{n-3}{2} \right\rceil$, as claimed.

□

In that way, the following statement is proved:

Corollary 3.11. *Let $G = [V_0, V_1, V_2, V_3, V_4] \in \mathcal{B}(n, 4)$ be the connected graph with the maximal Sombor index. Then $|V_0| = |V_3| = |V_4| = 1$, $|V_1| = \lceil \frac{n-3}{2} \rceil$ and $|V_2| = \lfloor \frac{n-3}{2} \rfloor$, i.e. $G = [1, \lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor, 1, 1]$.*

Remark 3.12. *If we define*

$$E_d^1(m_0, \ldots, m_d) = \sum_{k=1}^{d} T_k, \tag{3}$$

where

$$T_1 = m_0 m_1 \sqrt{(m_0 + m_2)^2 + m_1^2},$$
$$T_k = m_{k-1} m_k \sqrt{(m_{k-2} + m_k)^2 + (m_{k-1} + m_{k+1})^2}, \quad 2 \le k \le d-1,$$
$$T_d = m_{d-1} m_d \sqrt{(m_{d-2} + m_d)^2 + (m_{d-1} + 1)^2},$$

then it is evident that the same reasoning applied in the analysis of the function E for the case $d = 4$ with $m_0 = m_d = 1$ and $\sum_{i=0}^{d} m_i = S$ can be extended here. In particular, one can show that the maximum of E^1 is attained at

$$(m_0, m_1, m_2, m_3, m_4) = \left(1, 1, \lceil \tfrac{S-3}{2} \rceil, \lfloor \tfrac{S-3}{2} \rfloor, 1\right).$$

3.2. Bipartite Graphs of Prescribed Order and Higher Diameter $d \geq 5$

Lemma 3.13. *Let $d \geq 5$, $m_0 = m_d = 1$, and $\sum_{k=0}^{d} m_k = n$. Define the function $E_d(m_0, \ldots, m_d)$ as given in equation (2). Let $1 \leq i < j \leq d-1$ be indices such that $j - i \geq 3$. Fix all variables m_k, $k = 0, 1, \ldots, d$, except m_i and m_j, and define*

$$m_j = S - m_i, \quad \text{where} \quad S = n - \sum_{\ell \neq i,j} m_\ell.$$

Define the one-variable function

$$g(x) := E_d(\ldots, m_{i-1}, x, m_{i+1}, \ldots, m_{j-1}, S - x, m_{j+1}, \ldots).$$

Then $g(x)$ is strictly convex on $[1, S-1]$.

Proof. We distinguish three cases for the indices i and j:

Case 1: $i = 1$, $j = d-1$. Here, m_1 appears in T_1, T_2, T_3 and m_{d-1} in T_{d-2}, T_{d-1}, T_d. All other T_k are constant. Explicitly, for $d \geq 6$, we obtain that

$$\begin{aligned}
T_1(x) &= h_{m_0,(m_0+m_2)^2,0}(x),\\
T_2(x) &= h_{m_2,(m_0+m_2)^2,m_3}(x),\\
T_3(x) &= k_{m_2m_3,(m_2+m_4)^2,m_3}(x),\\
T_{d-2}(x) &= k_{m_{d-3}m_{d-2},(m_{d-4}+m_{d-2})^2,m_{d-3}}(S-x),\\
T_{d-1}(x) &= l_{m_{d-2},(m_{d-2}+m_d)^2,m_{d-3}}(x),\\
T_d(x) &= l_{1,(m_{d-2}+m_d)^2,0}(x).
\end{aligned}$$

For $d = 5$, observe that T_2 is a linear function of x, and therefore it is convex.

On the other hand, in this case we have $T_3(x) = T_{d-2}(x) = s_{m_2\,m_3,m_3,m_2,S}(x)$, which is also convex.

Case 2: $i = 1$, $j < d-1$. Here, m_1 appears in T_1, T_2, T_3, and m_j appears in $T_{j-1}, T_j, T_{j+1}, T_{j+2}$. All other T_k are constant. Explicitly,

$$\begin{aligned}
T_1(x) &= h_{m_0,(m_0+m_2)^2,0}(x),\\
T_2(x) &= h_{m_2,(m_0+m_2)^2,m_3}(x),\\
T_3(x) &= k_{m_2m_3,(m_2+m_4)^2,m_3}(x),\\
T_{j-1}(x) &= k_{m_{j-2}m_{j-1},(m_{j-3}+m_{j-1})^2,m_{j-2}}(S-x),\\
T_j(x) &= l_{m_{j-1},(m_{j-1}+m_{j+1})^2,m_{j-2}}(x),\\
T_{j+1}(x) &= l_{m_{j+1},(m_{j-1}+m_{j+1})^2,m_{j+2}}(x),\\
T_{j+2}(x) &= k_{m_{j+1}m_{j+2},(m_{j+1}+m_{j+3})^2,m_{j+2}}(S-x).
\end{aligned}$$

Case 3: $i > 1$, $j < d-1$. Then m_i appears in $T_{i-1}, T_i, T_{i+1}, T_{i+2}$ and m_j in $T_{j-1}, T_j, T_{j+1}, T_{j+2}$. If $|i-j| \geq 4$, the sets of affected summands are disjoint. Explicitly,

$$\begin{aligned}
T_{i-1}(x) &= k_{m_{i-2}m_{i-1},(m_{i-3}+m_{i-1})^2,m_{i-2}}(x),\\
T_i(x) &= h_{m_{i-1},(m_{i-1}+m_{i+1})^2,m_{i-2}}(x),\\
T_{i+1}(x) &= h_{m_{i+1},(m_{i-1}+m_{i+1})^2,m_{i+2}}(x),\\
T_{i+2}(x) &= k_{m_{i+1}m_{i+2},(m_{i+1}+m_{i+3})^2,m_{i+2}}(x),\\
T_{j-1}(x) &= k_{m_{j-2}m_{j-1},(m_{j-3}+m_{j-1})^2,m_{j-2}}(S-x),\\
T_j(x) &= l_{m_{j-1},(m_{j-1}+m_{j+1})^2,m_{j-2}}(x),\\
T_{j+1}(x) &= l_{m_{j+1},(m_{j-1}+m_{j+1})^2,m_{j+2}}(x),\\
T_{j+2}(x) &= k_{m_{j+1}m_{j+2},(m_{j+1}+m_{j+3})^2,m_{j+2}}(S-x).
\end{aligned}$$

If $|i-j|=3$, then we obtin that T_{i+1} is a linear function of x, and therefore it is convex. On the other hand, in this case we have $T_{i+2}(x)=T_{j-2}(x)=s_{m_{i+1}\,m_{i+2},m_{i+2},m_{i+1},S}(x)$, which is also convex.

Let us observe that the case $i>1$, $j=d-1$ is symmetric to the Case 2. By Lemma 2.6, each of the previously exposed terms is a convex function. Therefore, $g(x)$ is the sum of strictly convex functions, and hence it is itself strictly convex on $[1,S-1]$. □

Lemma 3.14. *Let $d\geq 5$, $m_0=m_d=1$, and $\sum_{k=0}^{d} m_k=n$. Let $E_d(m_0,\ldots,m_d)$ be the expression given by (2), as in Lemma 3.13. Fix indices i and j, $1\leq i<j\leq d-1$, with $j=i+2$, and fix all variables except m_i and m_{i+2}. Put*

$$m_i=x,\qquad m_{i+2}=S-x,$$

where $x\in[1,S-1]$ and $S=n-\sum_{\ell\neq i,i+2} m_\ell$. Define

$$g(x):=E_d(\ldots,m_{i-1},x,m_{i+1},S-x,m_{i+3},\ldots).$$

Then g is strictly convex on $[1,S-1]$.

Proof. Only the summands $T_{i-1},T_i,T_{i+1},T_{i+2},T_{i+3},T_{i+4}$ can depend on x after the substitution $m_i=x$, $m_{i+2}=S-x$; all other T_k are constant in x.

We write each affected summand explicitly and identify its canonical form.

1. If $i\geq 3$, then $T_{i-1}(x)=m_{i-2}m_{i-1}\sqrt{(m_{i-3}+m_{i-1})^2+(m_{i-2}+x)^2}$. Hence

$$T_{i-1}(x)=k_{\alpha_1,A_1,B_1}(x),\quad \alpha_1=m_{i-2}m_{i-1},\ A_1=(m_{i-3}+m_{i-1})^2,\ B_1=m_{i-2}.$$

If $i=2$, then $T_{i-1}(x)=h_{m_0,(m_0+m_2)^2,0}(x)$.

2. If $i\geq 2$, then $T_i(x)=m_{i-1}\,x\,\sqrt{(m_{i-2}+x)^2+(m_{i-1}+m_{i+1})^2}$. Hence

$$T_i(x)=h_{\alpha_2,A_2,B_2}(x),\quad \alpha_2=m_{i-1},\ A_2=(m_{i-1}+m_{i+1})^2,\ B_2=m_{i-2}.$$

If $i=1$, then $T_i(x)=h_{m_0,(m_0+m_2)^2,0}(x)$.

3. $T_{i+1}(x)=x\,m_{i+1}\sqrt{(m_{i-1}+m_{i+1})^2+(x+m_{i+2})^2}$. With $m_{i+2}=S-x$ the sum inside the radical becomes $x+(S-x)=S$, so the radical is constant. Thus

$$T_{i+1}(x)=C_{i+1}x$$

is linear in x, where $C_{i+1}=m_{i+1}\sqrt{(m_{i-1}+m_{i+1})^2+S^2}>0$.

4. Since $i+2=j\leq d-1$, it follows that $i\leq d-3$. Therefore, we obtain $T_{i+2}(x)=m_{i+1}(S-x)\sqrt{S^2+(m_{i+1}+m_{i+3})^2}$. Hence

$$T_{i+2}(x)=C_{i+2}(S-x)$$

is linear in x, with $C_{i+2}=m_{i+1}\sqrt{S^2+(m_{i+1}+m_{i+3})^2}>0$.

5. If $i\leq d-4$, then $T_{i+3}(x)=m_{i+2}m_{i+3}\sqrt{(m_{i+1}+m_{i+3})^2+(m_{i+2}+m_{i+4})^2}$. With $m_{i+2}=S-x$ this becomes

$$T_{i+3}(x)=\ell_{\alpha_5,A_5,B_5}(x),$$

where $\alpha_5=m_{i+3},\ A_5=(m_{i+1}+m_{i+3})^2,\ B_5=m_{i+4}$.

If $i=d-3$, then $T_{i+3}(x)=m_d\,(S-x)\sqrt{(m_{d-2}+m_d)^2+(S-x)^2}=l_{m_d,(m_{d-2}+m_d)^2,0}$.

6. If $i \le d-5$, then $T_{i+4}(x) = m_{i+3}m_{i+4}\sqrt{(m_{i+2}+m_{i+4})^2+(m_{i+3}+m_{i+5})^2}$. With $m_{i+2} = S - x$ this equals

$$T_{i+4}(x) = k_{\alpha_6,A_6,B_6}(S-x),$$

with $\alpha_6 = m_{i+3}m_{i+4},\ A_6 = (m_{i+3}+m_{i+5})^2,\ B_6 = m_{i+4}$. Since $t \mapsto k_{\alpha_6,A_6,B_6}(t)$ is strictly convex, the composition $x \mapsto k_{\alpha_6,A_6,B_6}(S-x)$ is convex as well.

Moreover, if $i = d-4$, then

$$T_{i+4}(x) = m_{d-1}\, m_d \sqrt{S-x+m_d)^2+m_{d-1}^2} = l_{m_d,(m_{d-2}+m_d)^2,0} = k_{m_{d-1}\, m_d, m_{d-1}^2, m_d}(S-x).$$

According to Lemma 2.6, each of the canonical functions $h_{\alpha,A,B}, k_{\alpha,A,B}, \ell_{\alpha,A,B,S}$ is strictly convex on $[1, S-1]$. Linear functions, appearing in items 3 and 4, are also convex. Therefore each of the six summands above is a convex or strictly convex function in x, and hence their sum $g(x)$ is strictly convex on $[1, S-1]$. This proves the lemma. □

For $d = 5$ put $(m_0, m_1, m_2, m_3, m_4, m_5) = (1, 1, x, S-x, 1, 1)$ with $S = n-4$, and define

$$G(x) := E_5(1, 1, x, S-x, 1, 1), \qquad x \in [2, S-2],$$

where the expression E_5 defined as in (2).

Theorem 3.15. *For $n \ge 8$ the function G attains its maximum at*

$$x = \frac{S}{2} = \frac{n-4}{2}.$$

Proof. With the substitution above, we obtain that

$$\begin{aligned}
T_1 &= \sqrt{(x+1)^2+1},\\
T_2 &= x\sqrt{(x+1)^2+(S+1-x)^2},\\
T_3 &= x(S-x)\sqrt{(x+1)^2+(S+1-x)^2},\\
T_4 &= (S-x)\sqrt{(x+1)^2+(S+1-x)^2},\\
T_5 &= \sqrt{(S+1-x)^2+1},
\end{aligned}$$

hence

$$G(x) = \sqrt{(x+1)^2+1} + \sqrt{(S+1-x)^2+1} + \big(S + x(S-x)\big)R(x),$$

where $R(x) = \sqrt{(x+1)^2+(S+1-x)^2}$ and

$$T_2 + T_3 + T_4 = \big(S + x(S-x)\big)R(x).$$

Step 1. By Cauchy–Schwarz, it holds that

$$\sqrt{(x+1)^2+1} + \sqrt{(S+1-x)^2+1} \le \sqrt{2}\sqrt{(x+1)^2+(S+1-x)^2+2}.$$

Thus

$$G(x) \le \sqrt{f(x)} + \sqrt{g(x)},$$

with

$$f(x) = 2\big((x+1)^2+(S+1-x)^2+2\big), \qquad g(x) = \big(S + x(S-x)\big)^2\big((x+1)^2+(S+1-x)^2\big).$$

Let $c = S/2$. The map $x \mapsto S-x$ swaps $(x+1)$ and $(S+1-x)$, so both bounds are equalities at $x = c$. Using the concavity inequality

$$\sqrt{y} \le \sqrt{y_0} + \frac{y-y_0}{2\sqrt{y_0}},$$

applied at $y_0 = f(c)$ and $y_0 = g(c)$, define

$$T(x) = \sqrt{f(c)} + \sqrt{g(c)} + \frac{f(x) - f(c)}{2\sqrt{f(c)}} + \frac{g(x) - g(c)}{2\sqrt{g(c)}}.$$

Then

$$G(x) \le \sqrt{f(x)} + \sqrt{g(x)} \le T(x) \quad \text{for all } x, \qquad T(c) = G(c).$$

Step 2. Write $x = c + y$ and set $z = y^2$. A direct simplification gives

$$f(c) = n^2 - 4n + 8 = (n-2)^2 + 4, \qquad \sqrt{g(c)} = \frac{n(n-2)(n-4)}{4\sqrt{2}},$$

and

$$f'(c+y) = 8y, \qquad g'(c+y) = -\,y\left(K - z\right)\left(n^2 - 4n + 8 + 12z\right),$$

where $K = \dfrac{n(n-4)}{4}$. Consequently

$$T'(c+y) = \frac{f'(c+y)}{2\sqrt{f(c)}} + \frac{g'(c+y)}{2\sqrt{g(c)}} = y\,\Phi_n(z),$$

with

$$\Phi_n(z) = \frac{4}{\sqrt{(n-2)^2+4}} - \frac{2\sqrt{2}}{n(n-2)(n-4)}\,(K - z)\left(n^2 - 4n + 8 + 12z\right).$$

This is a convex quadratic in z (its z^2–coefficient equals $6/\sqrt{g(c)} > 0$).

Step 3. On $x \in [1, S-1]$ we have $y \in [-\frac{S-2}{2}, \frac{S-2}{2}]$, hence

$$z \in \left[0,\ z_{\max}\right], \qquad z_{\max} = \left(\frac{S-2}{2}\right)^2 = \left(\frac{n-6}{2}\right)^2.$$

By convexity, $\max_{z\in[0,z_{\max}]} \Phi_n(z) = \max\{\Phi_n(0), \Phi_n(z_{\max})\}$.

First,

$$\Phi_n(0) = \frac{4}{\sqrt{(n-2)^2+4}} - \frac{\sqrt{2}}{2} \cdot \frac{n^2 - 4n + 8}{n-2} \le 0 \qquad (n \ge 6),$$

since $\sqrt{(n-2)^2+4} \ge n-2$ and $n^2 - 4n + 8 \ge 20$ at $n = 6$.

Second, using $K - z_{\max} = 2n - 9$ and $n^2 - 4n + 8 + 12z_{\max} = 4(n^2 - 10n + 29)$,

$$\Phi_n(z_{\max}) = \frac{4}{\sqrt{(n-2)^2+4}} - \frac{8\sqrt{2}}{n(n-2)(n-4)}\,(2n-9)\,(n^2 - 10n + 29) \le 0 \qquad (n \ge 6),$$

because $\sqrt{(n-2)^2+4} \ge n-2$, $(2n-9) > 0$, and $(n^2 - 10n + 29) = (n-5)^2 + 4 > 0$.

Therefore $\Phi_n(z) \le 0$ on $[0, z_{\max}]$, and hence

$$T'(c+y) = y\,\Phi_n(y^2) \begin{cases} > 0, & y < 0, \\ = 0, & y = 0, \\ < 0, & y > 0, \end{cases}$$

so T is strictly increasing on $[1, c)$ and strictly decreasing on $(c, S-1]$.

Step 4. Since $G(x) \le T(x)$ for all x and $G(c) = T(c)$, and T has its unique maximum at $x = c$, we get

$$G(x) \le T(x) \le T(c) = G(c) \qquad (x \in [1, S-1]).$$

Thus G attains its maximum at $x = \dfrac{S}{2} = \dfrac{n-4}{2}$. □

Remark 3.16. *It is evident that the same reasoning applied in the analysis of the function E for the case $d = 5$ with $m_0 = m_d = 1$ and $\sum_{i=0}^{d} m_i = S$ can be extended here. In particular, one can show that the maximum of E^1 is attained at*

$$(m_0, m_1, m_2, m_3, m_4, m_5) = \left(1, 1, \lceil \tfrac{S-3}{2} \rceil, \lfloor \tfrac{S-3}{2} \rfloor, 1, 1\right).$$

Theorem 3.17. *Let $E = E_d(m_0, \dots, m_d)$ be the expression defined as in (2), with $d \geq 5$, $m_0 = m_d = 1$ and $m_i \geq 1$, for all $1 \leq i \leq d-1$, and suppose the total sum of variables m_0, m_i, m_d, $1 \leq i \leq d-1$, is fixed:*

$$\sum_{i=0}^{d} m_i = n.$$

Then the maximum of E is attained for the following configuration

$$m_0 = m_1 = \cdots = m_{k-1} = m_{k+2} = \cdots = m_{d-1} = m_d = 1, \quad m_k + m_{k+1} = n - d + 1,$$

for some index $k \in \{1, \dots, d-2\}$.

Proof. We prove the statement by iterative application of Lemma 2.5.

Step 1 (First iteration): Consider the variables m_1 and m_{d-1}. Fix all other variables and define the one-variable function

$$g_1(x) = E_d(1, x, m_2, \dots, m_{d-2}, S - x, 1),$$

where $S = n - 2 - \sum_{i=2}^{d-2} m_i$ is the sum of the two free variables. By Lemma 3.13, g_1 is strictly convex on $[1, S-1]$ and hence, according to Lemma 2.5, it attains its maximum at an endpoint of this interval. Therefore, at the maximum of E, at least one of m_1 and m_{d-1} equals 1.

Step 2 (Iterative propagation): Suppose that after r iterations we have established

$$m_1 = \cdots = m_i = 1, \quad m_j = \cdots = m_{d-1} = 1,$$

for some $i < j$ with $j - i \geq 5$. Consider the next pair (m_{i+1}, m_{j-1}). Define

$$g_{r+1}(x) = E_d(\dots, m_{i-1}, m_i, x, \dots, m_{j-2}, S' - x, m_j, \dots),$$

where $S' = n - (i+2) - (d-j) - \sum_{\ell=i+2}^{j-2} m_\ell$ is the sum of the two free variables. Again, by Lemma 3.13, g_{r+1} is strictly convex in the interval $[1, S'-1]$, and, according to Lemma 2.5, its maximum is attained at an endpoint of this interval. Hence, either $m_{i+1} = 1$ or $m_{j-1} = 1$. This extends the region of variables fixed to 1 by at least one more index.

Step 3 (Termination): Repeat the propagation until $j - i = 2$, and then apply Lemma 3.14; at this point, only two consecutive inner variables remain unfixed. Let these be m_k and m_{k+1}. Then, by the total sum constraint,

$$m_k + m_{k+1} = n - 2 - \sum_{\ell \neq k, k+1} m_\ell = n - d + 1.$$

All other variables are fixed to 1, and exactly two consecutive inner variables sum to $n - d + 1$. Therefore, the configuration described in the statement is the global maximizer of E. □

Theorem 3.18. *Let $d \geq 3$ and $n \geq d + 1$. The maximum of the expression*

$$E_d(m_0, \dots, m_d) = \sum_{k=1}^{d} T_k,$$

defined as (2), under the constraints

$$m_0 = m_d = 1, \quad m_i \in \mathbb{N}, \quad \sum_{i=0}^{d} m_i = n,$$

is attained precisely when all variables are equal to 1 *except two consecutive ones, say* m_k, m_{k+1}, *for some* $1 \leq k \leq d-2$, *and these two satisfy*

$$m_k + m_{k+1} = n - d + 1, \qquad m_k \in \left\{ \left\lfloor \frac{n-d+1}{2} \right\rfloor, \left\lceil \frac{n-d+1}{2} \right\rceil \right\}.$$

Proof. We proceed by induction on d.

Base cases $3 \leq d \leq 7$.

If $d \in \{3, 4\}$, the statement follows directly from Corollaries 3.2 and 3.11.

According to Theorem 3.17, for $d = 5$, the maximum value of E must occur for a tuple of the form $(1, m_1, m_2, 1, 1, 1)$ or $(1, 1, m_2, m_3, 1, 1)$. Furthermore, Theorem 3.15 directly implies that this statement holds in the case of the latter tuple. For the first tuple, we obtain $E_5(1, x, n-4-x, 1, 1, 1) = E_4^1(1, x, n-4-x, 1, 1) + \sqrt{5}$. It is evident that the statement of the theorem follows directly by applying Remark 3.12.

For $d = 6$, the following equalities hold:

$$\begin{aligned} E_6(1, x, n-5-x, 1, 1, 1, 1) &= E_5(1, x, n-5-x, 1, 1, 1) + 2\sqrt{2}, \\ E_6(1, 1, x, n-5-x, 1, 1, 1) &= E_5^1(1, 1, x, n-5-x, 1, 1) + \sqrt{5}. \end{aligned}$$

According to the analysis presented in the preceding paragraph and in Remark 3.16, the maximum of the right-hand side in both equalities is attained for $x = \left\lfloor \frac{n-5}{2} \right\rfloor$. This implies that for the same value of x, the maximum of the left-hand side expressions is also attained.

For $d = 7$, the following equalities hold:

$$\begin{aligned} E_7(1, x, n-6-x, 1, 1, 1, 1, 1) &= E_6(1, x, n-6-x, 1, 1, 1, 1) + 2\sqrt{2}, \\ E_7(1, 1, x, n-6-x, 1, 1, 1, 1) &= E_6(1, 1, x, n-6-x, 1, 1, 1) + 2\sqrt{2}, \\ E_7(1, 1, 1, x, n-6-x, 1, 1, 1) &= E_6^1(1, 1, 1, x, n-6-x, 1, 1) + \sqrt{5}. \end{aligned}$$

According to the analysis presented in the previous section, the maximum of the right-hand side in each equality is attained when $x = \left\lfloor \frac{n-6}{2} \right\rfloor$. In particular, the maximum of $E_6^1(1, 1, 1, x, n-6-x, 1, 1)$ is attained at $x = \left\lfloor \frac{n-6}{2} \right\rfloor$ if and only if the maximum of $E_6(1, 1, 1, x, n-6-x, 1, 1)$ is attained at the same value of x. Therefore, it follows that for this value of x, the maxima of the left-hand side expressions are also attained.

Induction Hypothesis. Assume that the statement holds for some $d - 1 \geq 7$. In other words, for any admissible n', the maximizer of E_{d-1} is obtained when all entries are equal to 1, except for two consecutive entries whose sum is $n' - (d-1) + 1$. Moreover, these two entries are chosen to be as balanced as possible, that is, for $x = \lfloor (n' - d + 2)/2 \rfloor$.

Induction step.

Firstly, we may exploit the symmetry (reflection) of the chain by applying the index reversal

$$i \mapsto d - i,$$

which transforms the right-end pair (m_i, m_{i+1}) into the left-end pair (m_{d-i-1}, m_{d-i}) of the reflected chain. Therefore, without loss of generality, we may assume that $k+1 \leq \frac{d+1}{2}$. Since $d > 7$, we observe that $\frac{d+1}{2} < d-3$. Consequently, it follows that $k + 1 < d - 3$. From this inequality we deduce that $m_{d-3} = m_{d-2} = m_{d-1} = 1$.

By definition,

$$\begin{aligned} E_d(m_0,\dots,m_d) &= E_{d-1}(m_0,\dots,m_{d-1}) + m_{d-1}m_d\sqrt{(m_{d-2}+m_d)^2+m_{d-1}^2} \\ &+ m_{d-2}m_{d-1}\sqrt{(m_{d-3}+m_{d-1})^2+(m_{d-2}+m_d)^2} \\ &- m_{d-2}m_{d-1}\sqrt{(m_{d-3}+m_{d-1})^2+m_{d-2}^2} \\ &= E_{d-1}(m_0,\dots,m_{d-1})+2\sqrt{2}. \end{aligned}$$

Let $n' := n-1$. Removing the last variable $m_d = 1$ yields a reduced number of terms in the expression of length $d-1$ whose total sum of entries equals n'. The induction hypothesis is to be applied to this reduced chain E_{d-1} (with length $d-1$ and total sum n'). The pair (m_k, m_{k+1}) is strictly inside the reduced chain because the reduced chain has internal indices $1,\dots,d-2$. Hence the induction hypothesis applies directly to E_{d-1} with the same index k. Note also that the target sum for the pair on the reduced chain equals

$$m_k + m_{k+1} = n' - (d'-1) = n-d+1,$$

which is exactly the same value as in the original chain; thus the conclusion of the induction hypothesis transfers unchanged to E_d. □

Proposition 3.19. *Let $d \geq 6$, $t \geq 2$, and let $E(k;t)$ denote the value of the expression defined in (2) when $m_k = m_{k+1} = t$, $1 \leq k \leq d-3$, and every other inner $m_\ell = 1$. Define $\Delta_k(t) := E(k+1;t) - E(k;t)$. Then the following holds:*

1. *If $3 \leq k \leq d-4$, then*

$$\Delta_k(t) = 0 \quad \textit{for all } t > 1.$$

2. *For the leftmost positions $k = 1$ and $k = 2$, when $d \geq 6$, one obtains*

$$\Delta_1(t) = E(2;t) - E(1;t) = t\sqrt{(t+1)^2+t^2} - \sqrt{(t+1)^2+1} > 0,$$

and

$$\Delta_2(t) = E(3;t) - E(2;t) = \sqrt{(t+1)^2+4} - \sqrt{(t+1)^2+1} < 0 \quad (t \geq 2).$$

3. *If $k = d-3$ and $k = d-2$, then it holds that $\Delta_{d-2}(t) = \Delta_1(t)$ and $\Delta_{d-3}(t) = \Delta_2(t)$.*

Proof. All computations are elementary substitutions into the T_r formulas and straightforward cancellations. We give the algebraic derivations case by case.

Case (1) Suppose $3 \leq k \leq d-4$. With the pair at $(k, k+1)$ the only dependent indices are

$$\{k-1, k, k+1, k+2, k+3\},$$

and each of these indices lies strictly inside $\{2,\dots,d-1\}$ so the formula for T_r applies, for $2 \leq r \leq d-1$. Substituting $m_k = m_{k+1} = t$ and $m_i = 1$, $i \notin \{k, k+1\}$ yields

$$\begin{aligned} T_{k-1} &= \sqrt{4+(t+1)^2}, \\ T_k &= t\sqrt{2}\,(t+1), \\ T_{k+1} &= t^2\sqrt{2}\,(t+1), \\ T_{k+2} &= t\sqrt{2}\,(t+1), \\ T_{k+3} &= \sqrt{4+(t+1)^2}. \end{aligned}$$

The shifted pair at $(k+1, k+2)$ produces the same multiset of five terms (just shifted by one index), so $E(k+1;t)$ and $E(k;t)$ are identical and therefore $\Delta_k(t) = 0$.

(2a) Case $k = 1$**.** With the pair at $(1,2)$ the affected terms are those with the indices (for $d \geq 6$) are $1,2,3,4$. Substitution gives

$$E(1;t)\Big|_{\text{affected}} = t\sqrt{(t+1)^2 + t^2} + \sqrt{2}\,(t+1)(t^2+t) + \sqrt{(t+1)^2+4}.$$

For the pair located at $(2,3)$, the affected terms are $1,2,3,4,5$, which results in the following expression for $d \geq 6$:

$$E(2;t)\Big|_{\text{affected}} = \sqrt{(t+1)^2+1} + \sqrt{2}\,(t+1)(t^2+2t) + \sqrt{(t+1)^2+4}.$$

Subtracting gives the formula $\Delta_1(t) = t\sqrt{(t+1)^2+t^2} - \sqrt{(t+1)^2+1} + 2\sqrt{2}$, whence $\Delta_1(t) > 0$ for $t > 1$.

(2b) Case $k = 2$**.** For $d \geq 7$, considering the pair located at $(2,3)$, the five affected indices yield

$$E(2;t)\Big|_{\text{affected}} = \sqrt{(t+1)^2+1} + \sqrt{4+(t+1)^2} + \sqrt{2}\,(t+1)(t^2+2t),$$

while moving the pair to $(3,4)$ yields

$$E(3;t)\Big|_{\text{affected}} = 2\sqrt{4+(t+1)^2} + \sqrt{2}\,(t+1)(t^2+2t).$$

Subtracting gives

$$\begin{aligned}
\Delta_2(t) &= \sqrt{4+(t+1)^2} - \sqrt{1+(t+1)^2} + \sqrt{5} - 2\sqrt{2} \qquad (4)\\
&= \frac{(4+(t+1)^2)-(1+(t+1)^2)}{\sqrt{4+(t+1)^2}+\sqrt{1+(t+1)^2}} + \sqrt{5} - 2\sqrt{2}\\
&= \frac{3}{\sqrt{(t+1)^2+4}+\sqrt{(t+1)^2+1}} + \sqrt{5} - 2\sqrt{2}\\
&< \frac{3}{2(t+1)} + \sqrt{5} - 2\sqrt{2} \quad \text{for } t \geq 2\\
&\leq \frac{3}{6} + \sqrt{5} - 2\sqrt{2} < 0.
\end{aligned}$$

Each left-end formula has a mirror on the right end: replace index r by $d - r$. Thus the stated right-end identities hold. □

Proposition 3.20. *Let $d \geq 6$, $t \geq 2$, and let $E(k;t)$ denote the value of the expression in* (2) *when $m_k = t+1$, $m_{k+1} = t$ for some $1 \leq k \leq d-3$, and every other inner $m_\ell = 1$. Define $\Delta_k(t) := E(k+1;t) - E(k;t)$. Then:*

1. *If $3 \leq k \leq d-4$, then*

$$\Delta_k(t) = 0 \quad \textit{for all } t > 0.$$

2. *For $d \geq 6$,*

$$\Delta_1(t) = E(2;t) - E(1;t) = (t+1)\sqrt{(t+2)^2+(t+1)^2} + \sqrt{(t+2)^2+1} - \sqrt{2}\,(t+1)^2 > 0,$$

and for $d \geq 7$,

$$\Delta_2(t) = E(3;t) - E(2;t) = \sqrt{(t+2)^2+4} - \sqrt{(t+2)^2+1} > 0.$$

3. *By symmetry of the chain,*

$$\Delta_{d-2}(t) = \Delta_1(t) \quad \textit{and} \quad \Delta_{d-3}(t) = \Delta_2(t).$$

Proof. All steps follow by substituting the specified tuple into the T_r formulas and cancelling identical terms.

(1) $3 \le k \le d-4$**.** The only indices whose T_r change when the pair sits at $(k, k+1)$ are $r \in \{k-1, k, k+1, k+2, k+3\}$. With $m_k = t+1$, $m_{k+1} = t$ and all neighbors = 1, one computes

$$\begin{aligned} T_{k-1} &= \sqrt{4 + (t+2)^2}, \\ T_k &= (t+1)\sqrt{(t+2)^2 + (t+1)^2}, \\ T_{k+1} &= t(t+1)\sqrt{(t+1)^2 + (t+2)^2}, \\ T_{k+2} &= t\sqrt{(t+2)^2 + (t+1)^2}, \\ T_{k+3} &= \sqrt{(t+1)^2 + 4}. \end{aligned}$$

Shifting the pair one step to $(k+1, k+2)$ simply shifts this same multiset of five values along the chain (the two square-root arguments are the same two numbers in reversed order), so the partial sums coincide and hence $\Delta_k(t) = 0$.

(2a) $k = 1$**.** For $d \ge 6$ and the pair at $(1, 2)$ we have, on the affected block $r = 1, 2, 3, 4$,

$$E(1;t)\Big|_{\text{aff}} = \underbrace{\sqrt{2}\,(t+1)^2}_{T_1} + \underbrace{t(t+1)R}_{T_2} + \underbrace{tR}_{T_3} + \underbrace{\sqrt{(t+1)^2+4}}_{T_4},$$

where $R := \sqrt{(t+2)^2 + (t+1)^2}$. For the pair at $(2, 3)$ the affected block $r = 1, 2, 3, 4, 5$ yields

$$E(2;t)\Big|_{\text{aff}} = \sqrt{(t+2)^2 + 1} + (t+1)R + t(t+1)R + tR + \sqrt{(t+1)^2 + 4}.$$

Subtracting gives

$$\Delta_1(t) = (t+1)R + \sqrt{(t+2)^2 + 1} - \sqrt{2}\,(t+1)^2 + 2\sqrt{2}.$$

Since $R = \sqrt{(t+2)^2 + (t+1)^2} > \sqrt{(t+1)^2 + (t+1)^2} = \sqrt{2}\,(t+1)$, we get $(t+1)R - \sqrt{2}(t+1)^2 > 0$, hence $\Delta_1(t) > 0$.

(2b) $k = 2$**.** For $d \ge 7$ and $(2, 3)$ we already have the affected sum above. Moving to $(3, 4)$ changes only the two boundary terms, giving

$$E(3;t)\Big|_{\text{aff}} = \sqrt{4 + (t+2)^2} + (t+1)R + t(t+1)R + tR + \sqrt{(t+1)^2 + 4}.$$

Thus, according to inequality (4), we obtain the following inequality $\Delta_2(t) = \sqrt{(t+2)^2 + 4} - \sqrt{(t+2)^2 + 1} + \sqrt{5} - 2\sqrt{2} < 0$.

(3) Reflecting the chain (replace index r by $d - r$) maps $(1, 2)$ to $(d-2, d-1)$ and $(2, 3)$ to $(d-3, d-2)$, preserving the computed differences. Hence $\Delta_{d-2}(t) = \Delta_1(t)$ and $\Delta_{d-3}(t) = \Delta_2(t)$. □

From the two preceding propositions, it follows that E_d, for $d \ge 6$, attains its maximum for tuples of the form $(m_0, \ldots, m_k, m_{k+1}, \ldots, m_d)$, where $m_k = \lceil \frac{n-d+1}{2} \rceil$, $m_{k+1} = \lfloor \frac{n-d+1}{2} \rfloor$, and $m_i = 1$ for all $i \notin \{k, k+1\}$, specifically in the case $k = 2$. The same observation can be straightforwardly demonstrated in the case $d = 5$.

From Corollaries 3.11 and 3.2, together with Theorem 3.18 and Propositions 3.19 and 3.20, we now establish the main theorem. This result provides a complete characterization of all bipartite graphs that attain the maximal Sombor index for a fixed order and diameter.

Theorem 3.21. *Let $G = [V_0, V_1, \ldots, V_d] \in \mathcal{B}(n, d)$ be a connected bipartite graph with the maximal Sombor index. Then:*

- *If $d = 3$, the partitions satisfy $|V_0| = |V_3| = 1$, $|V_1| = \lceil \frac{n-2}{2} \rceil$, and $|V_2| = \lfloor \frac{n-2}{2} \rfloor$.*
- *If $d \ge 4$, then $|V_0| = |V_1| = |V_3| = \cdots = |V_d| = 1$, while $|V_2| = \lceil \frac{n-d+1}{2} \rceil$ and $|V_3| = \lfloor \frac{n-d+1}{2} \rfloor$.*

Conclusion

In summary, we have characterized the bipartite graphs of order n and diameter d that attain the maximum Sombor index. The principal contribution of this work is a structural description of the unique extremal graphs in $\mathcal{B}(n,d)$, obtained by combining new analytical methods with classical extremal graph theory arguments. This result provides a complete solution to the problem of how imposing a diameter constraint influences the maximum possible value of the Sombor index, thereby broadening the understanding of degree-based graph invariants under structural restrictions. A natural direction for further research is to extend this study to broader graph classes. In particular, it would be of interest to investigate the extremal Sombor index of multipartite graphs of a given order and diameter.

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