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Extremal Randic type indices

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Abstract

Vertex degree is one of the most important graph notions and many topological graph indices are degree based including the Randic type graph indices. These indices are calculated in terms of vertex degrees of all the edges in a graph. They have been proven to be very useful in chemical applications. It is an important problem called realizability to find all the graphs corresponding to a given set of non-negative integers as the vertex degrees. Although there are several algorithms about the realizability, there is no complete answer working in all cases. Two recently introduced algorithms called odd and even algorithms are proven already to be very useful for calculating the extremal values of the second Zagreb index. In this work, we apply the same algorithms to determine the extremal values of some Randic type topological graph indices. By knowing the extremal values of such indices, we can eliminate a large workload from the computational studies related to graphs and the modeled chemical and other structures.

Keywords: Randic index, topological graph index, omega invariant, cycle length, odd algorithm, Zagreb index of connected unicyclic graphs

2020 MSC: 05C07, 05C09, 05C30

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1. Introduction

We assume that G is a simple finite graph having n vertices and m edges. In such a graph G, the degree of a vertex v of G is defined to be the number of edges meeting at v. It is denoted by $d_G v$ or briefly by dv. If the neighbourhood of a vertex v has only one vertex, in such a case, the vertex v is called a pendant vertex, and it has degree 1.

Graphs are classified up to several graph parameters. One of these parameters is the number of independent cycles which is also named as the cyclomatic number of the graph. If a connected graph has no cycles, then it is a tree. If it has one, two, three, . . ., k-cycles, then it is called unicyclic, bicyclic, tricyclic, . . ., k-cyclic, respectively.

In [4], a new graph invariant was defined which is related to the cyclomatic number and Euler characteristics. See [1, 5, 6, 7, 16, 22, 25] for further details of omega invariant. It is shown that when the omega invariant is equal to zero, it happens that the size and order of the connected graph are equal and this only happens when the graph is unicyclic. Clearly, this case happens when the number of vertices is equal to the number of edges in the graph.

In [5], the authors found that the unique cycle in a connected unicyclic graph may have length as any integer between 1 and $n - a_1$. Here a_1 is the number of pendant vertices in the graph. In [5], it was also shown that when this unique cycle has its maximum length, which is $n-a_1$, the graph consists of a cycle of length $n-a_1$, and some pendant edges with one of their vertices is on the cycle. If v is such a vertex on the cycle having degree dv, then this vertex will

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be incident to $dv-2$ pendant edges as two neighbour vertices already are on the cycle, and all edges of the graph will either be such a pendant edge or an edge on the cycle. This specific form of the graph implies same advantages to us.

In [17], two new algorithms were given to find the extremal values of the second Zagreb index of such unicyclic graphs having maximum cycle length.

In this paper, we shall apply these two novel algorithms to some Randic type topological graph indices. In the proofs of our algorithms, we made use of the facts given in Lemma 1.1 and Lemma 1.2.

Lemma 1.1 (*cf.* [15])**.** *If $a \geq b$ and $x \geq y$, then*

$$ax + by \geq ay + bx.$$

A more general result known as the rearrangement inequality is used in both algorithms:

Lemma 1.2 (*cf.* [15] (Rearrangement inequality))**.** *If $a_1 \leq a_2 \leq \cdots \leq a_n$ and $b_1 \leq b_2 \leq \cdots \leq b_n$ are real numbers, then*

$$a_1b_1 + a_2b_2 + \cdots + a_nb_n \geq c_1b_1 + c_2b_2 + \cdots + c_nb_n \geq a_nb_1 + a_{n-1}b_2 + \cdots + a_1b_n$$

for any permutation $(c_1, c_2, \ldots, c_n)$ of $(a_1, a_2, \ldots, a_n)$.

This means that if we multiply pairs of integers taken from two given sets and add their products, the value obtained by multiplying the large one with large one and small one with small one is the largest result. This idea is used in our odd and even algorithms to discriminate between the algorithms giving extremal values of several topological graph indices where the index includes a sum of product of pairs of numbers. Using these lemmas, two new algorithms were recently given which are recalled below:

In [17], Ozden Ayna introduced two novel algorithms to find the minimum and maximum values of the second Zagreb index of connected unicyclic graphs with cycle length

$$n - a_1.$$

These algorithms are called odd and even algorithms. Let us recall them:

Theorem 1.3 (Odd algorithm)**.** *Let*

$$\Omega(D) = 0.$$

Amongst all realizations of D which are unicyclic and has maximum cycle length, the one constructed as below has the minimum second Zagreb index:

Step 1: *Label the vertices of the cycle by $v_1, v_2, \ldots, v_n$ in rotating order (clockwise or anticlockwise). Without loss of generality, we choose anticlockwise orientation.*

Step 2: *Assign the largest vertex degree d_1 to v_1.*

Step 3: *Assign the smallest vertex degree d_{n-a_1} to v_2 and the next smallest vertex degree d_{n-a_1-1} to v_{n-a_1}. Note that, when placing two smallest degrees to the next vertices to be labelled, we place the smaller one to the next unlabelled vertex anticlockwise and the larger one (or equal one) to the next unlabelled vertex clockwise.*

Step 4: *Assign the next largest vertex degree d_2 to v_3 and the remaining next largest vertex degree d_3 to v_{n-a_1-1}. Similarly to the previous step, when assigning next two largest degrees to the remaining vertices, we place the larger one to the next unlabelled vertex anticlockwise and the larger one (or equal one) to the next unlabelled vertex clockwise.*

Step 5: *Assign the next remaining smallest vertex degree d_{n-a_1-2} to v_4 and the next remaining smallest vertex degree to v_{n-a_1-2}.*

Step 6: *Assign similarly d_4 to v_5 and d_5 to v_{n-a_1-3}.*

Step 7: *Repeat the last two steps until all vertices are labelled by the remaining vertex degrees.*

Theorem 1.4 (Even algorithm)**.** *Let*

$$D = \left\{1^{(a_1)}, 2^{(a_2)}, \dots, \Delta^{(a_\Delta)}\right\}$$

be a degree sequence with

$$\Omega(D) = 0.$$

Let $G_i(n - a_1)$ be a connected realization of D. We know that as in minimum values case, $G_i(n - a_i)$ is unicyclic realization with maximum cycle length $n - a_1$. The maximum value of second Zagreb index is obtained for the graph constructed as below:

***Step 1:** Assign the largest vertex degree to a vertex, say v_1.*

***Step 2:** Assign the next largest vertex degree to one of the two vertices adjacent to v_1, say v_2.*

***Step 3:** Assign the next largest vertex degree to the adjacent vertex with largest vertex degree so far. This is v_1. So let us call this vertex by v_3.*

***Step 4:** For all the remaining vertex degrees, assign the largest value to the vertex which is adjacent to the larger one of the two vertices at both ends of the labelled vertices.*

In [17], Ozden Ayna obtained that the odd algorithm always gives the minimum second Zagreb index amongst all realizations of D. Similarly, the even algorithm gives us the maximum second Zagreb index. Now we try to understand the behaviour of odd and even algorithms for some other graph indices.

In this paper, we have concentrated on irregularity indices of certain unicyclic graphs as the total number is over 3000. We have determined that as in second Zagreb index case the odd algorithm always gives the maximum values of the irregularity indices under consideration.

2. Some Randic type graph indices

Topological graph indices are defined and studied for both mathematical reasons and applications. Since 1947, many examples have been defined and some of them are applied to different disciplines. One of these topological graph index families is called as Randic indices. The classical Randic index of a graph is one of the oldest graph indices in graph theory. It is defined in [18] as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{dudv}}.$$

By means of the bounds on the Randic energy, Liu et al. improved the existing results for the Randic spectral radius (*cf.* [14]). The aim of this paper on Randic energy is to establish relations with other known energies like normalized Laplacian energy and its signless form with Randic energy. So many new physical formulae depending on these energies can be computed just by means of Randic type energies easily. Randic energy exactly corresponds to the normalized Laplacian energy and the normalized signless-Laplacian energy. So many other numerical formulae such as Kirchhoff index, resistance distance and average page length which are directly related to normalized Laplacian and signless Laplacian can be obtained by Randic energy. Sharp upper and lower bounds for the spectral radius of a graph were recently obtained by Jahanbani et al. [12], and also see [2, 3, 9, 11, 13, 18, 19, 20, 23, 24] for more details.

Due to all those applications, people introduced new variants of Randic index which are usually called as Randic type indices. In this paper, we shall consider four of such variants which are the reciprocal Randix index

$$RR(G) = \sum_{uv \in E(G)} \sqrt{dvdv}$$

introduced in [8]; IRA, IRB and IRC indices defined by

$$IRA(G) = \sum_{uv \in E(G)} \left(d_u^{-\frac{1}{2}} - d_v^{-\frac{1}{2}}\right)^2,$$

$$IRB(G) = \sum_{uv\in E(G)} \left(d_u^{\frac{1}{2}} - d_v^{\frac{1}{2}}\right)^2$$

and

$$IRC(G) = \frac{1}{m} \sum_{uv\in E(G)} \sqrt{d_u d_v} - \frac{2m}{n},$$

where m and n are positive integers (*cf.* [21]). After some algebraic calculations, one can easily get

$$IRA(G) = n - 2R(G),$$

$$IRB(G) = M_1(G) - 2RR(G)$$

and

$$IRC(G) = \frac{RR(G)}{m} - \frac{2m}{n},$$

where m and n are positive integers.

Because of the similar nature of RR, IRA, IRB and IRC with the classical Randic index, the results for these Randic type indices will all be relevant to the results on $R(G)$. Therefore we now concentrate on the effect of odd and even algorithms on the Randic index:

Theorem 2.1. *The Randic index takes its maximum/minimum values amongst all simple connected unicyclic graphs having maximum cycle length for even/odd algorithm, respectively.*

Proof. Recall the definition of Randic index as

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{dudv}}.$$

By the rearrangement inequality given in Lemma 1.1, the sum of products for two edges

$$e = uv$$

and

$$f = rs$$

with the property that

$$du \leq dr$$

and

$$dv \leq ds$$

satisfy the following inequality:

$$dudv + drds \geq dudr + dvds.$$

Using the general case given in the Rearrangement inequality given in Lemma 1.2, we see that Randic index gets its minimum value for the realization obtained by odd algorithm. The same inequalities can be used to deduce the fact that Randic index gets its maximum value for the realization obtained by even algorithm. ☐

Note the similarity between the formulae for Randic and reciprocal Randic indices. Hence we get the result for reciprocal Randic index as below:

Theorem 2.2. *The reciprocal Randic index RR takes its maximum/minimum values amongst all simple connected unicyclic graphs having maximum cycle length for even/odd algorithm, respectively.*

Proof. The proof is similar to the one given for the second Zagreb index in [17] because of the similarity of both indices. Note that larger values of

$$dudv$$

correspond exactly to larger values of

$$\sqrt{dudv}.$$

Therefore, the same argument implies the result. □

Because of the reciprocal numbers in both definitions, one expects to use different algorithms to get the maximum/minimum values of Randic and reciprocal Randic indices, but interestingly, we need the same algorithm for both indices to get minimum and maximum values.

Finally we obtain the similar result for the remaining three Randic type graph indices. We start with IRA index:

Corollary 2.3. *IRA takes its maximum/minimum values amongst all simple connected unicyclic graphs having maximum cycle length for odd/even algorithm, respectively.*

Proof. It is well-known that

$$IRA(G) = \sum_{uv\in E(G)} \left(\frac{1}{\sqrt{du}} - \frac{1}{\sqrt{dv}} \right)^2 .$$

Therefore,

$$IRA(G) = n - 2R(G).$$

This means that IRA and R are anti-proportional. Hence, by Theorem 2.1, as the Randic index takes its minimum value for odd algorithm, IRA, on the contrary, takes its maximum value for odd algorithm and hence its minimum value for even algorithm. □

Interestingly enough, we can deduce the similar result for IRR and IRC indices by means of reciprocal Randic index instead of Randic index itself:

Corollary 2.4. *IRB and IRC take their maximum/minimum values for odd/even algorithm amongst all simple connected unicyclic realizations having maximum cycle length.*

Proof. Recall that

$$IRB(G) = \sum_{uv\in E(G)} \left(\sqrt{du} - \sqrt{dv} \right)^2$$

Thus, we get

$$IRB(G) = M_1(G) - 2RR(G),$$

where $M_1(G)$ denotes the first Zagreb index of a graph G, defined as follows (*cf.* [10]):

$$M_1(G) = \sum_{u\in V(G)} du^2.$$

As the set of vertex degrees is fixed in our special case of connected unicyclic graph realizations having maximum cycle length, $M_1(G)$ is also fixed for all such graphs. Hence RR and IRB indices are proportional reciprocally. Secondly, note that there is the following relation between IRC and RR indices:

$$IRC(G) = \frac{\sum_{uv\in E(G)} \sqrt{dudv}}{m} - \frac{2m}{n},$$

where positive integers m and n. Therefore, we have

$$IRC(G) = \frac{RR(G)}{m} - \frac{2m}{n}.$$

This relation shows that these two indices are directly proportional, implying the result. □

3. Applications

Although the history of graph theory starts with the centennial paper of Euler in 1736, there are many other works utilizing graphs in earlier centuries. But of course the most achievements are made in the last century together with the advances in computer technologies, both in terms of software and hardware. The first real application of topological graph indices is due to chemist Wiener [26], where he presented a comparative method based on a mathematical formula to compare and guess the boiling temperatures of the isomers of alkanes. Since then, this method is generalized and applied to many physico-chemical properties of chemical structures. Randic type topological indices which are calculated in terms of vertex degrees of all edges in a graph naturally gained an important place in this story together with Zagreb, Hosoya, GA, ABC, etc. index families.

Mathematical modeling with graphs has been applied to many intrinsic areas. Chemical structures form the most popular example. One can model a molecular structure by a graph by corresponding a vertex for each atom and an edge corresponding to each chemical bond. In such a way, we can form a graph corresponding to the given molecular structure.

Naturally, the applications of such a clever modeling could not be bounded by chemistry and this idea has been extended to many areas including pharmacology, pharmaceutical sciences, biology, physics, energy related topics, network sciences, city planning, shortest route problems, trade problems, industrial engineering problems, etc.

Once a newly defined topological graph index finds some interest and becomes popular with several applications, people usually try to obtain similar topological graph indices and meantime, this index produces a class of indices like Zagreb type or Randic type indices. Here the Randic type indices have been examined in details by means of two recently given algorithms.

4. Conclusions

For a given realizable degree sequence, it is possible to have a large number of graph realizations. A natural question is to ask the common properties of these realized graphs. Several algorithms have been given for some partial answers. Recently, two new algorithms called odd and even algorithms have been introduced and used for determining the extremal values of the second Zagreb index and also for some irregularity indices.

Here, we obtained some surprising results for the extremal values of five Randic type indices amongst all simple connected unicyclic realizations having maximum cycle length. Knowing the extremal values of such topological graph indices helps to reduce the computational work with theoretical graphs and also with the application areas, mainly chemistry, networks, neuroscience, etc. We also gave a section for the applications of such index classes.

We believe that the methods used here can be extended to other graph types and topological graph indices.

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