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The effect of omega invariant on some topological graph indices

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ABSTRACT. For a realizable set of non-negative integers, it is well-known that there are many ways of realizing it as a graph having this set as degree sequence. For a given degree sequence, a new graph invariant denoted by Ω which is related to the cyclomatic number and Euler characteristic is recently defined. It is already shown that this new invariant releases important combinatorial properties and gives direct information compared to the better known Euler characteristic on many normal or extremal problems related to the realizability, cyclicness, components, chords, loops, connectedness, etc. Many similar classification problems can be solved by means of Ω. Topological graph indices are used in applications of graph theory as they give us some mathematical results by means of some graph model of a real life situation which can frequently be used in other applied sciences. Therefore it is one of the main problems of graph theory to search for the possible values of these indices. Many problems dealing with the range of a topological index become easier if we could determine the lower and upper bounds for this topological index. In this paper, we study the change of several topological graph indices, the first and second Zagreb indices, forgotten index, sigma index and Narumi-Katayama index amongst all possible (fundamental) realizations of a given degree sequence.

1. SIGNIFICANCE OF THE WORK

Recently, a new graph invariant has been defined and shown to have a very informative nature about all the realizations of a given degree sequence. Topological graph indices have been defined and applied in the last 8 decades to obtain mathematical and chemical data and their number already exceeded 3000. Due to their applications, the values that a graph index attain is an open problem which has partial solutions for several indices and the problem is known as inverse problem. In this work, to help to solve inverse problem, we obtain lower and upper bounds for several frequently used topological graph indices and reduce the computation time that needed to solve the inverse problem.

2. INTRODUCTION

We study with finite undirected graphs $G = (V, E)$ with size $m = |E(G)|$ and order $n = |V(G)|$. The degree of a vertex $v \in V(G)$ is denoted by $d_G v$ or briefly d_v if there is no confusion. If the degree of v is one, then it is called a pendant vertex. The biggest vertex degree in G is denoted by Δ. If u and v are connected to each other by an edge e, this situation is denoted by $e = uv$ and the vertices u and v will be called adjacent vertices while the edge e is said to be incident with u and v. A graph is connected if there is a path between every two vertices. A graph that is not connected is called disconnected. A graph having no cycle will be called acyclic and the remaining graphs are called cyclic graphs. A graph having exactly one, two and three cycles is called unicyclic, bicyclic and

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tricyclic graph, respectively. An edge connecting a vertex to itself is called a loop, and two or more edges connecting two vertices will be called multiple edges.
A degree sequence is a set

$$DS(G) = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$$

with a_i's being non-negative integers. A graph G is called a realization of a set D if the degree sequence of G is equal to D. A realizable degree sequence has a large number of realizations. The most popular test of realizability is the Havel-Hakimi process [10, 11] and the realizability of multigraphs is studied in [3]. If we omit the connectedness condition, then every set of positive integers satisfying the Hand-Shaking lemma is realizable. So the interesting question is the realizability condition for connected graphs.

Let

$$D = \{1^{(a_1)}, 2^{(a_2)}, \cdots, \Delta^{(a_\Delta)}\}. \tag{2.1}$$

The invariant $\Omega(D)$ is defined [4] in terms of D as

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

The Ω is fixed for all the realizations of a given degree sequence and therefore is a graph invariant. For any graph G, the fact that $\Omega(G) = 2(m-n)$ was shown in [4] and therefore, Ω invariant is directly related to the cyclomatic number. In [4] and [5], several properties of this Ω invariant have been obtained. In [5], all the graphs are classified into three classes according to $\Omega \le -4, \Omega = -2$ and $\Omega \ge 0$. It is shown that many classification problems can be classified into these three groups of graphs and some new notion called fundamental realization is defined in each of these cases. Although the set of fundamental realizations is a subset of all realizations, they give us insight information on many general properties as they can be used as reference points in some extremal problems. For $\Omega \ge 0$, a connected realization having a cycle of length $a_2 + a_3 + a_4 + a_5 + \cdots + a_\Delta$, some loops, chords and a_1 pendant edges was called a cyclic fundamental realization. At the same reference, there are two more definitions for fundamental realizations when $\Omega = -2$ and $\Omega \le -4$, respectively called as the acyclic and mixed type fundamental realizations. Omega invariant is recently applied to the cyclicness of graphs in [7]. In [2], Ω invariant is calculated for the union, join and corona products. In [8, 16], Ω invariant is utilized to classify all the Fibonacci and Lucas graphs. The relation between Ω invariant and matching number of graphs is studied in [12, 18]. The relation between Ω invariant and the independence number of graphs in [14]. Also the effect of edge and vertex deletion on Ω invariant is studied in [6]. Several works related to topological graph indices are [1, 13, 15, 17].

3. Properties of Ω invariant

Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$. If D is realizable as a connected planar graph G, then the number r of faces was given by $r = \frac{\Omega(G)}{2} + 1$ in [4]. In the case of disconnected graphs, it is easy to see that Ω is additive over the set of the components of G. So a direct generalization to disconnected graphs with c components was given in [4] as $r = \frac{\Omega(G)}{2} + c$. The fact that $c \ge -\frac{\Omega(G)}{2}$ or equivalently, $c \ge n - m$ can be deduced from the above results. The relation between the Euler characteristic and Ω invariant was established in [4] as $\Omega(G) = 2(r - \chi(G))$. Hence the newly defined Ω invariant is closely related to the well-known Euler characteristic. Therefore one may expect the omega invariant to give information on same properties of graphs as χ does, but it is already shown that

Ω invariant give more information on many properties of a degree sequence or its graph realizations such as connectedness, forcibly connectedness, possibly connectedness, number of faces, chords, pendant edges, loops, multiple edges, components, etc., see [4], [5] and [7]. If $\Omega(D) \leq -4$, then it was shown in [4] that any realization G of a degree sequence D cannot be forcibly or potentially connected. The following result shows that every degree sequence D with $\Omega(D) \geq 0$ is potentially connected:

Theorem 3.1. *Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$. If $\Omega(D) \geq 0$, then D is potentially connected and its connected realizations are having a cycle of length $a_2 + a_3 + a_4 + a_5 + \cdots + a_\Delta$, loops, chords and a_1 pendant edges. That is, when $\Omega(D) \geq 0$, every connected realization of D must be cyclic.*

Proof. By construction. We give an algorithm to construct the required graph:
1) Draw a cycle with $a_3 + a_4 + \cdots + a_\Delta$ edges. Then we have a graph with degree sequence $\{2^{(a_3+a_4+\cdots+a_\Delta)}\}$.
2) If $a_1 > 0$, then add a_1 pendant edges to the vertices of the constructed cycle so that the choice of the vertices is made as distinct as possible. The resulting graph will have degree sequence $\{1^{(a_1)}, 2^{(a_3+a_4+\cdots+a_\Delta-a_1)}, 3^{(a_1)}\}$.
3) Add a total of $\Omega/2$ chords, loops and multiple edges conveniently to the vertices of this graph to get a new fundamental graph realization with degree sequence $\{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ which is the required result.
4) If $\Omega(D) = 0$, then we are done. If not, continue according to the priority which is adding chords as much as possible and if necessary, adding the rest as loops and if still needed, as multiple edges. $\square$

4. Change of graph indices

In this section, we shall determine the change of six important topological graph indices for the family of graph realizations of a given degree sequence. The following theorem given in [4] will be the main tool for our calculations in this section. It determines the possible connected realizations of a given degree sequence with zero Ω invariant:

Theorem 4.2. *Let $D = \{1^{(a_1)}, 2^{(a_2)}, \cdots, \Delta^{(a_\Delta)}\}$ where $a_1 > 0$ and $a_2, a_3, \cdots, a_\Delta \geq 0$. If $\Omega(D) = 0$, then D can be realized as a connected unicyclic graph where the length of this unique cycle could be anything between 1 and $a_2 + a_3 + \cdots + a_\Delta$.*

The main idea used in the proof was due to an algorithm based on a cut-and-paste process. Start with an $a_2 + a_3 + \cdots + a_\Delta$-gon $C = C_{a_2+a_3+\cdots+a_\Delta}$ so that all vertices on C are placed consecutively from smallest degree to largest degree. Using the fact that $\Omega(D) = 0$, it was shown that we can add one pendant edge to the vertices of degree 3, two pendant edges to the vertices of degree 4, three pendant edges to the vertices of degree 5, and finally $\Delta - 2$ pendant edges to the vertices of degree Δ. This is the fundamental realization defined in [5]. An algorithm was then defined to obtain all unicylic realizations having all positive integers between $a_2 + a_3 + \cdots + a_\Delta$ and 1 as cycle length. Let us denote the realizations obtained at each step of the algorithm by $C_{a_2+a_3+\cdots+a_\Delta-1}$, $C_{a_2+a_3+\cdots+a_\Delta-2}$, $\cdots$, C_1. For example, if $a_2 + a_3 + \cdots + a_\Delta = 8$, then starting with $C = C_8$, there are 7 steps giving $C_7, C_6, \cdots, C_1$ as possible cycles.

As the graphs are used in modelling some real life cases, instead of studying chemical, physical, social, etc. properties of such cases, we can use some mathematical formulae to calculate some number which we can comment to get information on the real life case. Such mathematical formulae are called topological graph indices and they are used in many applications since 1947. We now calculate the change of five important graph indices amongst all the connected realizations mentioned in Theorem 4.2. First we recall these indices. The first and second Zagreb indices, the forgotten index, the sigma index and the Narumi-Katayama index of a graph G were defined by

$$M_1(G) = \sum_{v\in V(G)} d_v^2, \tag{4.2}$$

$$M_2(G) = \sum_{uv\in E(G)} d_u \cdot d_v, \tag{4.3}$$

$$F(G) = \sum_{v\in V(G)} d_v^3 = \sum_{uv\in E(G)} (d_u + d_v)^2, \tag{4.4}$$

$$\sigma(G) = \sum_{uv\in E(G)} (d_u - d_v)^2, \tag{4.5}$$

$$NK(G) = \prod_{v\in V(G)} d_u. \tag{4.6}$$

Theorem 4.3. *Let the graph G be one of the realizations of the degree sequence D given in Theorem 4.2 so that $\Omega(D) = 0$. If $\Delta \leq 9$, then $M_2(G)$ has its smallest and largest values amongst all realizations given in Theorem 4.2 for C and C_1, respectively. If $\Delta \geq 10$, then $M_2(G)$ has its smallest and largest values amongst all realizations given in Theorem 4.2 for C_1 and C, respectively.*

Proof. We use the steps of above algorithm to prove the results. We start by a $a_2 + a_3 + \cdots + a_\Delta$-gon C. We first show that the number of pendant edges added to the vertices of C is equal to a_1. Indeed, this number is $a_3 + 2a_4 + 3a_5 + \cdots + (\Delta - 2)a_\Delta$ which is equal, by the definition, to $\Omega + a_1$ which is a_1 in this case. In C, there are a_3 $(1, 3)$-vertices, $2a_4$ $(1, 4)$-vertices, $3a_5$ $(1, 5)$-vertices, $\cdots$, $(\Delta - 2)a_\Delta$ $(1, \Delta)$-vertices, $a_2 - 1$ $(2, 2)$-vertices, $a_3 - 1$ $(3, 3)$-vertices, $\cdots$, $a_\Delta - 1$ (Δ, Δ)-vertices, one $(2, 3)$-vertex, one $(3, 4)$-vertex, $\cdots$, one $(\Delta - 1, \Delta)$-vertex, and finally one $(\Delta, 2)$-vertex. So the second Zagreb index of this realization is equal to

$$\begin{aligned} M_2(C) &= \textstyle\sum_{i=2}^{\Delta} \left[(a_i - 1) \cdot i^2 + a_i \cdot (i - 2) \cdot (1 \cdot i) + i \cdot (i - 1)\right] + 2\Delta - 2 \\ &= \textstyle\sum_{i=2}^{\Delta} 2i \cdot (i - 1) \cdot a_i - \frac{\Delta^2 - 3\Delta + 2}{2}. \end{aligned}$$

Next, we draw an $a_2 + a_3 + a_4 + \cdots + a_\Delta - 1$-gon by omitting one of the vertices, say v, having the smallest degree on C together with any pendant edges incident with it and the end vertices incident with these edges. To keep the $\Omega(G)$ unchanged, we add a new vertex which we call v again, onto one, say $uv_{a_2+a_3+\cdots+a_\Delta}$, of the $d_{a_2+a_3+\cdots+a_\Delta} - 2$ existing pendant edges. So the second Zagreb index of this new graph $C_{a_2+a_3+\cdots+a_\Delta-1}$ is

$$M_2(C_{a_2+a_3+\cdots+a_\Delta-1}) = \textstyle\sum_{i=2}^{\Delta} \left[(a_i - 1) \cdot i^2 + a_i \cdot (i - 2) \cdot i + i \cdot (i - 1)\right] + 3\Delta - 4.$$

Continuing in the same fashion, we reach to a 1-gon (loop) C_1 which has the second Zagreb index

$$M_2(C_1) = \textstyle\sum_{i=2}^{\Delta} 2i \cdot (i - 1) \cdot a_i - \frac{\Delta^2 + \Delta - 36}{2}.$$

Now define a function f such that

$$\begin{aligned} f(\Delta) &= M_2(C_{a_2+a_3+\cdots+a_\Delta}) - M_2(C_1) \\ &= 2\Delta - 19. \end{aligned}$$

First note that $f'(\Delta) = 2$ and f is always increasing. Also for $\Delta < 19/2$, $M_2(C_{a_2+a_3+\cdots+a_\Delta})$ $< M_2(C_1)$ and for $\Delta > 19/2$, $M_2(C_{a_2+a_3+\cdots+a_\Delta}) > M_2(C_1)$. This completes the proof.

□

Theorem 4.4. *Let the degree sequence D be realizable and let $\Omega(D) = 0$. Then*

i *the first Zagreb index of G is the same for all graphs G given in Theorem 4.2;*

ii *the forgotten index of G is the same for all graphs G given in Theorem 4.2.*
iii *the Narumi-Katayama index of G is the same for all graphs G given in Theorem 4.2.*

Proof. The first two indices are defined as the sum of powers of the vertex degrees. The third one is the product of all vertex degrees. As the degree sequence is the same for all the realizations, each of these three indices takes the same value. □

Finally we study the sigma index. Recall that the inverse problem for this irregularity index was settled in [9]. Now we have

Theorem 4.5. *Let the graph G be one of the realizations of the degree sequence D given in Theorem 4.2 so that $\Omega(D) = 0$. Then $\sigma(G)$ has its smallest and largest values amongst all realizations given in Theorem 4.2 for C_1 and C, respectively.*

Proof. By Theorem 4.2, to go from C_k to C_{k-1}, we carry a vertex u of degree du on the cycle C_k in graph G onto one of the pendant edges at the vertex w of degree dw in graph G^*, see Fig. 1.

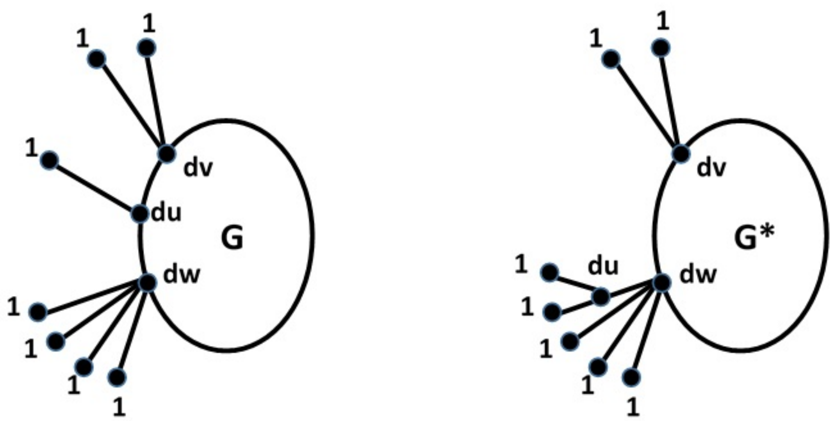

Figure 1. Carrying the vertex u in C_k onto a pendant edge at the vertex w in C_{k-1}

Recall that we had $du \leq dv \leq dw$ in the proof of Theorem 4.2. Note that

$$\begin{aligned}\sigma(G^*) - \sigma(G) &= (dv - dw)^2 + (du - 1)^2 - (du - dv)^2 - (dw - 1)^2 \\ &= -2(dv - 1)(dw - du).\end{aligned}$$

Note that $dv - 1 > 0$ and $dw - du > 0$ implying $\sigma(G^*) < \sigma(G)$. Therefore each time we carry a vertex onto a pendant edge as explained in the proof of Theorem 4.2, the sigma index gets smaller. Therefore we have the largest sigma index for the unicyclic graph C with the largest cycle length and smallest sigma index for the unicyclic graph C_1 having cycle length 1 amongst all fundamental realizations defined in Theorem 4.2. □

5. Results and discussion

Omega invariant of a degree sequence or of a graph has recently been introduced as a new graph invariant and is shown to have a very useful nature about all the realizations of a given degree sequence or of a given graph. It gives information on realizability, connectedness, cyclicness, chords, loops, components, etc. Over 3000 topological graph indices have been defined and applied in the last eight decades to study mathematical and chemical properties. Due to their applications, the values that a graph index attain is an open problem which has been solved partially for several well-known indices and the problem is known as the inverse problem for graph indices. In this work, to help with the solution of the inverse problem, lower and upper bounds for several frequently used topological graph indices are obtained and the computation time that needed to solve inverse problem is reduced.

6. Conclusions

Classical method of giving lower and upper bounds is applied to obtain limits on the values of several impactful topological indices. By the help of our results, it is possible to solve the inverse problem for the indices under investigation in polynomial time.

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