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Inverse degree index of graphs with a given cyclomatic number

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Abstract. We investigate how the inverse degree index of graphs depends on their cyclomatic number. In particular, we provide sharp lower bounds on the inverse degree index over all graphs on a given number of vertices with a given cyclomatic number. We also deduce some structural properties of extremal graphs. Some open questions regarding the upper bound over the same class of graphs are discussed and some possible further developments are indicated.

1. Introduction

Throughout this paper all graphs are connected and simple, that is, with no loops and multiple edges. Let G be a graph with the vertex set $V(G) = \{v_1, \dots, v_n\}$ and the edge set $E(G)$. The degree of a vertex v_i is denoted by d_i. A *tree* is a connected graph with no cycles and a *unicyclic graph* is a connected graph with exactly one cycle. For a connected graph G with n vertices and m edges its *cyclomatic number* $c(G)$ is defined as $c(G) = m - n + 1$. Hence, the cyclomatic number of trees and of unicyclic graphs is equal to 0 and 1, respectively. (For graphs which are not connected, the definition of their cyclomatic number is modified by replacing 1 with the number of connected components, but we will not consider such graphs here.) As usual, we denote the cycle and the path of order n by C_n and P_n, respectively.

The degree-based indices are among the oldest and the best researched classes of topological indices. The best known among them are the Randić index and the Zagreb indices, but there are also many others. Most of them have been studied for their possible applications in the QSAR and QSPR modeling. They are, however, investigated also for their intrinsic interest in classical graph theory. Nice examples are provided by [4, 5] and [6]. In this paper we are interested mostly in the inverse degree index which belongs to the class of indices obtained by summing given powers of degrees over all vertices. See [1] for an excellent recent survey.

The *inverse degree* of G is defined as

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

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Also the *Randić index* $R(G)$ and the *harmonic index* $H(G)$ of a graph G are defined as follows:

$$R(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_i d_j}}, H(G) = \sum_{v_iv_j \in E(G)} \frac{2}{d_i + d_j}.$$

The Randić index and its relationships with other graph-theoretic invariants have been extensively studied by many authors, for instance, see [2, 3, 7–14]. Its relationship with the harmonic index is valid for all graphs.

Theorem 1.1. *[12, 15] For every graph G of order n, the following inequalities hold:*

$$H(G) \leqslant R(G), R(G) \leqslant \frac{n}{2}$$

2. Trees and unicyclic graphs

In [8], the authors proved that if T is a tree, then $ID(T) \geqslant R(T)$ and $ID(T) \geqslant H(T)$. Here, we provide a simple proof for these results and also extend these results to unicyclic graphs.

Theorem 2.1. *Let T be a tree of order n. Then $ID(T) \geqslant \frac{n}{2} + 1$ and the equality holds if and only if $T = P_n$.*

Proof. We apply induction on n. For $n = 2$, the assertion is clear. Let T be a tree of order $n > 2$, with vertex set $V(T) = \{v_1, \ldots, v_n\}$ and $d_i = d(v_i)$. Now, let $v_1 \in V(T)$ be a pendant vertex and $v_1v_2 \in E(T)$. By the induction hypothesis we have:

$$ID(T \setminus v_1) \geqslant \frac{n-1}{2} + 1,$$

and the equality holds if and only if $T \setminus v_1 = P_{n-1}$. Therefore, the following holds:

$$\frac{1}{d_2 - 1} + \sum_{1=3}^{n} \frac{1}{d_i} \geqslant \frac{n-1}{2} + 1.$$

This implies that:

$$\frac{1}{2} + \frac{1}{d_2 - 1} + \sum_{i=3}^{n} \frac{1}{d_i} \geqslant \frac{n}{2} + 1,$$

and if $T \setminus v_1 \neq P_{n-1}$, then the inequality is strict. In order to show that $ID(T) \geqslant \frac{n}{2} + 1$, it suffices to prove,

$$ID(T) = \sum_{i=1}^{n} \frac{1}{d_i} \geqslant \frac{1}{2} + \frac{1}{d_2 - 1} + \sum_{i=3}^{n} \frac{1}{d_i}$$

or equivalently,

$$1 + \frac{1}{d_2} + \sum_{i=3}^{n} \frac{1}{d_i} \geqslant \frac{1}{2} + \frac{1}{d_2 - 1} + \sum_{i=3}^{n} \frac{1}{d_i}.$$

So it suffices to show that:

$$\frac{1}{2} + \frac{1}{d_2 - 1} \leqslant 1 + \frac{1}{d_2}, \text{ or } 0 \leqslant (d_2 + 1)(d_2 - 2).$$

Since $d_2 \geqslant 2$, $ID(T) \geqslant \frac{n}{2} + 1$ and if $d_2 > 2$, then $ID(T) > \frac{n}{2} + 1$. This implies that if $ID(T) = \frac{n}{2} + 1$, then $d_2 = 2$ and $T \setminus v_1 = P_{n-1}$. Hence $T = P_n$ and the proof is complete. □

Now, we generalize the previous result to unicyclic graphs.

Corollary 2.2. *For every unicyclic graph G of order n, $ID(G) \geqslant \frac{n}{2}$ and the equality holds if and only if $G = C_n$. Therefore, for every unicyclic graph G, $ID(G) \geqslant R(G) \geqslant H(G)$.*

Proof. We apply induction on n. For $n = 3$, the assertion is clear. Let G be a unicyclic graph of order $n > 3$, $V(G) = \{v_1, \ldots, v_n\}$ and $d_i = d(v_i)$. First note that for two positive integers $x, y \geqslant 2$, we have

$$\left(\frac{1}{x-1} + \frac{1}{y-1}\right) - \left(\frac{1}{x} + \frac{1}{y}\right) = \frac{1}{x(x-1)} + \frac{1}{y(y-1)} \leqslant \frac{1}{2} + \frac{1}{2}. \tag{1}$$

Since G is unicyclic, there exists an edge e such that $G \setminus e$ is a tree. Noting to (1) and Theorem 2.1, $ID(G \setminus e) - ID(G) \leqslant 1$. Therefore $ID(G) \geqslant \frac{n}{2}$. If $G = C_n$, then $ID(G) = \frac{n}{2}$. Now, assume that $ID(G) = \frac{n}{2}$. Therefore $ID(G \setminus e) = \frac{n}{2} + 1$ and by Theorem 2.1, $G \setminus e$ is P_n. Let u and v be the end vertices of P_n. If $e = uv$, then $G = C_n$. If $e = uw$ and $w \neq v$, then $ID(G) = \frac{n}{2} + \frac{1}{3}$, a contradiction. If $e = wt$, $w, t \notin \{u, v\}$, then $ID(G) = \frac{n}{2} + \frac{2}{3}$, a contradiction. The proof is complete. □

Remark 2.3. *If G is a graph of order n, then by the Cauchy-Schwarz inequality we have,*

$$\left(\sum_{i=1}^{n} d_i\right)\left(\sum_{i=1}^{n} \frac{1}{d_i}\right) \geqslant n^2.$$

Thus $ID(G) \geqslant \frac{n^2}{2m}$, where $m = |E(G)|$.

3. Graphs with a given cyclomatic number

In this section we look at the inverse degree index of graphs of larger cyclomatic numbers. We start with an observation on a structural property of graphs minimizing this index.

Lemma 3.1. *Let G be a connected graph of order n and cyclomatic number $c > 0$. If G contains a vertex of degree 1, then there is a graph G' of the same order n and with the same cyclomatic number such that $ID(G') < ID(G)$.*

Proof. Let G be a graph with cyclomatic number $c > 0$ and let $u \in V(G)$ be a vertex of G with $d_u = 1$. Then u must be an end-vertex of a path $wv_1 \ldots v_k u$, where $d_w > 2$, $d_{v_1} = \ldots = d_{v_k} = 2$. Hence the total contribution of the vertices of this path to $ID(G)$ is given by $\frac{1}{d_w} + \frac{k}{2} + 1$. Let x and y be two adjacent vertices on some cycle C_r of G. (Such a cycle exists since $c > 0$.) Now delete vertices of the path $v_1 \ldots v_k u$ and subdivide the edge xy by $k + 1$ new vertices $v'_1, \ldots, v'_k, u'$ of degree 2. The new graph, call it G', has order n and the same cyclomatic number as G. Moreover, there are only two vertices whose degrees differ in G and in G': the degree of w in G' decreases by one with respect to its degree in G, and the degree of u' in G' is 2, one more than d_u in G. By computing $ID(G) - ID(G')$ we see that contribution of all vertices except those two cancel. Hence,

$$ID(G) - ID(G') = \frac{1}{d_w} + 1 - \frac{1}{d_w - 1} - \frac{1}{2} = \frac{1}{d_w} - \frac{1}{d_w - 1} + \frac{1}{2} > 0,$$

since $d_w > 2$. This completes the proof. □

Hence a graph minimizing $ID(G)$ over all graphs of order n containing cycles cannot have pendent vertices. This is consistent with the fact that C_n minimizes $ID(G)$ over all unicyclic graphs.

Now we can formulate results on the inverse degree index of graphs with larger cyclomatic number. We first consider the case of rather small cyclomatic numbers and present detailed proof. A general case then follows along the same lines.

Theorem 3.2. *Let G be a connected graph of order n with cyclomatic number $c > 0$. If $c \leq \frac{n}{2} + 1$, then*

$$ID(G) \geq \frac{n}{2} - \frac{c-1}{3},$$

with equality if and only if G is a subcubic graph, i.e., $2 \leq \delta(G) \leq \Delta(G) \leq 3$. In particular, if $c = \frac{n}{2} + 1$, then $ID(G) \geq \frac{n}{3}$ with equality if and only if G is a cubic graph.

Proof. Let $u \in V(G)$ be a vertex of the largest degree k in G. The case $k = 1$ is ruled out by the condition $c > 0$, and the case $k = 2$ is either ruled out by the same condition for paths, or settled in the results about unicyclic graphs. Hence we may assume k is at least three.

Every vertex of a connected graph with a positive cyclomatic number which is not on one of its cycles either lies in some path connecting two cycles or in some tree rooted in a vertex of a cycle or of a cycle-connecting path. We call the paths connecting two cycles *internal paths*. Suppose that G contains a vertex which lies in a tree. Then, by repeatedly applying the procedure of Lemma 3.1 we can construct a graph G' with $ID(G') < ID(G)$ such that all vertices of G' lie on its cycles or on cycle-connecting paths. Hence we can assume that all vertices of our graph G lie on its cycles or on its internal paths. This implies that the smallest degree in G is at least 2. Moreover, the average degree of G cannot exceed 3. Otherwise, the sum of all degrees would exceed $3n$, meaning that $m > \frac{3n}{2}$ and leading to $c > \frac{n}{2} + 1$, contrary to our assumption.

Take a vertex $u \in V(G)$ of degree k. If $k > 3$, then there must be a vertex $x \in V(G)$ of degree 2. If there is exactly one vertex of degree 2 in G, then $k = 4$ and u is the only vertex in G of degree greater than 3. Then x is adjacent to at most two of the four neighbors of u. Let y be a neighbor of u not adjacent to x. By deleting the edge uy and adding the edge xy we obtain a cubic graph which minimizes $ID(G)$ and the assertion follows.

Let us now assume that there are at least two vertices, x and y, of degree 2 in G. Each of them can be adjacent to at most two neighbors of u. If one of the neighbors of u non-adjacent to x, say v, is of degree at least 3, delete the edge uv and add the edge vx. In this way we obtain a new graph, G', with the same number of vertices and the same cyclomatic number as G. By computing the difference

$$ID(G) - ID(G') = \frac{1}{d_u} + \frac{1}{2} - \frac{1}{d_u - 1} - \frac{1}{3} = \frac{1}{2} - \frac{1}{3} - \left(\frac{1}{d_u - 1} - \frac{1}{d_u}\right) > 0,$$

since $\frac{1}{x-1} - \frac{1}{x}$ is strictly decreasing on $[2, \infty)$.

If all neighbors of u are of degree 2, then either there is a path $uv_1 \dots v_l w$ in which all internal vertices are of degree 2 and $d_w \geq 3$, or there is a cycle $uv_1 \dots v_l u$ in which all internal vertices are of degree 2 such that v_1 is not adjacent to x. In both cases, by deleting the edge uv_1 and adding the edge $v_1 x$, we can construct a graph on the same number of vertices and with the same cyclomatic number as G but with strictly smaller inverse degree index. Hence a graph minimizing $ID(G)$ cannot contain a vertex of degree greater than 3.

Let now G' be a graph of order n with all vertices of degree 2 or 3 and with the cyclomatic number c. It follows immediately that G must contain exactly $2(c-1)$ vertices of degree 3. Each of them contributes $\frac{1}{3}$ to $ID(G)$, while each of the remaining $n - 2(c-1)$ vertices contributes $\frac{1}{2}$. The assertion now follows by adding all contributions, since for any graph G of order n and cyclomatic number c we have

$$ID(G) \geq ID(G') = \frac{n - 2(c-1)}{2} + \frac{2(c-1)}{3} = \frac{n}{2} - \frac{c-1}{3}.$$

□

The above results provide a complete characterization of bicyclic graphs minimizing the inverse degree index.

Corollary 3.3. *Let G be a connected bicyclic graph of order n. Then $ID(G) \geq \frac{n}{2} - \frac{1}{3}$, with equality if and only if G is either a Θ-graph or G consists of two cycles connected by a path.*

(A graph G of order n is a Θ-*graph* if it has two vertices of degree 3 and $n-2$ vertices of degree 2 which lie on three internally disjoint paths connecting the two vertices of degree 3. One of the paths may be a single edge. The simplest Θ-graph is $K_4 - e$.)

By a completely analogous rewiring argument we can prove the lower bound on the inverse degree index for graphs of arbitrary cyclomatic numbers. We leave out the details.

Theorem 3.4. *Let G be a connected graph of order n with cyclomatic number c. If, for some $k \geq 1$, we have*

$$(k-1)\frac{n}{2} + 1 < c \leq k\frac{n}{2} + 1,$$

then

$$ID(G) \geq \frac{n}{2} - \frac{c-1}{k+2}.$$

In particular, for $c = k\frac{n}{2} + 1$, we have $ID(G) \geq \frac{n}{k+2}$ with equality if and only if G is $(k+2)$-regular.

4. Concluding remarks

In this paper we have studied the relationship between the cyclomatic number of connected graphs and their inverse degree index. We have derived sharp lower bounds on the inverse degree index of graphs with a given cyclomatic number and obtained some information on minimizing graphs. As a consequence, we have recovered some results on relationships between the inverse degree index and some other degree-based indices of graphs with low cyclomatic numbers.

It would be interesting to investigate the upper bounds on the inverse degree index of graphs with a given cyclomatic number c. Intuitively, one would expect that $ID(G)$ will be maximized by the graphs with the largest possible number of leaves, each contributing one. If c happens to be a triangular number $T_p = \frac{p(p+1)}{2}$, the most economic (in terms of the number of vertices) way to achieve it is to take K_{p+2} and then attach the remaining $n-p-2$ vertices to one of its vertices. For such a graph $G(n,c)$ one easily obtains $ID(G(n,c)) = n-(p+2)+1+\frac{1}{n-1} = n-p-1+\frac{1}{n-1}$. Taking into account that $p = \frac{1}{2}\left(-1+\sqrt{8c+1}\right)$, one obtains $ID(G(n,c)) \sim n - \frac{1}{2} - \sqrt{2c}$ for large values of n and c.

If c is not a triangular number, things become slightly more complicated. Suppose $T_p < c \leq T_{p+1}$. Then there must exist $0 \leq k \leq p$ such that $c = T_{p+1} - k$. For a big enough order n we construct a graph $G(n,c)$ by taking a copy of K_{p+3} and removing from it k edges, all incident with the same vertex v. That leaves at least one vertex, say u, of degree $p+2$. To this vertex u we attach $n-p-3$ vertices of degree one. Hence our graph has one vertex v of degree $p+2-k$, k vertices of degree $p+1$, $p+1-k$ vertices of degree $p+2$, one vertex u of degree $n-1$ and $n-p-3$ vertices of degree 1. Its inverse degree index is then given by

$$ID(G(n,c)) = n-p-3+\frac{1}{n-1}+\frac{p^3+(5-k)p^2+(8-k)p+4-k^2}{(p+1)(p+2)(p+2-k)},$$

where $p = \frac{\sqrt{8(c+k)+1}-3}{2}$. One can see that the rightmost fraction becomes 1 for $k=0$ and that it remains between 1 and 3/2 for all values of $0 \leq k \leq p$. We believe that the above expression is a sharp upper bound on the inverse degree index over all graphs of order n with the cyclomatic number equal to c. However, we have not worked out the details.

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