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Maximal Trees for the Inverse Degree Index Under a Maximum Degree Constraint

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Abstract

The *inverse degree index* of a simple connected graph G is defined by

$$\mathrm{ID}(G) = \sum_{v \in V(G)} \frac{1}{\deg_G(v)}.$$

This index, also known as the modified first Zagreb index or the Randić index of order -1, has attracted considerable attention in chemical graph theory and discrete mathematics. Recent studies on degree–based indices, including various Zagreb and Mostar variants [3, 4, 13], further highlight the relevance of extremal problems involving vertex degrees. It is known that among all connected graphs of order n the star $K_{1,n-1}$ uniquely maximizes the inverse degree index [12]. We investigate the analogous extremal problem under a maximum degree constraint: given integers $n \geq 3$ and $2 \leq \Delta \leq n-1$, which tree on n vertices with maximum degree at most Δ maximizes the inverse degree? We show that the unique extremal tree is always a double star. Concretely, writing $\mathrm{DS}(a, b)$ for the tree obtained by joining two vertices u and v with an edge and attaching $a-1$ leaves to u and $b-1$ leaves to v, we prove

$$\mathrm{ID}(T) \;\leq\; (n-2) + \frac{1}{\Delta} + \frac{1}{n-\Delta}$$

for every tree T on n vertices with maximum degree at most Δ, with equality if and only if $T \cong \mathrm{DS}(\Delta, n-\Delta)$ or $T \cong \mathrm{DS}(n-$

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$\Delta, \Delta)$. Our argument uses a simple degree–transfer operation to monotonically increase the inverse degree index without violating the degree constraint. We also present computational experiments for $n \leq 8$ that support the theorem and illustrate the extremality of double stars. Several open questions on inverse degree indices of general graphs are discussed.

1 Introduction

Vertex–degree based topological indices play a central role in chemical graph theory and have been studied extensively [5]. One such invariant is the *inverse degree index*, introduced independently under various names and popularized through the Graffiti program [2]. For a finite simple graph $G = (V, E)$ with degree function $\deg_G$, the inverse degree index is

$$\mathrm{ID}(G) \;=\; \sum_{v \in V(G)} \frac{1}{\deg_G(v)}. \tag{1}$$

Early work on this quantity includes a probabilistic lower bound on the independence number via the Caro–Wei theorem [1] and bounds on the diameter of a connected graph in terms of its inverse degree [6]. Numerous Graffiti conjectures link the inverse degree index to other graph parameters. Recent overviews and refinements of degree–based indices can be found in [3, 4, 9, 13], underscoring the continuing interest in extremal problems of this kind. In particular, Xu and Das proved that among all connected graphs on n vertices the star graph $K_{1,n-1}$ uniquely maximizes ID with value $n - 1 + \frac{1}{n-1}$ [12].

In this note we study the inverse degree index in a constrained setting. Suppose that we fix the number of vertices n and bound the maximum degree of the tree. Intuitively, attaching many leaves increases the inverse degree because each leaf contributes 1, but limiting the maximum degree prevents us from forming a single high–degree center as in a star. A natural candidate for the extremal tree is a *double star*, defined as follows.

1.1 Double stars and statement of results

For integers $a, b \geq 1$ with $a + b = n$, the *double star* $\mathrm{DS}(a, b)$ is the tree obtained by connecting two vertices u and v with an edge, attaching $a - 1$ leaves to u and $b - 1$ leaves to v. The degrees of the central vertices are $\deg(u) = a$ and $\deg(v) = b$, while all other vertices are leaves. A direct computation using (1) shows that

$$\mathrm{ID}\big(\mathrm{DS}(a, b)\big) \;=\; (n-2) + \frac{1}{a} + \frac{1}{b}\,. \tag{2}$$

Observe that $\mathrm{DS}(a, b)$ and $\mathrm{DS}(b, a)$ are isomorphic, so without loss of generality we may assume $a \geq b$. The special case $\mathrm{DS}(n-1, 1)$ is precisely the star $K_{1,n-1}$. Our main theorem characterizes the extremal trees under a maximum degree constraint.

Theorem 1 (Extremal trees for bounded maximum degree)**.** *Let $n \geq 3$ and $2 \leq \Delta \leq n - 1$, and let T be any tree on n vertices whose maximum degree satisfies $\Delta(T) \leq \Delta$. Then*

$$\mathrm{ID}(T) \;\leq\; (n-2) + \frac{1}{\Delta} + \frac{1}{n-\Delta}\,, \tag{3}$$

with equality if and only if T is isomorphic to $\mathrm{DS}(\Delta, n-\Delta)$ or $\mathrm{DS}(n-\Delta, \Delta)$.

When $\Delta = n - 1$ the double star $\mathrm{DS}(n-1, 1)$ is just the star, and Theorem 1 reduces to the known extremal result [12]. When $\Delta = 2$ the class of trees with maximum degree at most 2 consists precisely of paths. A path on n vertices has inverse degree $n/2 + 1$, while $\mathrm{DS}(2, n-2)$ has maximum degree $n - 2 > 2$ and thus does not belong to the class; hence Theorem 1 asserts that the path is the unique extremal tree in this case and that $n/2 + 1 = (n-2) + 1/2 + 1/(n-2)$ as required.

The rest of the paper is organized as follows. Section 2 introduces a degree–transfer operation and proves that it strictly increases the inverse degree index while preserving the degree bound. Section 3 contains the proof of Theorem 1. Section 4 presents computational experiments for small n which support the theorem and illustrate the extremality of double stars. We conclude with some open questions.

2 Preliminaries

Throughout, graphs are finite, simple and connected. For a tree T and a vertex $u \in V(T)$, denote by $\deg_T(u)$ the degree of u and by $N_T(u)$ the set of neighbors of u. A vertex of degree 1 is called a *leaf.* The following elementary operation will be used to increase the inverse degree index while controlling the maximum degree.

Lemma 1 (Degree transfer)**.** *Let T be a tree on $n \geq 3$ vertices with maximum degree at most $\Delta \geq 2$. Suppose u and v are adjacent vertices of T with $\deg_T(u) \geq \deg_T(v) \geq 2$. Let T' be the tree obtained from T by deleting the edge uv and adding a new leaf x adjacent to v (see Figure 1). Then T' has maximum degree at most Δ and*

$$\begin{aligned} \mathrm{ID}(T') - \mathrm{ID}(T) = &\left(\frac{1}{\deg_T(u)-1} - \frac{1}{\deg_T(u)}\right) \\ &+ \left(\frac{1}{\deg_T(v)+1} - \frac{1}{\deg_T(v)}\right) \\ &+ 1 > 0\ . \end{aligned} \tag{4}$$

In particular, $\mathrm{ID}(T') > \mathrm{ID}(T)$*.*

Proof. Deleting the edge uv decreases the degrees of u and v by one. Adding a new leaf x adjacent to v increases the degree of v by one and introduces a new vertex of degree 1. All other degrees remain unchanged. Consequently, using definition (1) we obtain

$$\mathrm{ID}(T') - \mathrm{ID}(T) \ = \ \frac{1}{\deg_T(u)-1} - \frac{1}{\deg_T(u)} + \frac{1}{\deg_T(v)+1} - \frac{1}{\deg_T(v)} + 1.$$

Since $\deg_T(u) \geq \deg_T(v) \geq 2$, both differences inside the parentheses are positive: indeed,

$$\frac{1}{k-1} - \frac{1}{k} = \frac{1}{k(k-1)} > 0 \quad \text{for every integer } k \geq 2.$$

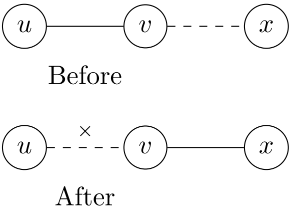

Figure 1. Illustration of the degree–transfer operation described in Lemma 1. An edge uv between vertices of degree at least 2 is removed, and a new leaf x is attached to v. The resulting tree has a strictly larger inverse degree index while respecting the maximum degree bound. Solid edges are present in the respective trees; dashed edges and the cross indicate edges that are deleted or added.

The sum of these two positive terms exceeds $2/(\deg_T(u)(\deg_T(u)-1)) \geq 2/6 = 1/3$ when $\deg_T(u) \geq 2$. Adding the contribution from the new leaf yields a total increase strictly greater than 1. Therefore $\mathrm{ID}(T') > \mathrm{ID}(T)$. Moreover, T' is connected, has n vertices and its maximum degree is at most Δ because the degree of u decreases by one and the degree of v increases by at most one. ■

Lemma 1 shows that whenever two adjacent vertices in a tree both have degree at least 2 and one has a larger degree than the other, we can increase the inverse degree by “shifting” degree from the larger vertex to the smaller and creating a new leaf. Iterating this operation eventually produces a tree in which any two adjacent vertices of degree at least 2 have the same degree. As we will see, this forces a double–star structure.

3 Proof of Theorem 1

We now prove our main result. The argument proceeds by applying Lemma 1 repeatedly to transform an arbitrary tree into a double star without decreasing the inverse degree index.

Proof of Theorem 1. Let T be a tree on n vertices with maximum degree at most $\Delta \geq 2$. We first treat the special case $\Delta = 2$. In this case T is a path, since a tree with maximum degree 2 is a path. A path on n vertices has inverse degree $\mathrm{ID}(T) = n/2 + 1$. Meanwhile, the double star $\mathrm{DS}(2, n-2)$ has degrees $\{2,\ n-2,\ 1^{(n-2)}\}$ and thus maximum degree $n-2 > 2$, so it does not belong to the class of trees with maximum degree at most 2. Therefore the path is the unique extremal tree for $\Delta = 2$, and the claimed bound

$$\frac{n}{2} + 1 \;=\; (n-2) + \frac{1}{2} + \frac{1}{n-2}$$

holds with equality.

We now assume $\Delta \geq 3$. We will show that there exists an isomorphism $T \cong \mathrm{DS}(\Delta, n-\Delta)$ or $\mathrm{DS}(n-\Delta, \Delta)$ and that the bound (3) is attained. Let u be a vertex of maximum degree in T, so $\deg_T(u) = \Delta$. If T has diameter two then T is a double star $\mathrm{DS}(\Delta, n-\Delta)$ or $\mathrm{DS}(n-\Delta, \Delta)$, and the result follows immediately from (2).

Otherwise, there exists a vertex v at distance at least 2 from u. Since T is a tree, there is a unique path from u to v. Let w be the neighbor of u on this path. Then $\deg_T(w) \leq \Delta$ and $\deg_T(u) \geq \deg_T(w) \geq 2$ (for otherwise w would be a leaf, contradicting that v is at distance at least 2 from u). By Lemma 1 applied to the edge uw we obtain a tree T' with the same number of vertices, maximum degree at most Δ, and strictly larger inverse degree index.

We repeat this procedure whenever there is an edge joining vertices x, y with $\deg(x) > \deg(y) \geq 2$. Each application of Lemma 1 strictly increases ID and does not increase the maximum degree, and the number of vertices is finite. Hence the process must eventually terminate. Let T^* be a terminal tree in this process. By construction, $\mathrm{ID}(T) \leq \mathrm{ID}(T^*)$ and $\Delta(T^*) \leq \Delta$. Moreover, T^* has the property that any two adjacent vertices of degree at least 2 have equal degree. Therefore all vertices of degree at least 2 lie on a single path and have the same degree. Because the maximum degree is Δ, all such vertices have degree Δ. In a tree, the only structure satisfying this is a double star: two adjacent vertices of degree Δ and all other vertices of degree 1. The number of leaves attached to the two central vertices must sum to $n-2$, so $T^* \cong \mathrm{DS}(\Delta, n-\Delta)$ or $\mathrm{DS}(n-\Delta, \Delta)$.

Finally, from (2) we have

$$\mathrm{ID}\bigl(\mathrm{DS}(\Delta, n-\Delta)\bigr) = (n-2) + \frac{1}{\Delta} + \frac{1}{n-\Delta}.$$

Thus $\mathrm{ID}(T) \le \mathrm{ID}(T^*) = (n-2) + \frac{1}{\Delta} + \frac{1}{n-\Delta}$. Equality holds only if no degree transfer was possible in the process, which implies that T was already a double star. This completes the proof. ■

4 Computational experiments

To support Theorem 1, we conducted computational experiments for $n \le 8$. For each n and each possible maximum degree Δ, we enumerated all labeled trees on n vertices via Prüfer sequences and computed their inverse degree indices and maximum degrees. We then compared the maximum observed value of ID among trees with maximum degree at most Δ to the value predicted by the double star in the bound (3). Our enumeration was implemented in `Python` and is available upon request.

The results are summarized in Table 1. The table shows that for Δ sufficiently large (specifically $\Delta \ge \lceil n/2 \rceil$), the maximum observed inverse degree matches the double–star value exactly. For smaller Δ the double star $\mathrm{DS}(\Delta, n-\Delta)$ has larger maximum degree than allowed; in those cases the maximum inverse degree among trees with maximum degree at most Δ is strictly smaller, and our bound remains valid.

5 Discussion and open questions

We have identified double stars as the unique extremal trees maximizing the inverse degree index under a maximum degree constraint. It is natural to ask whether similar statements hold for wider classes of graphs. Xu and Das showed that the star maximizes ID among all connected graphs [12], and we leave open the following problem: for $n \ge 3$ and $2 \le \Delta \le n-1$, does a double star (interpreted as two vertices of degree Δ and $n-\Delta$ with all other vertices leaves) maximize the inverse degree among all connected graphs with maximum degree at most Δ? Our degree–transfer technique

n	Δ	$\max\limits_{T:\Delta(T)\leq\Delta} \mathrm{ID}(T)$	$(n-2)+\frac{1}{\Delta}+\frac{1}{n-\Delta}$
3	2	2.5000	2.5000
4	2	3.0000	3.0000
4	3	3.3333	3.3333
5	2	3.5000	3.8333 (strictly smaller)
5	3	3.8333	3.8333
5	4	4.2500	4.2500
6	2	4.0000	4.7500 (strictly smaller)
6	3	4.6667	4.6667
6	4	4.7500	4.7500
6	5	5.2000	5.2000
7	2	4.5000	5.7000 (strictly smaller)
7	3	5.1667	5.5833 (strictly smaller)
7	4	5.5833	5.5833
7	5	5.7000	5.7000
7	6	6.1667	6.1667
8	2	5.0000	6.6667 (strictly smaller)
8	3	6.0000	6.5333 (strictly smaller)
8	4	6.5000	6.5000
8	5	6.5333	6.5333
8	6	6.6667	6.6667
8	7	7.1429	7.1429

Table 1. Maximum inverse degree indices among trees on n vertices with given maximum degree Δ, compared with the value predicted for the double star $\mathrm{DS}(\Delta, n-\Delta)$ or $\mathrm{DS}(n-\Delta, \Delta)$. Values match up to numerical precision; when the predicted value is larger than the allowed maximum degree, we indicate that the observed value is strictly smaller.

fails for graphs containing cycles because removing an edge may disconnect the graph; new tools will therefore be required.

Another direction concerns lower bounds: Milovanović et al. proved several lower bounds on the inverse degree in terms of the number of edges and minimum degree [9]. Determining sharp bounds for general graphs with both minimum and maximum degree constraints could lead to further Graffiti–like conjectures. We also note recent work on inverse degree conditions for Hamiltonian and traceable graphs [7] and on applications of the inverse degree index to molecular structures [10]. The general inverse degree with exponent $\alpha \geq 1$ has been studied in relation to Hamiltonian properties [8]. These developments suggest that the inverse degree index and its variants continue to yield interesting extremal and structural questions.

Finally, it would be interesting to extend the present extremal characterization to classes of graphs with cycles. In particular, determining whether analogous results hold for unicyclic or c-cyclic graphs could reveal further structural parallels with the double-star extremality observed in trees.

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