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INVERSE PROBLEM FOR ALBERTSON IRREGULARITY INDEX

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ABSTRACT. Graph indices have attracted great interest as they give us numerical clues for several properties of molecules. Some indices give valuable information on the molecules under consideration using mathematical calculations only. For these reasons, the calculation and properties of graph indices have been in the center of research. Naturally, the values taken by a graph index is an important problem called the inverse problem. It requires knowledge about the existence of a graph having index equal to a given number. The inverse problem is studied here for Albertson irregularity index as a part of investigation on irregularity indices. A class of graphs is constructed to show that the Albertson index takes all positive even integers. It has been proven that there exists at least one tree with Albertson index equal to every even positive integer but 4. The existence of a unicyclic graph with irregularity index equal to m is shown for every even positive integer m except 4. It is also shown that the Albertson index of a cyclic graph can attain any even positive integer.

Keywords: Inverse problem, Albertson index, irregularity index, topological graph index.

AMS Subject Classification: 05C07, 05C10, 05C30.

1. Introduction and preliminaries

Throughout this paper, let $G = (V, E)$ be a connected, undirected and unweighted graph with $| V(G) |= n$ vertices and $| E(G) |= m$ edges having no isolated vertices, unless otherwise stated. For a vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$ or d_v. A vertex with degree one is called a pendant vertex and we shall use the term pendant edge for an edge having a pendant vertex.

Topological graph indices have been defined and used in many areas in the last few decades to study several properties of different objects such as atoms and molecules solely by means of some mathematical techniques. Several topological graph indices have been defined and studied by many mathematicians and chemists as most graphs are generated from molecules by replacing atoms with vertices and bonds between them with edges.

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These indices are defined as invariants measuring several physical, chemical, pharmaceutical, biological properties of graphs which are modelling real situations. They can be grouped mainly into three classes according to the way they are defined; by vertex degrees, by distances or by matrices.

Two of the earliest defined topological graph indices are called the first and second Zagreb indices defined in 1972 by Gutman and Trinajstic, [15], and are often referred to due to their uses in QSAR and QSPR studies. In [7], some results on the first Zagreb index together with some other indices are given. In [8], the multiplicative versions of these indices are studied. Some relations between Zagreb indices and some other indices such as ABC, GA and Randic indices are obtained in [18]. Zagreb indices of subdivision graphs were studied in [21] and these were calculated for the line graphs of the subdivision graphs in [20]. In [26], all versions of Zagreb indices of subdivision graphs were studied and in [25], several inequalities on Zagreb indices of r-subdivision graphs were obtained. The effect of cut edges and cut vertices on some topological indices is investigated in [30]. In [23], the (a,b)-Zagreb index of some derived networks was considered. The sum-edge characteristic polynomials of graphs was investigated in [19]. In [2], the Narumi–Katayama index of the subdivision graphs was studied. In [5, 6], the complexity of graphs is studied and in [22], total edge irregularity strength of graphs is discussed.

The existence of the inverse problems in many areas of science, and naturally mathematics, is quite important, and the one for the graph theory is a recent one. The inverse problem for graph indices is the one about the existence of a graph having index equal to a given non-negative integer. This problem which formed the beginning of what is now called the inverse problem for graph indices was first proposed in [16]. In [24], the inverse problem for the first Zagreb index $M_1(G)$ was solved by showing that all positive even integers except for 4 and 8 are equal to the first Zagreb index of a special type of graph called caterpillar graph. In [28], Wagner showed that each integer greater than 469 is the Wiener index of a special graph class called starlike trees. In [29], all 49 positive integer values which are not the Wiener index of any tree are listed. Some more results for the Wiener index was obtained in [3] and [9] and in [12], Goldman et. al. gave the final result for Wiener index: Except 2 and 5, all positive integers can be the Wiener index of at least one graph.

If all vertices of a graph have the same degree, then the graph is called regular. Regularity makes calculations easier in many occasions and regular graphs usually form examples or counterexamples in many areas of graph theory. A graph which is not regular, that is which has at least two unequal vertex degrees, is called irregular. Irregularity may occur slightly or strongly. As a result of this, several measures for irregularity have been defined and used by some authors. The most throughly investigated ones are the Albertson index (which is also called irregularity index, third Zagreb index or Kekule index) defined as

$$Alb(G) = \sum_{uv \in E(G)} |d_u - d_v|, \tag{1}$$

see [1], [10], [11], the Bell index

$$B(G) = \sum_{v \in V(G)} \left(d_v - \frac{2m}{n} \right)^2, \tag{2}$$

see [4] and [11] and the sigma index

$$\sigma(G) = \sum_{uv \in E(G)} (d_u - d_v)^2. \tag{3}$$

In [14], the inverse problem for σ index was completely solved. In [27], the inverse problem is answered for Bell index. In [13], Gutman et.al. compared the irregularity indices for chemical trees, and the inverse problem for four topological indices were studied in [17]. Recently, the problem for the second Zagreb index $M_2(G)$, forgotten Zagreb index $F(G)$, and the hyper-Zagreb index $HM(G)$ were completely solved in [31]. For the second Zagreb index $M_2(G)$, 10 values of positive integers which cannot be the second Zagreb index of any graph were found. Similarly, it was found that there are 10 values of positive even integers which cannot be the forgotten index of any graph. In the same paper, also the 50 values of positive even integers which cannot be the hyper-Zagreb index of any graph were determined.

In this paper, we study the inverse problem for the Albertson irregularity index. We shall show that it must be even for any simple (without loops and multiple edges) graph. We shall also study the inverse problem for trees, unicyclic graphs and cyclic graphs.

2. Albertson irregularity index

Now we can obtain some properties of the Albertson index which will be used to solve the inverse problem. First we have,

Theorem 2.1. *The Albertson index $Alb(G)$ of a simple graph G is even.*

Proof. Recalling the definitions of Albertson and sigma indices, the result follows by the fact that the sigma index of a simple graph is even and the parities of each term $|d_u - d_v|$ and $(d_u - d_v)^2$ in these sums are the same, see [14]. □

The effect of adding a new edge to a graph on its Albertson index can be determined as follows:

Theorem 2.2. *Let G be a connected simple graph having at least three vertices. Let the neighbours of the vertex u with degree $d_G u = t > 1$ be $v_1,\ v_2,\ \cdots,\ v_t$ with degrees $d_G 1,\ d_G 2,\ \cdots,\ d_G t$, respectively. Let k be a positive integer such that $d_G i \leq d_G u$ for $i = 1,\ 2,\ \cdots,\ k$ with $k \leq t$, and $d_G i > d_G u$ for $i = k+1,\ k+2,\ \cdots,\ t$. Then $Alb(G)$ increases by $2k$ when a new pendant edge e is added to G at u.*

By the definition of $Alb(G)$, we can omit calculating the terms $|d_u - d_v|$ corresponding to the edges with $d_u = d_v$. We can apply this fact to paths and cycles. Whenever there are n consecutive vertices on a path all having degree 2, replacing these n vertices with a single vertex of degree 2 does not change the Albertson index. In [14], this simplification method was named as path reduction. Similarly, if there are n successive vertices on a cycle all having degree 2, we can replace them with a single vertex of degree 2. This is called cyclic reduction, see Fig. 1. These two reduction ideas are very useful in eliminating or reducing the graphs under question in calculating the $Alb(G)$. We can replace all branches of length at least two with an edge as they have the same irregularity index.

For example, if we want to calculate the Albertson index of the tadpole graphs $T_{5,4}$, $T_{7,3}$ or in general $T_{r,s}$, with $r \geq 3$ and $s \geq 1$, instead, we can calculate only the Albertson index of $T_{3,2}$ as all of these indices are the same after path and cyclic reduction.

FIGURE 1. Cyclic reduction

3. Inverse problem for the Albertson index

In [24], Tavakoli and Rahbarnia had made use of a special type of tree called caterpillars to solve the inverse problem for the first Zagreb index $M_1(G)$. They added a new pendant edge to increase $M_1(G)$ regularly by 4 and they obtained infinitely many positive integers corresponding to constructed graph family. In [14], the authors constructed a new class of graphs denoted by $C_{a,b}$ named as comb graphs obtained by adding one pendant edge to each of the b adjacent vertices $v_2, v_3, \cdots, v_{b+1}$ of a path P_{a+b+1} having vertices $v_1, v_2, \cdots, v_{a+b+1}$, see Fig. 2.

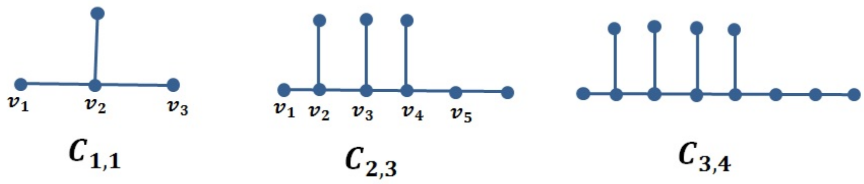

FIGURE 2. Some $C_{a,b}$ graphs

To solve the inverse problem for the Albertson irregularity index, we first have

Transformation 1. Let G be a graph possessing a vertex v of degree $d_G v \geq 3$. Let u be a pendant vertex of G adjacent to v. Construct the graph G^* by attaching two new pendant edges to u, cf. Fig. 3.

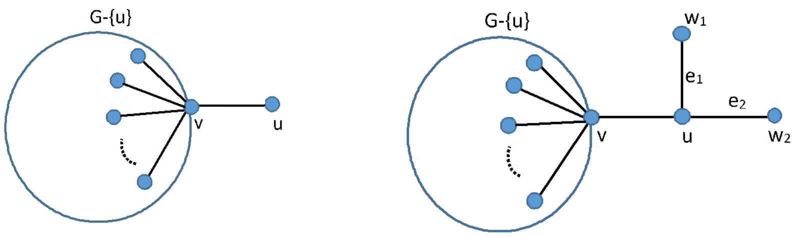

FIGURE 3. Transformation 1 giving G^*

The following result says that applying Transformation 1 to a connected simple graph having a pendant vertex increases the Albertson index by 2:

Lemma 3.1. *For any connected simple graph G different than the null graphs and path graphs,*

$$Alb(G^*) = Alb(G) + 2. \tag{4}$$

Proof. As $d_G v \geq 3$ and as $Alb(G) = d_G v - 1 + \sum_{xy \in E(G-\{u\})} |d_G x - d_G y|$ and $Alb(G^*) = d_G v - 3 + 2 + 2 + \sum_{xy \in E(G-\{u\})} |d_G x - d_G y|$, we obtain the required result. □

Note that we had the condition that v is a vertex of degree at least 3 in defining Transformation 1. If we omit this condition and allow that $d_G v$ could be any positive integer, then we would have

$$Alb(G) = Alb(G - u) + d_G v - 1, \tag{5}$$

for the graph G on the left in Fig. 3. The graph $G + \{e_1, e_2\}$ on the right has

$$Alb(G + \{e_1, e_2\}) = Alb(G - u) + |d_G v - 3| + 4. \tag{6}$$

Then we have,

$$Alb(G + \{e_1, e_2\}) - Alb(G) = |d_G v - 3| - d_G v + 5. \tag{7}$$

Now we have several cases to consider: If $d_G v = 1$, then G is P_2 which has Albertson irregularity index equal to 2, and $G + \{e_1, e_2\}$ is $S_4 = C_{1,1}$. In this case, the increase of Albertson irregularity index is 6 by Eq. (2). If $d_G v = 2$, then our graph G is as in Fig. 4. Here the increase is 4 by Eq. (2).

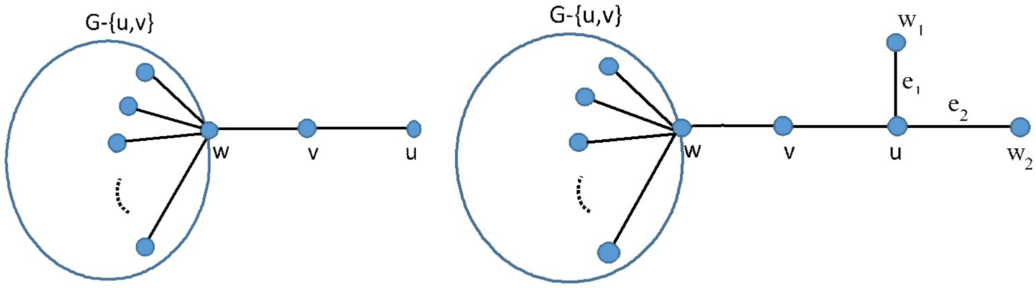

FIGURE 4. Transformation 1 with $d_G v = 2$ gives G^*

If $d_G v = 3$, then the increase of Albertson index is equal to 2. Therefore starting with graph $C_{1,1}$ which has Albertson index 6, we obtain the graphs $C_{1,2}$, $C_{1,3}$, $\cdots$, $C_{1,s}$ with Albertson indices 8, 10, $\cdots$, $2s + 4$, respectively. That is, all even integers greater than 4 can be attained by the Albertson index Alb. Also the path graph P_n has Albertson index 2, and the tadpole graph $T_{3,1}$ has $Alb(T_{3,1}) = 4$. As all regular graphs have Albertson index equal to 0, we have just proved the following.

Theorem 3.1. *For every even non-negative integer m, there is at least one graph G such that $Alb(G) = m$.*

Note that amongst all graphs that are used in obtaining Theorem 3.3, only the tadpole graph $T_{3,1}$ is not acyclic. So we can immediately state the following result for trees:

Corollary 3.1. *For every even positive integer $m \neq 4$, there is at least one tree T such that $Alb(T) = m$.*

Finally, we ask the same question for unicyclic graphs. That is what positive integer values can be attained by the *Alb* index of a unicyclic graph. We construct a graph class to give the result. Consider a cyclic graph C_n for $n \geq 3$ and add one pendant edge to each of the n vertices of C_n. The resulting graph, that we shall denote by $Th(C_n)$ is called the thorn graph of C_n in some sources, see Fig. 5. In $Th(C_n)$, all the vertices on the cycle have degree 3 and all other vertices have degree 1. Therefore each of the n edges on the cycle contributes $|3-3| = 0$ and each of the n pendant edges contributes $|3-1| = 2$ to $Alb(Th(C_n))$. Also the tadpole graph $T_{3,1}$ has the Albertson index 4. Therefore we proved the following result:

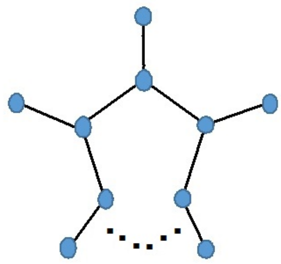

FIGURE 5. Thorn graph of C_n

Theorem 3.2. *For every even positive integer $m = 2n \geq 4$, there is at least one unicyclic graph G such that $Alb(G) = m$.*

As the graph in Fig. 6 has Albertson index 2, we have

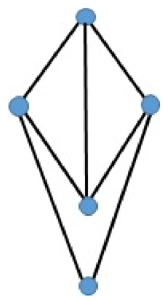

FIGURE 6. A tricyclic graph with Albertson index 2

Theorem 3.3. *For every even positive integer $m = 2n$, there is at least one cyclic graph G such that $Alb(G) = m$.*

The Albertson index has an interesting property which does not hold for other topological indices: Clearly because of cyclic and path reductions, the graph obtained by adding a new pendant edge to an existing pendant vertex of a graph G or increasing the number of edges in an existing cycle would have the same Albertson index with the graph G. As we can repeatedly apply these reductions infinitely many times, we obtain the following result:

Corollary 3.2. *For each fixed non-negative even integer $m \neq 4$, there exist infinitely many connected simple graphs G with $Alb(G) = m$.*

That is, each even positive integer except 4 can be attained as the Albertson index of infinitely many graphs.

4. Results and discussion

We used the fact that modelling a molecule by a graph gives the required information on the properties of the molecule by means of some mathematical calculations made on the graph. To achive this, we need to calculate the values of the index under consideration and also determine which values are attained by this index. This latter problem is called the inverse problem for graph indices. In this paper, inverse problem is solved for the Albertson irregularity index. It is shown that the Albertson index takes all the even integer values. For every positive even integer m but 4, the existence of a tree with Albertson index m is shown. Also, results on Albertson index of unicyclic and cyclic graphs are obtained. The other graph types such as bicyclic, threecyclic, etc are not considered as the ones studied here are enough to solve the inverse problem. In a sequel paper, the values of Albertson index could be calculated for other graph types.

Disclosure statement

No potential conflict of interest was reported by the authors.

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