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INVERSE DEGREE, RANDIĆ INDEX AND HARMONIC INDEX OF GRAPHS

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Let G be a graph with vertex set V and edge set E. Let d_i be the degree of the vertex v_i of G. The inverse degree, Randić index, and harmonic index of G are defined as $ID = \sum_{v_i \in V} 1/d_i$, $R = \sum_{v_i v_j \in E} 1/\sqrt{d_i\, d_j}$, and $H = \sum_{v_i v_j \in E} 2/(d_i + d_j)$, respectively. We obtain relations between ID and R as well as between ID and H. Moreover, we prove that in the case of trees, $ID > R$ and $ID > H$.

1. INTRODUCTION

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v_i \in V(G)$ is denoted by d_i.

The inverse degree first attracted attention through conjectures of the computer program Graffiti [**8**]. This vertex–degree–based graph invariant is defined as

$$ID = ID(G) = \sum_{v_i \in V(G)}^{n} \frac{1}{d_i}\,.$$

Motivated by a Graffiti conjecture [**8**], Zhang et al. [**23**] established upper and lower bounds on $ID(T) + \beta(T)$ for any tree T, where β is the number of independent edges. Hu et al. [**12**] determined the extremal graphs with respect to ID among all connected graphs of order n and with m edges. Dankelmann et al. [**5**] determined a relation between ID and edge-connectivity. In the same paper a bound is established on the diameter in terms of ID. Mukwembi [**16**]

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further improved this bound. In addition, Li and Shi [**15**] improved the bound for trees and unicyclic graphs. Chen and Fujita [**2**] obtained a nice relation between diameter and inverse degree of a graph, which settled a conjecture in [**16**]. Recently Xu et al. [**22**] determined upper and lower bounds on inverse degree in terms of chromatic number, clique number, independence number, matching number, edge-connectivity, and number of cut edges. In [**4**], the authors found some lower and upper bounds on ID and characterized the extremal graphs. Moreover, in the same paper, the inverse degree was compared with other degree–based graph invariants.

The Randić index $R(G)$ is defined as

$$R = R(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{d_i\, d_i}}\,.$$

For details of this much studied vertex–degree-based graph invariant see [**10, 13, 14, 17, 20**] and the references cited therein.

The harmonic index was introduced by Fajtlowicz [**8**] as

$$H = H(G) = \sum_{v_i v_j \in E(G)} \frac{2}{d_i + d_j}\,.$$

Favaron et al. [**9**] considered the relationship between the harmonic index and graph eigenvalues. Zhong [**24**] found the minimum and maximum values of the harmonic index for connected graphs and trees, and characterized the corresponding extremal graphs. Other related results can be found in [**7, 18, 19, 25**].

The main contribution of the present paper is in establishing relations between the inverse degree and Randić index, as well as between the inverse degree and harmonic index. Moreover, we prove that in the case of trees, the inverse degree is greater than both the Randić and harmonic index.

In order to start our considerations, assume that $|V(G)| = n$ and $|E(G)| = m$ and that $V(G) = \{v_1, v_2, \ldots, v_n\}$. A vertex is said to be pendent if its degree is one. The edge incident with a pendent vertex is said to be a pendent edge. The smallest and greatest vertex degree of the graph G are denoted by δ and Δ, respectively.

Other undefined graph theoretical notation and terminology can be found in [**1**].

2. RELATION BETWEEN INVERSE DEGREE AND RANDIĆ INDEX

We now present a relation between ID and R of a graph G.

Theorem 1. *Let G be a connected graph of order n with maximum degree Δ and minimum degree δ. Then*

$$R(G) \leq \frac{\Delta}{2}\, ID(G) - \frac{\Delta - \delta}{4\Delta\delta^2\,(\delta+1)} - \frac{1}{2}\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\delta+1}}\right)^2 \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right) \tag{1}$$

with equality holding if and only if G is regular.

Proof. First we have to show that

$$(2)\qquad \sum_{v_iv_j\in E(G)} \frac{1}{\sqrt{d_i\,d_j}} \leq \frac{1}{2}\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i}+\frac{1}{d_j}\right)-\frac{1}{2}\left(\frac{1}{\sqrt{\delta}}-\frac{1}{\sqrt{\delta+1}}\right)^2\left(\frac{1}{\sqrt{\delta}}-\frac{1}{\sqrt{\Delta}}\right)$$

with equality holding if and only if G is a regular graph.

For regular graphs $\Delta = \delta$, and thus the equality in (2) holds. Otherwise, $\Delta \neq \delta$. Then for any edge $v_iv_j \in E(G)$,

$$\frac{1}{\sqrt{d_i}} - \frac{1}{\sqrt{d_j}} \geq \frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\delta+1}} \qquad \text{and} \qquad \frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} < 1$$

implying

$$\begin{aligned}\sum_{v_iv_j\in E(G)}\left[\frac{1}{2}\left(\frac{1}{d_i}+\frac{1}{d_j}\right)-\frac{1}{\sqrt{d_i\,d_j}}\right] &= \frac{1}{2}\sum_{v_iv_j\in E(G)}\left(\frac{1}{\sqrt{d_i}}-\frac{1}{\sqrt{d_j}}\right)^2\\ &> \frac{1}{2}\left(\frac{1}{\sqrt{\delta}}-\frac{1}{\sqrt{\delta+1}}\right)^2\left(\frac{1}{\sqrt{\delta}}-\frac{1}{\sqrt{\Delta}}\right).\end{aligned}$$

Therefore we get the result in (2).

Next we have to show that

$$(3)\qquad 2\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \leq \sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i^2}+\frac{1}{d_j^2}\right)(d_i+d_j)-\frac{\Delta-\delta}{\Delta\delta^2\,(\delta+1)}$$

with equality holding if and only if G is regular.

For regular graphs $\Delta = \delta$, and equality in (3) holds. Otherwise, $\Delta \neq \delta$. Since G is connected, one can easily see that

$$\begin{aligned}&\sum_{v_iv_j\in E(G)}\left[\left(\frac{1}{d_i^2}+\frac{1}{d_j^2}\right)(d_i+d_j)-2\left(\frac{1}{d_i}+\frac{1}{d_j}\right)\right]\\ =&\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_j^2}-\frac{1}{d_i^2}\right)(d_i-d_j)\geq\frac{1}{\delta^2}-\frac{1}{(\delta+1)^2}>\left(\frac{1}{\delta}-\frac{1}{\delta+1}\right)\left(\frac{1}{\delta}-\frac{1}{\Delta}\right)\end{aligned}$$

which directly leads to (3).

Using the above results, we have

$$R(G) = \sum_{v_iv_j\in E(G)}\frac{1}{\sqrt{d_i\,d_j}}$$

$$
\begin{aligned}
(4) \qquad & \leq \frac{1}{2} \sum_{v_iv_j \in E(G)} \left(\frac{1}{d_i} + \frac{1}{d_j} \right) - \frac{1}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\delta+1}} \right)^2 \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right) \\
& \leq \frac{1}{4} \sum_{v_iv_j \in E(G)} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) (d_i + d_j) - \frac{\Delta - \delta}{4\Delta\delta^2 (\delta+1)} \\
& - -\frac{1}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\delta+1}} \right)^2 \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right) \\
& \leq \frac{\Delta}{2} \sum_{v_iv_j \in E(G)} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) - \frac{\Delta - \delta}{4\Delta\delta^2 (\delta+1)} \\
(5) \qquad & - \frac{1}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\delta+1}} \right)^2 \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right) \\
& = \frac{\Delta}{2} \sum_{i=1}^{n} \frac{1}{d_i} - \frac{\Delta - \delta}{4\Delta\delta^2 (\delta+1)} - \frac{1}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\delta+1}} \right)^2 \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right) \\
& = \frac{\Delta}{2} ID(G) - \frac{\Delta - \delta}{4\Delta\delta^2 (\delta+1)} - \frac{1}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\delta+1}} \right)^2 \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right).
\end{aligned}
$$

The first part of the proof is done.

The equality holds in (4) if and only if G is a regular graph. The equality holds in (5) if and only if $d_i = \Delta$ for all $v_i \in V(G)$, that is, G is a regular graph. Hence, the equality holds in (1) if and only if G is regular. □

Corollary 1. *Let G be a connected graph of order n with maximum degree Δ. Then*

$$R(G) \leq \frac{\Delta}{2} ID(G)$$

with equality holding if and only if G is regular.

Theorem 2. *Let G be a connected graph of order n, size m, with maximum degree Δ, and minimum degree δ. Then*

$$R(G) + \frac{m}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right)^2 \leq \frac{\delta}{2} ID(G) - \frac{m}{4} \left(\frac{1}{\delta^2} - \frac{1}{\Delta^2} \right) (\Delta - \delta) \tag{6}$$

with equality holding if and only if G is a regular graph.

Proof. For any edge $v_iv_j \in E(G)$,

$$\left(\frac{1}{\sqrt{d_i}} - \frac{1}{\sqrt{d_j}} \right)^2 + \left(\frac{1}{\sqrt{d_i}} + \frac{1}{\sqrt{d_j}} \right)^2 = 2 \left(\frac{1}{d_i} + \frac{1}{d_j} \right)$$

that is,

$$\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \leq \left(\frac{1}{\sqrt{\delta}}-\frac{1}{\sqrt{\Delta}}\right)^2+\frac{2}{\sqrt{d_i\,d_j}}$$

with equality holding if and only if $d_i=\delta$, $d_j=\Delta$ (or $d_j=\delta$, $d_i=\Delta$).

Using the above result, we have

$$2\,R(G)+\left(\frac{1}{\sqrt{\delta}}-\frac{1}{\sqrt{\Delta}}\right)^2 m \geq \sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \tag{7}$$

with equality holding if and only if G is a regular or a semiregular graph.

Now,

$$\sum_{v_iv_j\in E(G)}\left[\left(\frac{1}{d_j^2}+\frac{1}{d_i^2}\right)(d_i+d_j)-2\left(\frac{1}{d_i}+\frac{1}{d_j}\right)\right]$$

$$=\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_j^2}-\frac{1}{d_i^2}\right)(d_i-d_j)\leq m\left(\frac{1}{\delta^2}-\frac{1}{\Delta^2}\right)(\Delta-\delta)$$

with equality holding if and only if G is regular or semiregular. Combining the above result with (7), we get

$$\begin{aligned}
&R(G)+\frac{m}{2}\left(\frac{1}{\sqrt{\delta}}-\frac{1}{\sqrt{\Delta}}\right)^2\\
\geq\ &\frac{1}{4}\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_j^2}+\frac{1}{d_i^2}\right)(d_i+d_j)-\frac{m}{4}\left(\frac{1}{\delta^2}-\frac{1}{\Delta^2}\right)(\Delta-\delta)\\
\geq\ &\frac{\delta}{2}\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i^2}+\frac{1}{d_j^2}\right)-\frac{m}{4}\left(\frac{1}{\delta^2}-\frac{1}{\Delta^2}\right)(\Delta-\delta) \qquad (8)\\
=\ &\frac{\delta}{2}\sum_{i=1}^{n}\frac{1}{d_i}-\frac{m}{4}\left(\frac{1}{\delta^2}-\frac{1}{\Delta^2}\right)(\Delta-\delta)\\
=\ &\frac{\delta}{2}\,ID(G)-\frac{m}{4}\left(\frac{1}{\delta^2}-\frac{1}{\Delta^2}\right)(\Delta-\delta)\,.
\end{aligned}$$

The first part of the proof is done. Equality in (8) holds if and only if $d_i=\delta$ for all $v_i\in V(G)$, that is, G is a regular graph as G is connected. Hence, the equality holds in (6) if and only if G is a regular graph. □

We now provide a relation between H and ID.

Theorem 3. *Let G be a connected graph of order n with maximum degree Δ. Then*

$$H(G) \le \frac{\Delta}{2}\, ID(G) \tag{9}$$

with equality if and only if G is regular.

Proof. For any edge $v_iv_j \in E(G)$, we have $(d_i - d_j)^2 \ge 0$, that is, $(d_i + d_j)^2 \ge 4d_i\, d_j$, that is, $\frac{1}{d_i} + \frac{1}{d_j} \ge \frac{4}{d_i + d_j}$ with equality if and only if $d_i = d_j$. Using this result, we get

$$H(G) = \sum_{v_iv_j \in E(G)} \frac{2}{d_i + d_j} \le \frac{1}{2} \sum_{v_iv_j \in E(G)} \left(\frac{1}{d_i} + \frac{1}{d_j}\right) \tag{10}$$

$$\le \frac{\Delta}{2} \sum_{v_iv_j \in E(G)} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2}\right) \tag{11}$$

$$= \frac{\Delta}{2} \sum_{i=1}^{n} \frac{1}{d_i} = \frac{\Delta}{2}\, ID(G)\,.$$

Equality holds in (10) if and only if $d_i = d_j$ for all edges $v_iv_j \in E(G)$, that is, G is a regular graph as G is connected. Equality holds in (11) if and only if $d_i = \Delta$ for all $v_i \in V(G)$, that is, G is regular. Hence, equality holds in (9) if and only if G is regular. □

Theorem 4. *Let G be a connected graph of order n with $d_i \ge d_j \ge \sqrt{d_i} + 1$ for any edge $v_iv_j \in E(G)$. Then $ID(G) < H(G)$.*

Proof. For any edge $v_iv_j \in E(G)$, we have $d_i \ge d_j \ge \sqrt{d_i} + 1$, that is, $(d_i - 1)^2 \ge (d_j - 1)^2 \ge d_i$, that is, $d_i^2 \ge d_j^2 > d_i + d_j$. Since G is a connected graph, using this result, we have

$$d_i^2\,(d_j^2 - d_i - d_j) + d_j^2\,(d_i^2 - d_i - d_j) > 0$$

that is,

$$2d_i^2\, d_j^2 > (d_i^2 + d_j^2)(d_i + d_j)$$

that is,

$$\frac{2}{d_i + d_j} > \frac{1}{d_i^2} + \frac{1}{d_j^2} \quad \text{for any edge } v_iv_j \in E(G)\,.$$

Hence

$$H(G) = \sum_{v_iv_j \in E(G)} \frac{2}{d_i + d_j} > \sum_{v_iv_j \in E(G)} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2}\right) = \sum_{i=1}^{n} \frac{1}{d_i} = ID(G)\,.$$

This completes the proof of the theorem. □

Corollary 2. *Let G be a graph of order n. If $d_i \geq \sqrt{n-1}+1$ for all i $(1 \leq i \leq n)$, then $ID(G) < H(G)$.*

Proof. Since $d_i \geq \sqrt{n-1}+1$ for all i $(1 \leq i \leq n)$, for each edge $v_i v_j \in E(G)$, we have

$$d_i \geq d_j \geq \sqrt{n-1}+1 \geq \sqrt{d_i}+1\,.$$

□

3. COMPARING INVERSE DEGREE, RANDIĆ AND HARMONIC INDICES OF TREES

In this section, we prove that in the case of trees, the inverse degree is greater than the Randić index and that the same holds also for the harmonic index.

First note that

$$ID(K_{1,n-1}) = n-1+\frac{1}{n-1} > \sqrt{n-1} = R(K_{1,n-1})\,.$$

whereas for $n > 4$,

$$R\left(K_{\frac{n}{2},\frac{n}{2}}\right) = \frac{n}{2} > 2 = ID\left(K_{\frac{n}{2},\frac{n}{2}}\right).$$

Therefore, in the general case ID and R are incomparable. On the other hand, for trees we have the following:

Theorem 5. *Let T_n be a tree of order n. Then $ID(T_n) > R(T_n)$.*

Proof. By means of computer aided checking, it can be verified that $ID(T_n) > R(T_n)$ holds for $n \leq 10$. We therefore assume that $n \geq 11$ and prove the theorem by induction on n.

Assume that $ID(T_i) > R(T_i)$ is true for any i, $i = 1, 2, \ldots, n-1$. We demonstrate that it remains true for $i = n$. Let v_n be a pendent vertex of T_n such that $v_{n-1}v_n \in E(T_n)$ and $T_n = T_{n-1} - \{v_n\}$. First we assume that $d_{n-1} \geq 3$ in T_n. Then

$$\begin{aligned} ID(T_n) &= ID(T_{n-1}) + 1 - \frac{1}{d_{n-1}\,(d_{n-1}-1)} \\ R(T_n) &= R(T_{n-1}) + \frac{1}{\sqrt{d_{n-1}}} - \sum_{v_j:\, v_{n-1}v_j \in E(T_n),\, j\neq n} \frac{\sqrt{d_{n-1}}-\sqrt{d_{n-1}-1}}{\sqrt{d_{n-1}\,(d_{n-1}-1)\,d_j}} \end{aligned}$$

which implies

$$ID(T_n) - R(T_n) = ID(T_{n-1}) - R(T_{n-1}) + 1 - \frac{1}{d_{n-1}\,(d_{n-1}-1)}$$

$$- \frac{1}{\sqrt{d_{n-1}}} + \sum_{v_j:\, v_{n-1}v_j \in E(T_n),\, j \neq n} \frac{\sqrt{d_{n-1}} - \sqrt{d_{n-1}-1}}{\sqrt{d_{n-1}\left(d_{n-1}-1\right) d_j}}$$

$$> 0, \quad \text{as } d_{n-1} \geq 3.$$

Next we need to consider the case $d_{n-1} = 2$. If $T_n \cong P_n$, then $ID(T_n) < R(T_n)$. Otherwise, let T_k be a tree of order k ($k \leq n-2$) with $v_k v_{k+1} \in E(T_n)$ such that $T_n - \{v_k v_{k+1}\} = T_k \cup P_{n-k}$, where $P_{n-k} : v_{k+1}v_{k+2}\ldots v_{n-1}v_n$ and $d_{k+1} = d_{k+2} = \cdots = d_{n-1} = 2$, $d_k \geq 3$, $d_n = 1$. Then

$$ID(T_n) = ID(T_k) + \frac{n-k+1}{2} - \frac{1}{d_k\left(d_k - 1\right)}$$

$$R(T_n) = R(T_k) + \frac{n-k-2}{2} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d_k}} - \sum_{v_j:\, v_k v_j \in E(T_n),\, j \neq k+1} \frac{\sqrt{d_k} - \sqrt{d_k - 1}}{\sqrt{d_k\left(d_k-1\right) d_j}}.$$

From the above results, we obtain

$$ID(T_n) - R(T_n) = ID(T_k) - R(T_k) + \frac{3}{2} - \frac{1}{d_k\left(d_k-1\right)} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2d_k}} + \sum_{v_j:\, v_k v_j \in E(T_n),\, j \neq k+1} \frac{\sqrt{d_k} - \sqrt{d_k - 1}}{\sqrt{d_k\left(d_k-1\right) d_j}}$$

$$> 0, \quad \text{as } d_k \geq 3.$$

This completes the proof of this theorem. □

In a similar manner,

$$ID(K_{1,n-1}) = n - 1 + \frac{1}{n-1} > \frac{2(n-1)}{n} = H(K_{1,n-1})$$

$$H\left(K_{\frac{n}{2},\frac{n}{2}}\right) = \frac{n}{2} > 2 = ID\left(K_{\frac{n}{2},\frac{n}{2}}\right).$$

implying that in the general case, ID and H are incomparable.

Theorem 6. *Let T_n be a tree of order n. Then $ID(T_n) > H(T_n)$.*

Proof. According to a result by Xu [**21**], $R(G) \geq H(G)$. By Theorem 5, $ID(T_n) > R(T_n)$. Theorem 6 follows. □

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