



## Inverse Problem for Bell Index

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**Abstract.** Due to their applications in many branches of science, topological graph indices are becoming more popular every day. Especially as one can model chemical molecules by graphs to obtain valuable information about the molecules using solely mathematical calculations on the graph. The inverse problem for topological graph indices is a recent problem proposed by Gutman and is about the existence of a graph having its index value equal to a given non-negative integer. In this paper, the inverse problem for Bell index which is one of the irregularity indices is solved. Also a recently defined graph invariant called omega invariant is used to obtain several properties related to the Bell index.

### 1. Introduction

Let  $G = (V, E)$  be an undirected, connected and unweighted graph having  $|V(G)| = n$  vertices and  $|E(G)| = m$  edges without isolated vertices. The degree of a vertex  $v \in V(G)$  is denoted by  $d_G(v)$  or  $d_v$ . A vertex of degree one will be called a pendant vertex.

Graph indices have been defined in the last few decades to study several properties of atoms and molecules by means of some mathematical techniques. Nearly three hundreds graph indices are defined by mathematicians and chemists as molecular graphs are obtained from molecules by replacing atoms with vertices and bonds between them with edges. In this way, every chemical molecule can be modelled by a graph and studying this graph helps us to obtain information on the properties of the molecule without needing money and time-consuming experiments. These indices are invariants measuring several physical, chemical or biological properties of graphs. Two popular graph indices are called the first and second Zagreb indices defined by Gutman and Trinajstić, [9]. In [3], the first Zagreb index is related to some other indices. In [4], multiplicative versions of these indices are considered. Zagreb indices are related to  $ABC$ ,  $GA$  and Randić indices in [12]. In [15], Zagreb indices of subdivision graphs were obtained and in [14], inequalities for Zagreb indices of  $r$ -subdivision graphs were found.

Inverse problems have very fundamental role in many areas of science and the one for the graph theory is a new one. The inverse problem for graph indices is about the existence of graphs having index equal

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to an integer and was first proposed in [10]. The inverse problem for the first Zagreb index  $M_1(G)$  was solved in [13] and for Wiener index in [16]. Inverse problem for four topological indices were studied in [11]. 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 [17].

If the degree of all vertices of a graph are equal, then the graph is regular. Regularity has many advantages in graph theory. A graph which is not regular is called irregular. Several measures for irregularity are used and the most investigated ones are the Albertson index

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

[1] and [7], the Bell index

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

[2] and [7] and the sigma index

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

In [8], the inverse problem for  $\sigma$  index is solved. In this paper, we study the inverse problem for Bell index.

## 2. Inverse problem for Bell index

In this section, we investigate the inverse problem for the Bell index  $B(G)$ . As with all irregularity indices, we know that  $G$  is regular iff  $B(G) = 0$ . Let  $\bar{d}$  denote the average vertex degree of a connected simple graph  $G$ . First we obtain the relation between the Bell index and the first Zagreb index:

**Theorem 2.1.** *The relation between the Bell index  $B(G)$  and the first Zagreb index  $M_1(G)$  is*

$$B(G) = M_1(G) - \bar{d}(4m - n\bar{d}).$$

*Proof.* By the definition, we can write

$$\begin{aligned} B(G) &= \sum_{v \in V(G)} (d_v - \bar{d})^2 \\ &= \sum_{v \in V(G)} d_v^2 - 2\bar{d} \sum_{v \in V(G)} d_v + \sum_{v \in V(G)} \bar{d}^2 \\ &= M_1(G) - \bar{d}(4m - n\bar{d}). \end{aligned}$$

□

The following is a well known property of a connected simple graph:

**Lemma 2.2.** *Let  $G$  be a connected simple graph with order  $n$  and size  $m$ . Then*

$$n - 1 \leq m \leq \frac{n(n-1)}{2}.$$

Let  $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \dots, \Delta^{(a_\Delta)}\}$ . If there is at least one graph having the elements of  $D$  as its vertex degrees, then  $D$  is called realizable. In [5], an invariant number denoted by  $\Omega(G)$  for a given degree sequence and all its realization graphs was defined and some of its properties were studied. The motivation to define  $\Omega$  was its similarity to the number of leaves (pendant vertices) of a tree. This number closely related to the cyclomatic number of the graph gives direct information on all the realizations of a given degree sequence:

**Definition 2.3 ([5]).** Let  $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \dots, \Delta^{(a_\Delta)}\}$  be a realizable degree sequence and its realization be the graph  $G$ . The  $\Omega(G)$  of  $G$  is defined in terms of the degree sequence as

$$\begin{aligned} \Omega(G) &= a_3 + 2a_4 + 3a_5 + \dots + (\Delta - 2)a_\Delta - a_1 \\ &= \sum_{i=1}^{\Delta} (i - 2)a_i. \end{aligned}$$

$\Omega(G)$  has the following important computational property:

**Theorem 2.4 ([5]).** For any graph  $G$ ,

$$\Omega(G) = 2(m - n).$$

In the same paper, the number  $r$  of the closed regions (faces) which are bounded by the edges of the graph  $G$  was formulized. Note that a closed region could be bounded by any  $n$ -cycle ( $n$ -gon) where  $n \geq 3$ , a loop (1-gon) or a pair of multiple edges (2-gon). Hence

**Theorem 2.5 ([5]).** Let  $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \dots, \Delta^{(a_\Delta)}\}$ . If  $D$  is realizable as a connected planar graph  $G$ , then the number  $r$  of closed regions is given by

$$r = \frac{\Omega(G)}{2} + 1.$$

For example, for all trees including path and star graphs, we have  $\Omega(G) = -2$ , for all unicyclic graphs  $\Omega(G) = 0$ , for all bicyclic graphs  $\Omega(G) = 2$ , and for all graphs having  $k$  cycles, we have  $\Omega(G) = 2k - 2$ , giving the number of faces as 0, 1, 2 and  $k$ , respectively.

In [6], some extremal problems on the numbers of components and loops of all realizations of a given degree sequence were given. We now apply this new invariant  $\Omega$  to Bell irregularity index. First we prove

**Lemma 2.6.** The necessary and sufficient condition for the average vertex degree of a connected simple graph to be greater than 2 is that  $\Omega(G) \geq 2$ .

*Proof.* Let the average vertex degree of a connected simple graph  $G$  be denoted by  $\bar{d}$ .  $\bar{d} > 2$  iff  $m > n$  iff  $G$  has at least two cycles iff  $\frac{\Omega(G)}{2} + 1 \geq 2$  by Theorem 2.5 iff  $\Omega(G) \geq 2$ .  $\square$

As we consider the integer values of the Bell index, we shall assume that the average vertex degree  $\bar{d}$  of  $G$  is an integer. In general, if  $n|2m$ , then  $\bar{d}$  is a positive integer. In particular, when  $n$  is odd and  $n|m$ , then  $\bar{d}$  is a positive integer. As the average vertex degree plays an important role in the study of the inverse problem for Bell index, we shall now study some properties of it by means of the omega invariant. We first have

**Lemma 2.7.** A tree  $T_n$  with  $n$  vertices has integer average vertex degree iff  $n|2$ .

*Proof.* Let  $G \cong T_n$  be a tree with  $n$  vertices. Then it is well known that  $n = m + 1$ . Then the average vertex degree is

$$\bar{d} = \frac{2m}{n} = \frac{2(n-1)}{n} = 2 - \frac{2}{n}$$

and for this number to be an integer we must have  $n|2$ .  $\square$

That is, amongst all trees, only those with 1 or 2 vertices, that is, graphs having a single vertex and a single edge, respectively, can have integer average vertex degree.

The following result gives the necessary and sufficient conditions for a graph being unicyclic in terms of average vertex degree and can be proven by easy calculations:

**Theorem 2.8.** Let  $G$  be a connected graph. Adding a pendant edge to  $G$  does not change the average vertex degree iff  $G$  is unicyclic. That is

$$\overline{d_{G+e}} = \bar{d}_G \Leftrightarrow r = 1.$$

The following are immediate consequences of Theorem 2.4, 2.8 and Lemma 2.2:

**Corollary 2.9.** *If  $G$  is a connected unicyclic graph, then  $\overline{d}_G = 2$ .*

**Corollary 2.10.** *The necessary and sufficient condition for  $\Omega(G) = 0$  is  $\overline{d}_G = 2$ .*

**Corollary 2.11.** *Let  $G$  be a connected simple graph. Then  $G$  is unicyclic iff  $m = n$ .*

**Corollary 2.12.** *If  $\Omega(G) = 0$ , then  $n \geq 3$ .*

**Corollary 2.13.** *Let  $G$  be a connected simple graph with average vertex degree  $\overline{d}_G \geq 2$ . Then*

$$\Omega(G) = (\overline{d}_G - 2)n.$$

Let  $G$  be a connected unicyclic graph and let  $u \in V(G)$  have degree  $d_G u$ . Then it can easily be shown that adding a pendant edge to  $G$  at  $u$  increases the Bell index of  $G$  by  $2d_G u - 2$ . Hence if  $G$  is a connected unicyclic graph and if  $u \in V(G)$  is a pendant vertex so that  $d_G u = 1$ , then adding a new pendant edge to  $G$  at  $u$  does not change the Bell index. Similarly, if  $G$  is a connected graph having at least three vertices and if  $u$  and  $v$  are two non-adjacent vertices having degree  $d_G u$  and  $d_G v$ , respectively, then adding a new edge  $e = uv$  to  $G$ , the obtained graph  $G + e$  has non-integer average vertex degree.

We are now in a position to solve the inverse problem for the Bell index. For this, we need the following tool:

**Transformation 2.14.** *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. 1.*

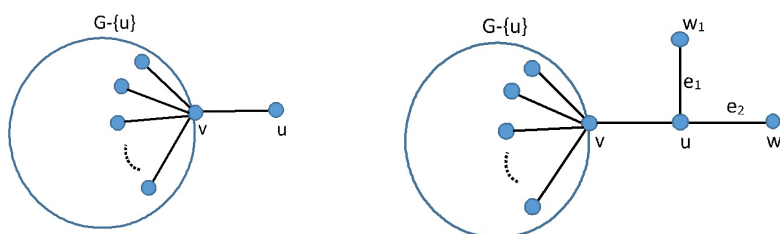


Figure 1: Transformation 2.14 giving  $G^*$

The following result says that applying Transformation 2.14 to a connected simple graph having a pendant vertex and average vertex degree  $\overline{d} = 2$  increases the Bell index by 2:

**Lemma 2.15.** *Let  $G$  be a connected simple graph having a pendant vertex and  $\overline{d} = 2$ . Transformation 2.14 increases the Bell index by 2. That is,*

$$B(G^*) = B(G) + 2. \tag{1}$$

*Proof.* First we prove that Transformation 2.14 does not effect the average vertex degree  $\overline{d} = 2$  and so all the graphs constructed by successively applying Transformation 2.14 would have the same average vertex degree 2: Average vertex degree of  $G$  is 2 by the assumption:

$$2 = \frac{\sum_{x \in V(G)} d_G x}{n} = \frac{\sum_{x \in V(G-u)} d_G x + d_G u}{n} = \frac{\sum_{x \in V(G-u)} d_G x + 1}{n}$$

and hence  $\sum_{x \in V(G-u)} d_G x = 2n - 1$ . Similarly the average vertex degree of  $G^*$  is

$$\begin{aligned} \bar{d} &= \frac{\sum_{x \in V(G-u)} d_{G^*} x + d_{G^*} u + d_{G^*} w_1 + d_{G^*} w_2}{n + 2} \\ &= \frac{\sum_{x \in V(G-u)} d_G x + d_G u + d_G w_1 + d_G w_2}{n + 2} \\ &= \frac{2n - 1 + 3 + 1 + 1}{n + 2} \\ &= 2. \end{aligned}$$

Now

$$\begin{aligned} B(G^*) - B(G) &= \sum_{x \in V(G^*)} (d_x - 2)^2 - \sum_{x \in V(G)} (d_x - 2)^2 \\ &= \sum_{x \in V(G-u)} (d_x - 2)^2 + (d_u - 2)^2 + (d_{w_1} - 2)^2 + (d_{w_2} - 2)^2 \\ &\quad - \sum_{x \in V(G-u)} (d_x - 2)^2 - (d_u - 2)^2 \\ &= 2. \end{aligned}$$

□

Under the assumption that the average vertex degree is an integer, the Bell index of any connected simple graph can only take even values:

**Theorem 2.16.** *Let  $G$  be a connected simple graph with integer average vertex degree. Then  $B(G)$  is always even.*

*Proof.* If  $\bar{d}$  is even, for each vertex  $v_i$  of degree  $d_i$ , we know that  $(d_i - \bar{d})^2$  is either even or odd. The number of odd ones is even by handshaking lemma implying that  $B(G)$  is even. Let secondly  $\bar{d}$  be odd. As the sum of all vertex degrees is even, the product  $n \cdot \bar{d}$  must also be even. Then  $n$  must be even. In this case, as the number of odd  $d_i$ 's is even, the number of even  $d_i$ 's must also be even. For each odd vertex degree  $d_i$ ,  $(d_i - \bar{d})^2$  is even and for each even vertex degree  $d_i$ ,  $(d_i - \bar{d})^2$  is odd. So even times odd numbers and even times even numbers add up to an even number, so  $B(G)$  is again even. □

In fact when the average degree is 1, the values of the Bell index are more limited:

**Corollary 2.17.** *If  $G$  is a graph with average vertex degree 1, then  $B(G) = 0$ .*

*Proof.* Let  $\bar{d} = 1$ . As we do not allow isolated vertices, all vertices must have degree 1. Hence we have  $B(G) = 0$ . □

We can give an alternative proof of Theorem 2.16 by means of the first Zagreb index:

*Proof.* Let the degrees of  $G$  be  $d_1, d_2, \dots, d_n$ . Then  $B(G) = 2k + 1$ ,  $k$  is an integer iff  $2k + 1 = \sum_{i=1}^n (d_i - \bar{d})^2$  iff  $(2k + 1)n^2 = \sum_{i=1}^n (n \cdot d_i - 2m)^2$  iff  $(2k + 1)n = n \cdot M_1(G) - 4m^2$  iff  $M_1(G) = \frac{4m^2}{n} + 2k + 1$  iff  $M_1(G)$  is odd iff  $\sum_{i=1}^n d_i^2$  is odd iff  $\sum_{i=1}^n d_i$  is odd, which is a contradiction. □

The following is a useful property:

**Corollary 2.18.** *If  $G$  is a connected simple graph with integer average vertex degree  $\bar{d}$ , then*

$$n \geq \bar{d} + 1.$$

*Proof.* By Lemma 2.2, we have

$$n - 1 \leq m \leq \frac{n(n - 1)}{2}$$

implying

$$n - 1 \leq \frac{n \cdot \bar{d}}{2} \leq \frac{n(n - 1)}{2}$$

and hence the result is obtained.  $\square$

Now we are ready to give another main result of this paper:

**Theorem 2.19.** *Let the average vertex degree  $\bar{d}$  of a connected simple graph  $G$  be a positive integer. Then the Bell index of a connected simple graph can take all non-negative even integer values.*

*Proof.* First, the Bell index of the tadpole graph  $T_{3,1}$  is 2, see Fig. 2. Applying Transformation 2.14 repeatedly,

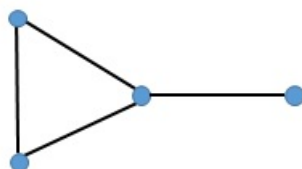


Figure 2: Tadpole graph  $T_{3,1}$  has Bell index 2

we get the graphs in Fig. 3 with Bell indices 4, 6, 8,  $\dots$ . Interestingly enough, all these graphs have average vertex degree 2. Finally the cycle graph  $C_n$  has  $B(C_n) = 0$   $\square$

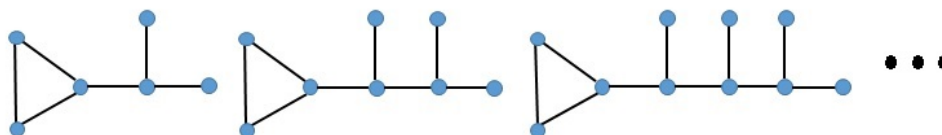


Figure 3: Graphs with Bell index 4, 6, 8,  $\dots$

In fact, to prove Theorem 2.19, one does not need to look at all the connected simple graphs with integer average vertex degree. Considering only those connected simple graphs with  $\bar{d} = 2$  would be enough to reach the target:

**Corollary 2.20.** *Let  $A_2$  be the set of all connected simple graphs with average vertex degree 2. The Bell index of any graph in  $A_2$  can take all non-negative even integer values.*

If the average vertex degree is 3, we have

**Theorem 2.21.** *Let  $G$  be a connected simple graph with average vertex degree 3. Then  $B(G)$  can take the values  $18k(2k - 1)$  for a positive integer  $k$ .*

*Proof.* If  $\bar{d} = 3$ , then

$$B(G) = \sum_{i=1}^n (d_i - 3)^2 = M_1(G) - 12m + 9n.$$

As  $2m = 3n$  by the assumption, we have  $B(G) = M_1(G) - 6m$ . Hence

$$B(G) = \sum_{i=1}^n d_i^2 - 3 \cdot \sum_{i=1}^n d_i = \sum_{i=1}^n d_i \left( \sum_{i=1}^n d_i - 3 \right) = 2m(2m - 3) = 9n(n - 1) = 18k(2k - 1)$$

as  $n$  must be even, say  $2k$  for an integer  $k$ .  $\square$

Similarly, if the average vertex degree is 4, we have

$$B(G) = M_1(G) - 16(m - n) = M_1(G) - 8\Omega(G) = M_1(G) - 8m = M_1(G) - 16n = \sum_{i=1}^n d_i \left( \sum_{i=1}^n d_i - 8 \right) = 4n(n - 4).$$

Here we can at least consider the complete graphs as connected simple graphs with average vertex degree 4. Hence we have proved

**Theorem 2.22.** *Let  $G$  be a connected simple graph with average vertex degree 4. Then  $B(G)$  can take the values  $4n(n - 4)$  where  $n$  is the order of  $G$ .*

### 3. Conclusion

In this paper, one of the recent problems of graph theory related to the most applicative area of it called the inverse problem is solved for the Bell index, one of the irregularity indices. As this index depends on the average vertex degree, the properties of this specific number is studied by means of a recently defined graph invariant called omega.

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