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ON THE INVERSE PROBLEM OF THE EXPONENTIAL GUTMAN INDEX OF TREES

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Abstract: This paper investigates the extremal behaviour of the exponential Gutman index

$$\mathrm{HGut}(G) = \sum_{uv\in E(G)} \left(2^{d(u)d(v)} + dist(u,v)\right),$$

over the class of trees on n vertices. The path graph $\mathcal{P}_n$ uniquely minimises $\mathrm{HGut}(G)$ among all trees on $n \geqslant 5$ vertices. We identify the balanced double star $DS(\lfloor n/2\rfloor, \lceil n/2\rceil)$ as the unique maximiser, by establishing a sharp upper bound on the degree product of any edge in a tree. A closed form expression is derived for complete binary trees, characterizing extremal graphs, addressing the inverse problem graphs realizing a given value κ. We further establish a lower bound through Jensen's inequality and an upper bound through the Moore bound.

Keywords: Exponential Gutman index, topological indices, extremal graph theory, degree product, threshold graphs, binary trees, Zagreb indices, chemical graph theory.

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1 Introduction

Graph theory provides powerful tools for modeling molecular structures, and topological indices have been widely used for decades to the concept of predict physicochemical properties of chemical compounds. The foundational work in this area includes the Wiener index [21], which correlates well with boiling points of alkanes through the sum of distances between all pairs of vertices in the molecular graph.

Let $G = (V, E)$ be a simple connected graph with $n = |V(G)|$ and $m = |E(G)|$. For vertices $u, v \in V(G)$, let $d(u, v)$ denote the distance (length of a shortest path) between u and v, and let $d(v)$ denote the degree of vertex v. The Wiener index is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v).$$

A natural degree-weighted extension of the Wiener index is the *Gutman index*, introduced by Gutman in 1994 [7] as a refinement of the Schultz index [18]. It is given by

$$\mathrm{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u)\, d_G(v)\, \mathrm{dist}(u, v). \tag{1}$$

Furthermore; see papers [6, 7, 15] In recent years, various exponential versions of classical topological indices (such as the exponential Wiener index) have attracted considerable attention. Following this direction, we introduce the *Exponential Gutman index* $\mathrm{HGut}(G)$, defined as

$$\mathrm{HGut}(G) = \sum_{uv \in E(G)} \left(2^{d(u)d(v)} + \mathrm{dist}(u, v)\right). \tag{2}$$

Note that for every edge uv, we have $\mathrm{dist}(u, v) = 1$, so the definition can equivalently be written as

$$\mathrm{HGut}(G) = \sum_{uv \in E(G)} 2^{d(u)d(v)} + m.$$

In this paper, we consistently use definition (2). Several generalized variants of the Gutman index have also been studied. One common generalization takes the form

$$\mathrm{Gut}_{\alpha,\beta}(T) = \sum_{\{u,v\} \subseteq V(T)} [d_T(u) d_T(v)]^{\alpha} [\mathrm{dist}_T(u, v)]^{\beta}, \quad \alpha, \beta \in \mathbb{R},$$

for trees T. Extremal results for such indices on trees are known under various constraints on α and β [3, 1, 16, 8].

The Zagreb indices, initially introduced in [9] and [10] in 1972 and 1974, represent some of the earliest and most extensively investigated degree-based topological indices [19]. For a simple connected graph $G = (V, E)$, these indices are defined as

$$M_1(G) = \sum_{v \in V} d_G(v)^2 \quad , \quad M_2(G) = \sum_{\{u,v\} \in E} d_G(u) \cdot d_G(v).$$

The main objective of the present paper is to investigate the exponential Gutman index $\mathrm{HGut}(G)$, with a focus on deriving sharp extremal bounds in terms of classical invariants (n, m, Δ, d, Wiener index, Zagreb indices), characterizing extremal graphs, addressing the inverse problem (graphs realizing a given value κ). We study extremal values of this index among trees of order n, examine its behavior on specific families of graphs, and explore some of its basic properties.

We present our main results in three parts. First, we derive sharp bounds connecting the Gutman index with other well-known topological indices. Next, we determine extremal graphs with respect to the Gutman index under fixed degree sequences. Finally, we address the inverse problem concerning graphs that are uniquely determined by their Gutman index.

2 Preliminaries

All graphs considered are simple, connected, and undirected. A *tree* on n vertices has exactly $n-1$ edges. The *path* $\mathcal{P}_n$ and the *star* $K_{1,n-1}$ are the two extremal trees with respect to many degree-based and distance-based indices. The *double star* $\mathrm{DS}(a, b)$ (with $a, b \geqslant 1$ and $a+b = n$) consists of two adjacent vertices (the *centres*) of degrees a and b, respectively, with $a - 1$ pendant neighbours of the first centre and $b - 1$ pendant neighbours of the second; it has $n = a + b$ vertices and $n - 1$ edges. Observe that $\mathrm{DS}(n - 1, 1) = K_{1,n-1}$ (the star) and $\mathrm{DS}(1, n - 1)$ is its mirror. As usual, $d(v)$ denotes the degree of a vertex v, and $d(u, v)$ denotes the distance between vertices u and v. We denote by $\mathcal{S}_n$ the star on n vertices and by $\mathcal{P}_n$ the path on n vertices. For the classical Gutman index, the following extremal results on trees are known: the star $\mathcal{S}_n$ minimizes and the path $\mathcal{P}_n$ maximizes the index. Explicit formulas are:

$$\mathrm{Gut}(\mathcal{S}_n) = (n - 1)(2n - 3), \qquad \mathrm{Gut}(\mathcal{P}_n) = \frac{1}{3}(n - 1)(2n^2 - 4n + 3).$$

These results can be found in [3, 16] and related works.

Two classical families of graph realizations make this intuition precise.

Definition 1 (Threshold graph realization [2, 13])**.** *Given a graphical degree sequence $\mathscr{D}$, the* threshold graph realization $\mathrm{TH}(\mathscr{D})$ *is the unique (up to isomorphism) threshold graph with degree sequence $\mathscr{D}$.*

Threshold graphs are constructed greedily, by starting from a single vertex, each new vertex is added either as an *isolated* vertex (connected to nobody) or as a *dominating* vertex (connected to all existing vertices), chosen so that the running degree sequence matches $\mathscr{D}$.

We will also make use of the following well-known tools.

Proposition 1 (Jensen's Inequality [4]). *If $f\colon I \to \mathbb{R}$ is a convex function on an interval I and $x_1, \dots, x_k \in I$, then*

$$f\left(\frac{x_1 + \cdots + x_k}{k}\right) \leq \frac{f(x_1) + \cdots + f(x_k)}{k}.$$

Equality holds if and only if f is affine on $\{x_1, \dots, x_k\}$ or all x_i are equal.

Proposition 2 (Moore Bound [12]). *The maximum number of vertices $b(\Delta, d)$ in a Δ-regular graph of diameter d is given by*

$$b(\Delta, d) = \begin{cases} 2 & \text{if } \Delta = 1, \\ 2d + 1 & \text{if } \Delta = 2, \\ 1 + \Delta \dfrac{(\Delta - 1)^d - 1}{\Delta - 2} & \text{if } \Delta \geq 3. \end{cases}$$

Since the term $2^{d(u)d(v)}$ grows extremely fast with the product of degrees, the value of $\mathrm{HGut}(G)$ is dominated by edges connecting high-degree vertices. This makes HGut highly sensitive to the presence of adjacent high-degree vertices, but also causes many non-isomorphic graphs to potentially share the same value when only low-degree edges are present. Note that calculating $\mathrm{HGut}(G)$ can be done in linear time $O(m)$ once the degree sequence is known.

Observation 1. *Non-isomorphic graphs can have the same* HGut *value.*

For example, the path $\mathcal{P}_4$ and the star $K_{1,3}$ both yield $\mathrm{HGut} = 24$. This shows that HGut is *not* a complete isomorphism invariant.

A *perfect binary tree* T_h of height $h \geqslant 1$ is defined recursively: T_0 consists of a single root vertex. For $h \geq 1$, the root has two children, and each of the two subtrees is a perfect binary tree of height $h-1$. The tree T_h has exactly $n = 2^{h+1} - 1$ vertices.

2.1. Statement Problem. The Exponential Gutman index $\mathrm{HGut}(G)$ exhibits interesting behavior due to the rapid growth of the term $2^{d(u)d(v)}$. Several natural questions remain open and deserve further investigation.

(1) Determine the maximum and minimum values of $\mathrm{HGut}(G)$ among all connected graphs on n vertices with m edges. For a fixed degree sequence, it is expected that the threshold graph maximizes the index while a suitable bipartite realization minimizes it. Rigorous proofs for general degree sequences are still needed.
(2) The path $\mathcal{P}_n$ uniquely minimizes $\mathrm{HGut}(T)$ among all trees on n vertices. Characterize the trees that maximize HGut.

3 Main Results

Unlike the classical Gutman index, the exponential Gutman index depends only on degree products along edges.

Proposition 3. *If $G \cong \mathcal{C}_n$. Then,* $\mathrm{HGut}(G) = 16n$.

Proof. Assume that $G \cong \mathcal{C}_n$ is the cycle graph on $n \geqslant 3$ vertices, then $\mathrm{HGut}(C_n) = 16n$. □

In fact, according to Proposition 3, if $G \cong \mathcal{P}_n$, and $n \geqslant 4$, then $\mathrm{HGut}(G) = 16n - 40$. Hence, $\mathcal{P}_n$ has two pendant edges of type $(1, 2)$, and $n-3$ internal edges of type $(2, 2)$.

Proposition 4. *Let $a, b \geq 1$ with $a + b = n$. Then*

$$\mathrm{HGut}\big(\mathrm{DS}(a, b)\big) \;=\; 2^{ab} + (a-1)\cdot 2^{a} + (b-1)\cdot 2^{b}. \tag{3}$$

Proof. Since $\mathrm{DS}(a, b)$ has one central edge of type (a, b) contributing 2^{ab}, then there are $a-1$ pendant edges of type $(a, 1)$ each contributing 2^a, and $b-1$ pendant edges of type $(b, 1)$ each contributing 2^b. □

The extremely rapid growth of the function 2^x suggests that the value of $\mathrm{HGut}(G)$ contain significant contributions about the multiset of edge degree-products $\mathcal{M}(G) = \{d(u)d(v) \mid uv \in E(G)\}$.

Proposition 5. *Let G and H be two graphs. If $\mathcal{M}(G) \neq \mathcal{M}(H)$. Then,* $\mathrm{HGut}(G) = \mathrm{HGut}(H)$.

Proposition 6. *The index* $\mathrm{HGut}(G)$ *does not uniquely determine the graph G up to isomorphism. In particular, it is not a complete graph invariant.*

Based on Propositions 5 and 6, we noticed that among graphs with sufficiently large maximum degree product, the exponential terms dominate so strongly that different multisets of edge degree-products are very likely to produce distinct values of $\mathrm{HGut}(G)$.

Lemma 1. *Let T_h be the perfect binary tree of height $h \geqslant 1$ with $n = 2^{h+1}-1$ vertices. Then*

$$\mathrm{HGut}(T_h) = 260n - 1660 \tag{4}$$

Proof. If $h = 1$, then T_1 has a root of degree 2 connected to two leaves of degree 1 where $T_1 \cong \mathcal{P}_3$. Thus, all edges are of type $(2, 1)$, contributing 4 and according to Proposition 3, $\mathrm{HGut}(T_1) = 8$.

In the perfect binary tree with $h \geqslant 2$, the root has degree 2, all non-root internal vertices have degree 3 and there are 2^h leaves of degree 1. In this case, we noticed that the edges can be classified into three types as *2 edges* of type (2,3) such that from the root to its two children, and 2^h *edges* of type (3,1) established from the last internal level to the leaves. Therefore, at levels $1, \ldots, h-1$: each has degree 3. Then, there are $2^h - 2$ such non-root internal vertices. Thus, the edges between level ℓ and level $\ell + 1$ for $\ell = 1, \ldots, h-2$ are of type $(3, 3)$. Hence, there are $2^h - 4$ such edges. Thus,

$$\begin{aligned}
\mathrm{HGut}(T_h) &= 2\cdot 2^{2\cdot 3} + (2^h - 4)\cdot 2^{3\cdot 3} + 2^h \cdot 2^{3\cdot 1}\\
&= 2\cdot 2^6 + (2^h - 4)\cdot 2^9 + 2^h\cdot 2^3\\
&= 128 + 512\cdot 2^h - 2048 + 8\cdot 2^h\\
&= 520\cdot 2^h - 1920.
\end{aligned}$$

Then, by applying value of n, the relationship (4) holds. □

To determine which trees on a fixed number of vertices minimise and maximise HGut, we should be move to establishing the most basic property of HGut among Lemma 2.

Lemma 2. *Let G and H be two graphs. If $G \cong H$, then* $\mathrm{HGut}(G) = \mathrm{HGut}(H)$.

Proof. Let $ad : V(G) \to V(H)$ be a graph isomorphism. Then ad preserves adjacency, degrees, and distances. In particular, for every edge $uv \in E(G)$, we have $d_G(u) = d_H(ad(u))$, $d_G(v) = d_H(ad(v))$, and $\mathrm{dist}_G(u, v) = \mathrm{dist}_H(ad(u), ad(v)) = 1$. Therefore,

$$\begin{aligned}\mathrm{HGut}(G) &= \sum_{uv\in E(G)} \left(2^{d_G(u)d_G(v)} + 1\right)\\ &= \sum_{ad(u)ad(v)\in E(H)} \left(2^{d_H(ad(u))d_H(ad(v))} + 1\right)\\ &= \mathrm{HGut}(H).\end{aligned}$$

Thus, HGut is an isomorphism invariant. □

Furthermore, by establishing the Exponential Gutman indeximplies that the converse through Lemma 2 is not true. This shows that HGut is *not* a complete graph invariant.

Actually, by utilizing Proposition 5, the term $\mathrm{HGut}(G) = \mathrm{HGut}(H)$ holds even when the multisets differ, due to carry-over effects in the base-2 representation. For example, two edges with degree product p contribute $2 \cdot 2^p = 2^{p+1}$, which equals the contribution of a single edge with degree product $p + 1$. Nevertheless, since the term $2^{d(u)d(v)}$ grows so quickly, collisions become relatively rare for graphs with high maximum degree or large number of edges.

We now investigate extremal properties of HGut among trees.

Theorem 1. *Among all trees on n vertices, the path $\mathcal{P}_n$ is a strong candidate for the minimum value of* HGut.

Proof. The path graph contains only edges of types $(1, 2)$ and $(2, 2)$, whose contributions are respectively 4 and 16. Suppose that T is a tree on n vertices that is not a path. Then T contains at least one vertex of degree at least 3. Consequently, at least one edge uv satisfies $d_u\, d_v \geqslant 3$. Assume the result holds for every tree on n vertices where $n \geqslant 5$. Let T be an arbitrary tree on n vertices. Choose any leaf u of T and let $v = N_T(u)$ be its unique neighbour. Another tree derived from T as $T' = T - u$, the tree on $n - 1$ vertices obtained by deleting u and the edge uv. In this case, suppose that $k = d_T(v)$ be the degree of v in T. Then, $d_{T'}(v) = k - 1$, and the neighbours of v in T other than u are $w_1, \ldots, w_{k-1}$, with degrees $d_{w_1}, \ldots, d_{w_{k-1}}$ in T, it remains unchanged in T'. Thus, we should be comparing between $\mathrm{HGut}(T)$

and $\mathrm{HGut}(T')$. For satisfies this purpose, we noticed that the edge uv is present in T but not in T'; it contributes $2^{k\cdot 1} = 2^k$. Thus, each edge vw_i changes its contribution from $2^{k\cdot d_{w_i}}$ in T to $2^{(k-1)d_{w_i}}$ in T'. Therefore,

$$\mathrm{HGut}(T) = \mathrm{HGut}(T') + 2^k + \sum_{i=1}^{k-1}\left[2^{k\,d_{w_i}} - 2^{(k-1)d_{w_i}}\right]. \tag{5}$$

Thus, according to Proposition 3, if $G \cong \mathcal{P}_n$, and $n \geqslant 4$, $\mathrm{HGut}(T') \geqslant \mathrm{HGut}(\mathcal{P}_{n-1})$, and $\mathrm{HGut}(\mathcal{P}_{n-1}) = 16n - 56$. Hence,

$$\Delta_k := 2^k + \sum_{i=1}^{k-1} 2^{(k-1)d_{w_i}}(2^{d_{w_i}} - 1), \tag{6}$$

where $\Delta_k \geqslant 16$.

Case $k = 2$**.** There is exactly one neighbour w_1 of v in T'. Since T' is a connected tree on $n \geqslant 5$ vertices with v a leaf of degree k), the vertex w_1 must have degree $d_{w_1} \geqslant 2$ in T' equivalently, in T. Then, $\Delta_2 = 4 + 2^{d_{w_1}}(2^{d_{w_1}} - 1)$ it implies that

$$\Delta_2 = 4 + 2^{2d_{w_1}} - 2^{d_{w_1}}.$$

Since $d_{w_1} \geqslant 2$, we have $2^{2d_{w_1}} - 2^{d_{w_1}} \geqslant 12$. Thus, $\Delta_2 \geqslant 16$, with equality if and only if $d_{w_1} = 2$.

Case $k = 3$**.** We have two neighbours w_1, w_2 of v in T'. Since $n \geqslant 5$, not both can be leaves in T'; otherwise T would have $n \leqslant 4$ vertices, contradicting $n \geqslant 5$ with $T' = K_{1,2}$); at least one, say w_2, satisfies $d_{w_2} \geq 2$. If $d_{w_1} = 1$, $\Delta_3 = 8 + 4(2^1 - 1) + 2^{2d_{w_2}}(2^{d_{w_2}} - 1)$. Thus,

$$\Delta_3 = 8 + 4 + (2^{2d_{w_2}} - 2^{d_{w_2}}),$$

where $\Delta_3 \geqslant 16$. If $d_{w_1} \geqslant 2$ also, $\Delta_3 \geqslant 16$.

If $k \geqslant 4$. We have $2^k \geqslant 16$ and the sum is non-negative, so $\Delta_k \geqslant 16$. Thus, in all cases $\Delta_k \geqslant 16$, establishing (6) and hence $\mathrm{HGut}(T) \geqslant \mathrm{HGut}(\mathcal{P}_{n-1}) + 16 = \mathrm{HGut}(\mathcal{P}_n)$.

Moreover, the presence of a branching vertex increases the degree products of adjacent edges compared with the path structure. Since the exponential function is strictly increasing, every such increase raises the total value of the sum HGut. □

Lemma 3. *Let T be a tree on n vertices and let $uv \in E(T)$. Removing uv from T yields two components of sizes t and $n - t$. Then*

$$d_u \cdot d_v \;\leqslant\; t(n-t) \;\leqslant\; \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil.$$

Equality $d_u d_v = \lfloor n/2 \rfloor \lceil n/2 \rceil$ holds if and only if $t = \lfloor n/2 \rfloor$, $d_u = t$, $d_v = n-t$, where $T = \mathrm{DS}\left(\lfloor n/2 \rfloor, \lceil n/2 \rceil\right)$ and uv is its central edge.

Proof. In the component of size s containing u, the vertex u is adjacent to at most $t - 1$ other vertices in that component with v. Thus, $d_u \leqslant t$. Since $d_v \leqslant n - t$ yields $d_u \,.\, d_v \leqslant t(n-t)$. In this case, the term $t(n-t)$ is maximised over integers $1 \leqslant t \leqslant n - 1$ where $t = \lfloor n/2 \rfloor$, it implies that

$t(n-t) = \lfloor n/2 \rfloor \lceil n/2 \rceil$. Hence, for the equality condition, $d_u = t$ needs the vertex u to be connected to all $t-1$ other vertices in its component, so that component is a star with centre u and $t-1$ leaves. Similarly, if $d_v = n-t$ forces the other component to be a star with centre v and $n-t-1$ leaves. Therefore $T = \mathrm{DS}(t, n-t) = \mathrm{DS}\big(\lfloor n/2 \rfloor, \lceil n/2 \rceil\big)$. □

Based on Lemma 3, we have $\mathrm{HGut}\big(\mathrm{DS}(a,b)\big) = 2^{ab} + (a-1)\cdot 2^a + (b-1)\cdot 2^b$, which it will utilize in next theorem.

Theorem 2. *Let $a = \lfloor n/2 \rfloor$ and $b = \lceil n/2 \rceil$. Then, among all trees on $n \geqslant 4$ vertices,*

$$\mathrm{HGut}(T) \;\leqslant\; \mathrm{HGut}\big(\mathrm{DS}(a,b)\big) \tag{7}$$

with equality if and only if $T = \mathrm{DS}(a,b)$, for $n \geqslant 5$ or $T \in \{P_4, K_{1,3}\}$, for $n = 4$.

Proof. By Lemma 3, every edge uv of T satisfies $d_u d_v \leqslant ab$. The, $2^{d_u d_v} \leqslant 2^{ab}$. Thus, if $T = \mathrm{DS}(a,b)$, then $\mathrm{HGut}(T) = 2^{ab} + (a-1)2^a + (b-1)2^b$ where it established among Proposition 4.
Case 1: For $n = 4$, we noticed that both $\mathcal{P}_4 = \mathrm{DS}(2,2)$ and $K_{1,3} = \mathrm{DS}(1,3)$, and there are no other trees on 4 vertices.
Case 2: For $n \geqslant 5$, we find that $\mathrm{HGut}(\mathrm{DS}(a,b)) > \mathrm{HGut}(T)$ for any $T \ncong \mathrm{DS}(a,b)$. Thus, by utilizing Lemma 3, every edge of T has degree product at most $ab-1$. Since the maximum ab is achieved only at the central edge of $\mathrm{DS}(a,b)$. Thus

$$\mathrm{HGut}(T) \;\leqslant\; (n-1)\cdot 2^{ab-1}.$$

Claim 1. $\mathrm{HGut}(\mathrm{DS}(a,b)) > (n-1)\cdot 2^{ab-1}$ for $n \geqslant 5$.

Since $2^{ab} > (n-1)\cdot 2^{ab-1}$ where $2 > n-1$, and $n < 3$, this crude bound is not sufficient on its own. We instead compare $\mathrm{DS}(a,b)$ directly with the double star $\mathrm{DS}(a-1, b+1)$, which by Lemma 3 has the largest edge degree product among all trees other than $\mathrm{DS}(a,b)$,

$$\begin{aligned}&\mathrm{HGut}(\mathrm{DS}(a,b)) - \mathrm{HGut}(\mathrm{DS}(a-1, b+1))\\ &\quad= \big[2^{ab} - 2^{(a-1)(b+1)}\big] + \big[a\cdot 2^{a-1}\big] - \big[(b+1)\cdot 2^b\big].\end{aligned}$$

Since $b \geqslant a$ implies $(a-1)(b+1) = ab + (a-b-1) \leqslant ab-1$, we have

$$2^{ab} - 2^{(a-1)(b+1)} \;=\; 2^{(a-1)(b+1)}\big(2^{b-a+1}-1\big) \;\geqslant\; 2^{(a-1)(b+1)}.$$

Thus, by considering $a \geqslant 2$ and $b \geqslant 3$ where $n \geqslant 5$, $ab \geqslant 6$ and $(a-1)(b+1) \geqslant 4$. Then, $2^{(a-1)(b+1)} \geqslant 16$. Thus, $2^{(a-1)(b+1)}(2^{b-a+1}-1) > (b+1)\cdot 2^b - a\cdot 2^{a-1}$ holds for all a, b with $a + b = n \geqslant 5$ and $a \leqslant b$. ♦

Therefore, for any non-$\mathrm{DS}(a,b)$ tree T has maximum edge degree product at most $(a-1)(b+1)$, then the product for $\mathrm{DS}(a-1, b+1)$. Then, according to case 1, case 2 and Claim 1, we have $\mathrm{HGut}(T) \leqslant \mathrm{HGut}(\mathrm{DS}(a-1, b+1)) < \mathrm{HGut}(\mathrm{DS}(a,b))$, which completing the proof. □

To establish the maximum term it needs to verified value in Theorem 2, for $n = 5, 6, 7$ by direct computation in Table 1. Hence, it emphasizes that the star graph does not maximize HGut among trees.

n	Tree T	Degree sequence	$\mathrm{HGut}(T)$
5	$\mathcal{P}_5$	$(1, 2, 2, 2, 1)$	40
5	$K_{1,4}$	$(4, 1, 1, 1, 1)$	64
5	$\mathrm{DS}(2, 3)$	$(3, 2, 1, 1, 1)$	84
6	P_6	$(1, 2, 2, 2, 2, 1)$	56
6	"Broom"	$(1, 2, 2, 3, 1, 1)$	100
6	"Spider"	$(3, 2, 2, 1, 1, 1)$	144
6	$K_{1,5}$	$(5, 1, 1, 1, 1, 1)$	160
6	$\mathrm{DS}(2, 4)$	$(4, 2, 1, 1, 1, 1)$	308
6	$\mathrm{DS}(3, 3)$	$(3, 3, 1, 1, 1, 1)$	544

Таблица 1. All non-isomorphic trees on $n = 5, 6$ vertices with their HGut values, confirming that $\mathrm{DS}\big(\lfloor n/2 \rfloor, \lceil n/2 \rceil\big)$ is the unique maximum and $\mathcal{P}_n$ is the unique minimum.

Indeed, for $n \geqslant 5$, we find that $\mathrm{HGut}(K_{1,n-1}) = (n-1) \cdot 2^{n-1}$, where it bounded by $\mathrm{HGut}\big(\mathrm{DS}(a, b)\big) \geqslant 2^{ab} = 2^{\lfloor n^2/4 \rfloor}$, and $\lfloor n^2/4 \rfloor > n - 1$ for all $n \geq 5$, so $2^{ab} \gg (n-1) \cdot 2^{n-1}$. For example, according to Table 1, at $n = 6$, $\mathrm{HGut}(K_{1,5}) = 160$ while $\mathrm{HGut}(\mathrm{DS}(3, 3)) = 544$. This contrasts sharply with the classical Gutman index, where $K_{1,n-1}$ is the minimum and $\mathcal{P}_n$ is the maximum. The exponential amplification of degree products fundamentally changes the extremal structure.

3.1. Bounds Among Classical Invariants. In this subsection, we began with lower bound among Jensen's inequality by Lemma 4 and the upper bound among the Moore bound had established by Lemma 5.

Lemma 4. *Let G be a graph with $m \geqslant 1$ edges and let $M_2(G)$ be the second Zagreb index. Then*

$$\mathrm{HGut}(G) \;\geqslant\; m \cdot 2^{\,M_2(G)/m}, \tag{8}$$

with equality if and only if $d_u\, d_v$ is constant over all edges $uv \in E(G)$.

Proof. The function $f(x) = 2^x$ is strictly convex on $\mathbb{R}$. Applying Proposition 1 to the m values $\lambda_{uv} = d_u d_v$ gives

$$\frac{1}{m} \sum_{uv \in E(G)} 2^{\lambda_{uv}} \;\geqslant\; 2^{\frac{1}{m}\sum_{uv \in E(G)} \lambda_{uv}} = 2^{M_2(G)/m}.$$

By using transform as multiply both sides by m yields (8). Since f is strictly convex, equality holds if and only if all $d_u d_v$ are equal. In this case, the graph is *edge-regular* with respect to degree products. This holds in particular for every regular graph and every biregular bipartite graph. □

Lemma 5. *Let G be a connected graph with maximum degree $\Delta \geq 1$ and diameter $d \geq 1$. Then, according to Proposition 2,*

$$\mathrm{HGut}(G) \;\leqslant\; 2^{\Delta^2} \cdot \frac{\Delta}{2} \cdot b(\Delta, d). \tag{9}$$

Proof. For every edge uv one has $d_u \leq \Delta$ and $d_v \leq \Delta$, so $2^{d_u d_v} \leq 2^{\Delta^2}$. Hence

$$\mathrm{HGut}(G) \leq m \cdot 2^{\Delta^2}.$$

Since G has maximum degree Δ and diameter d, according to Proposition 2, the Moore bound gives $n \leqslant b(\Delta, d)$. Thus, $2m \leqslant \Delta\, n \leqslant \Delta\, b(\Delta, d)$. Thus, we have $m \leqslant \frac{\Delta}{2}\, b(\Delta, d)$. Thus, the relationship (9) holds. □

The upper bound in Lemma 5 is approached (though not attained for most parameters) only when G is close to a Moore graph, where Δ-regular is formed of diameter d, with $n = b(\Delta, d)$ vertices. Known Moore graphs include complete graphs $K_{\Delta+1}$ $(d = 1)$, and odd cycles where $\Delta = 2$.

Actually, together Lemmas 4 and 5 provide significantly sharper bounds than the naive estimates $2m \leqslant \mathrm{HGut}(G) \leqslant m \cdot 2^{\Delta^2}$, because the lower bound is tight for regular graphs and the upper bound incorporates structural constraints.

3.2. Extremal Values for Fixed Degree Sequences. In this subsection, consider G be a simple connected graph on n vertices with degree sequence $\mathscr{D} = (d_1 \geq d_2 \geq \cdots \geq d_n)$. We study which graph realizations of $\mathscr{D}$ attain the maximum or minimum value of

$$\mathrm{HGut}_s(G) \;:=\; \sum_{uv \in E(G)} 2^{d_u d_v},$$

which is the combinatorially significant part of $\mathrm{HGut}(G)$. Intuitively, $\mathrm{HGut}_s(G)$ is large when edges connect vertices of large degree to each other, and small when large degree vertices are matched to small degree vertices.

Proposition 7. *Let $\mathscr{D}$ be a graphical degree sequence. Among all connected realizations G of $\mathscr{D}$, the threshold graph realization* $\mathrm{TH}(\mathscr{D})$ *attains the maximum value of* $\mathrm{HGut}_s(G)$.

Proof. We use a swap argument based on the rearrangement inequality for convex functions (see, e.g., [14]). Suppose G is a connected realization of $\mathscr{D}$ that is *not* a threshold graph. Then there exist four distinct vertices a, b, c, d with $d_a \geq d_b$, $d_c \geq d_d$, such that $ac \in E(G)$, $bd \in E(G)$, but $bc \notin E(G)$ and $ad \notin E(G)$ (this configuration characterizes non-threshold graphs; see [2]). Consider the *2-switch* that replaces edges $\{ac, bd\}$ with $\{bc, ad\}$ (or $\{ab, cd\}$, depending on the configuration); this operation preserves the degree sequence. Since $d_a \geq d_b$ and $d_c \geq d_d$, we have $d_a d_c + d_b d_d \geqslant d_a d_d + d_b d_c$. Then,

$$2^{d_a d_c} + 2^{d_b d_d} \geqslant 2^{d_a d_d} + 2^{d_b d_c}.$$

Hence the 2-switch from $\{bc, ad\}$ to $\{ac, bd\}$ does not decrease $\mathrm{HGut}_s(G)$. Thus, according to [2], we conclude that $\mathrm{TH}(\mathscr{D})$ is a local maximum of $\mathrm{HGut}_s(G)$ over all realizations of $\mathscr{D}$. □

The 2-switch argument among Proposition 7 shows that *some* threshold realization maximizes $\mathrm{HGut}_s(G)$. Since $\mathscr{D}$ has a unique threshold realization which occurs for most sequences, the maximizer is unique. For degree sequences with multiple threshold realizations, all of them attain the same value of $\mathrm{HGut}_s(G)$.

For the minimum, the situation is more subtle such that not every degree sequence has a bipartite realization. Thus, we state the result conditionally.

Proposition 8. *Let $\mathscr{D}$ be a graphical degree sequence.*

(1) *If $\mathscr{D}$ has a bipartite realization $\mathrm{BR}(\mathscr{D})$, then among all connected bipartite realizations of $\mathscr{D}$, those in which high-degree vertices are in opposite parts of the bipartition minimize $S(G)$.*
(2) *Among* all *connected realizations of $\mathscr{D}$, a minimizer exists but need not be bipartite; it is, however, a graph in which the edges of largest degree-product are avoided as much as possible.*

Proof. According to Proposition 7, we will utilize it for same 2-switch argument applied in reverse.
(1). In this case, by replacing an edge ac with a, c both of large degree, with an edge connecting a large-degree vertex to a small-degree vertex decreases $2^{d_a d_c}$ by strict convexity. Hence, we find that the largest degree vertices in each part are *not* adjacent minimizes $\mathrm{HGut}_s(G)$.
(2). Since $\mathrm{HGut}_s(G)$ is a continuous function of a discrete edge set. Then, a minimum over the finite set of realizations always exists. Thus, large degree product edges follows from the same convexity argument. □

A fully rigorous treatment of both extremal problems for all degree sequences requires a careful application of the *rearrangement inequality* or *majorization* (in the sense of Hardy–Littlewood–Pólya; see [14, 11]). In particular, one needs to verify that the sequence of degree products $(d_u d_v)_{uv \in E(G)}$ is majorized by the corresponding sequence for $\mathrm{TH}(\mathscr{D})$, which would then imply $S(G) \leq S(\mathrm{TH}(\mathscr{D}))$ for all convex f by the Schur-convexity of the symmetric sum. We leave the complete majorization proof as a direction for future work.

3.3. On the Inverse Problem and Uniqueness. Given a positive integer κ, determine all graphs G up to isomorphism satisfying $\mathrm{HGut}(G) = \kappa$. This is a natural question for any graph index.

We first show that HGut is *not* a complete graph invariant, i.e., it does not distinguish all non-isomorphic graphs. For example, $\mathrm{HGut}_s(\mathcal{P}_4) = \mathrm{HGut}_s(K_{1,3}) = 24$ even though $\mathcal{P}_4 \ncong K_{1,3}$. Despite the above counterexample, collisions appear to become increasingly rare as the value of the index grows. The reason is the extremely rapid growth of $2^{d_u d_v}$ as a single edge between two vertices of degree k contributes 2^{k^2}, which dominates the entire sum for all smaller edges.

Assume that $d_u d_v = \lambda_{uv}$ and all other edges ab satisfy $d_a\, d_b < \lambda_{uv}$. Then,

$$\mathrm{HGut}_s(G) \;=\; 2^{\lambda_{uv}} + R(G),$$

where $R(G) < (m-1)\cdot 2^{\lambda_{uv}-1}$. Thus, the term $2^{\lambda_{uv}}$ determines a narrow range in which any other graph H with $\mathrm{HGut}_s(H) = \mathrm{HGut}_s(G)$ should be also have its maximum edge degree product equal to λ_{uv}. Thus, this severely constrains the structure of graphs that can produce the same index value.

We note that Conjecture 1 is analogous to known results for other graph polynomials and indices: for example, almost all trees are determined by their chromatic polynomial [17], and similar almost all graphs are determined by their spectrum results hold for the adjacency matrix [20]. Whether HGut behaves similarly is an interesting open question.

Characterizing all values κ that are attained by some graph, and all graphs that attain a given value, remains open. We record two natural questions.

Question 1. *For which positive integers κ does there exist a graph G with* $\mathrm{HGut}(G) = \kappa$*?*

Equivalently based on Question 1, what is the image of HGut over the class of all connected graphs?

Question 2. *Is the set $\{G : \mathrm{HGut}(G) = \kappa\}$ finite for every κ? For fixed n, is there an effective algorithm to determine all n-vertex graphs with a prescribed value of* HGut*?*

To determine behavior under graph operations, we must study how $\mathrm{HGut}(G)$ changes under standard graph operations. We also propose the following conjecture concerning eventual uniqueness.

Conjecture 1. *There exists a constant κ_0 such that depending only on the class of graphs under consideration, e.g., trees on $n \geqslant 3$ vertices.*

Actually, according to Conjecture 1 and based on 2, for all $\kappa \geqslant \kappa_0$, there is at most one graph G (up to isomorphism) with $\mathrm{HGut}(G) = \kappa$. The heuristic support for Conjecture 1 is the following. For κ to be achieved by two non-isomorphic graphs G and H, their multisets of edge degree products $\{\lambda_{uv} : uv \in E\}$ must produce equal $\mathrm{HGut}_s(G)$. Since the terms $2^{\lambda_{uv}}$ grow doubly exponentially in the maximum degree, distinct multisets of degree products generically yield distinct sums of powers of two; collisions require a precise cancellation that becomes increasingly unlikely as κ increases.

4 Conclusion

We have studied the exponential Gutman index $\mathrm{HGut}(G)$ for trees. In this paper, we emphasize that the path graph $\mathcal{P}_n$ minimises HGut among all trees on $n \geqslant 4$ vertices, with $\mathrm{HGut}(\mathcal{P}_n) = 16n - 40$. Also, the balanced double star $\mathrm{DS}(\lfloor n/2 \rfloor, \lceil n/2 \rceil)$ maximises HGut for $n \geqslant 5$, among the sharp edge degree product bound of Lemma 3. In particular, the star $K_{1,n-1}$ does *not* maximise HGut; it is far from optimal because the exponential amplification favours adjacent high degree vertices over the star's hub leaf structure. Through Lemma 1, for complete binary trees, showing $\mathrm{HGut}(T_h) = 260n - 1660$ for height $h \geqslant 2$. The bounds of HGut had established as lower bound by utilizing Jensen's inequality amng Lemma 4) and an upper bound by utilizing the Moore bound among Lemma 5.

These results and formulas support efficient computation and deeper analysis of distance-degree invariants, enabling future studies on optimal degree arrangements in general graphs.

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