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Energy of Some Unicyclic Graphs and Omega Invariant

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Abstract

[1] [2] A unicyclic graph is a graph which contains exactly one cycle. In a connected unicyclic graph, the number of edges must be equal to the number of vertices. Energy of a graph had been defined by Gutman nearly five decades ago as the sum of the absolute values of the eigenvalues of the adjacency matrix, which are the roots of the so-called characteristic polynomial, of the graph. In this paper, our aim is to obtain the characteristic polynomials corresponding to unicyclic graphs having the same given degree sequence using the concept of omega invariant $\Omega(G)$ of a graph G which was recently defined by Delen and Cangul. We also obtained some of the terms of the characteristic polynomials of these graphs. In particular, we deduce a formula for the specific unicyclic graphs $T_{r,1}$.

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1 Introduction and notions

In this work, we shall deal with connected undirected simple graphs. In mathematics, and in particular, in spectral graph theory, the concept of graph energy was defined by Gutman in 1978, see [9]. The graph energy of a graph G is denoted by $E = E(G)$. It can be used to estimate the total π-electron energy of a molecule in Chemistry using molecular graphs. Since its definition, there has been a lot of advancements in mathematical chemistry related to the application areas of the notion of energy. In recent years, many authors introduced several variants of energy by using other graph matrices in place of adjacency matrix. See [2] for further information on spectral graph theory and energy.

In [3], Delen and Cangul introduced a new graph invariant called omega invariant which is denoted by $\Omega(G)$ for a graph G or for some given degree sequence D. This number Ω which is related to well-known Euler characteristic for a given graph or degree sequence helps us to decide about many combinatorial, graph theoretical, structural and topological properties that the graph or all realizations of the degree sequence has. For some properties and applications of the omega invariant, see [1, 4, 5, 6, 7, 8, 11, 12, 13].

Let G be a graph with the vertex set $V(G)$ and edge set $E(G)$. Let $|V(G)| = n$ be the order of the graph G and let $|V(G)| = m$ be the size of the graph G. If $v \in V(G)$, then the degree of v in G is denoted by $d_G(v)$ and is defined to be the number of vertices in G which are adjacent to v. Here, we briefly use dv instead of $d_G(v)$. For undefined terminologies we refer [10].

A connected graph containing no cycles is called a tree. A graph having one, two, three cycles is called unicyclic, bicyclic and tricyclic graph, respectively and for higher number of cycles, similar naming can be done. In this paper, we calculated the energy of some unicyclic graphs with the help of a new graph invariant $\Omega(G)$. So, we have obtained the characteristic polynomials corresponding to all unicyclic graphs having the same degree sequence using the concept $\Omega(G)$. We also tried to find some of the general terms for the characteristic polynomials of these graphs.

The energy of a graph is defined as the sum of the absolute values of the eigenvalues of the adjacency matrix $A(G)$ of the graph in [9]. If $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the eigenvalues of $A(G)$, then the energy of a graph G is denoted by $E(G)$ and given by

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

The set of distinct eigenvalues $\lambda_1 > \lambda_2 > \cdots > \lambda_r$ of a graph G with their multiplicities being $m_1, m_2, \cdots, m_r$ is called the spectrum of G and it is denoted by

$$\text{Spec(G)} = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_r \\ m_1 & m_2 & \cdots & m_r \end{pmatrix}.$$

The adjacency matrix of a graph G is a square matrix and denoted by $A(G) = [a_{ij}]$ of order n where

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise,} \end{cases}$$

[9].

The characteristic polynomial of $A(G)$ is defined as

$$det(A(G) - \lambda I),$$

where I is the identity matrix. That is, this polynomial is the one that has the eigenvalues of the adjacency matrix as its roots.

The most studied graph polynomial is the characteristic polynomial of its adjacency matrix [2]. After this particular one, th eLaplacian and incidency matrices come next and these are followed by over a hundred other graph matrices.

There has been a huge number of research articles dealing with graphs having a specified number of cycles in the last few decades. A unicyclic graph which is the main object of this work is a graph which contains exactly one cycle. In a connected unicyclic graph, the number of edges is equal to the number of vertices as it can be understood from its name.

The minimum vertex degree in a graph G is denoted by $\delta = \delta(G)$, and the maximum vertex degree is denoted by $\Delta = \Delta(G)$. In an undirected graph G, the degree sequence of G is a monotonic non-decreasing sequence of non-negative integers which are the vertex degrees of G. That is, the degree sequence of a graph is just the set of vertex degrees. That is, the degree sequence of a graph G is $DS(G) = \{0^{(a_0)}, 1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \ldots, \Delta^{(a_\Delta)}\}$.

As a graph invariant, the omega invariant was defined recently in [3] as follows: Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ be a set. The omega invariant $\Omega(D)$ of D is defined only in terms of the vertex degrees as

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

Similarly, the omega invariant can be defined for a graph G similarly.

The Ω values of some well-known graph classes such as path, cycle, star, complete, complete bipartite and tadpole graphs are as follows: $\Omega(P_n) = -2,\ \Omega(C_n) = 0,\ \Omega(S_n) = -2,\ \Omega(K_n) = n(n-3),\ \Omega(K_{r,s}) = 2[rs - (r+s)],\ \Omega(T_{r,s}) = 0,\ \Omega(T) = -2.$

Let $D = \{0^{(a_0)}, 1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \ldots, \Delta^{(a_\Delta)}\}$ be a set. If there is a graph having this set as the set of all of its vertex degrees, then D is called realizable. That is, for a realizable set D, there exists at least one graph having degree sequence D. A graph G is a realization of the set D if the degree sequence of G is equal to D. There are a lot of algorithms to determine the realizability of a given set. But by means of the omega invariant, it is possible to decide the realizability of D much more easily: We have that for $D = \{0^{(a_0)}, 1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \ldots, \Delta^{(a_\Delta)}\}$, if $\Omega(D)$ is even, then D is realizable. This is because of the fact that for any graph G, $\Omega(G)$ is even. Therefore, if $\Omega(D)$ is odd for a degree sequence D, then D is not realizable.

2 Main results

In this section, we obtained some observations on the characteristic polynomials and their coefficients of all unicyclic realizations of a given degree sequence. We first note that the omega invariant of a unicyclic graph is zero. Our main results are as follows:

Theorem 2.1. *Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ and $\Omega(D) = 0$. That is, let all connected realizations of D be unicyclic. The maximum length l_{max} of the unique cycle in any graph realization G of D is equal to*

$$l_{max} = a_2 + a_3 + \cdots + a_\Delta = n - a_1.$$

That is, the maximum possible length of the unique cycle is equal to the sum of the multiplicities of vertex degrees $2, 3, 4, \cdots, \Delta$.

Proof. Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ be the degree sequence of a graph G. Then the number of vertices of any graph realization of D is the same and equal to n which is $n = a_1 + a_2 + a_3 + \cdots + a_\Delta$. In [3], it was proven as Corollary 3.6 that if $\Omega(G) = 0$, then any realization of D has no chords, loops nor multiple edges. Therefore, all the vertices of degree at least two will be on the unique cycle of the unicyclic realization of D. This means that only the vertices of degree 1 are excluded. That is, there are $n - a_1$ vertices on the cycle which gives the result. □

Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ be a realizable degree sequence with $a_1 + a_2 + \cdots + a_\Delta = n$ and its realizations be the graphs $G_1, G_2, \cdots$. Then, the highest power of the variable in the characteristic polynomial is n, that is the degree of the characteristic polynomial is the number of vertices as well-known.

In [3], the graphs are grouped into three families according to the value of omega invariant as $\Omega(D) \leq -4$, $\Omega(D) = -2$ or $\Omega(D) \geq 0$. For each family, a new type of realization called the fundamental realization was given in the same work. As we are considering the unicyclic graphs which correspond to the second case, in particular, to the case of $\Omega(D) = 0$, we shall recall the definition of the fundamental realization as follows: When $\Omega(D) = 0$, all connected realizations of D are unicyclic and the length of this unique cycle can be any integer between 1 and $l_{max} = a_2 + a_3 + \cdots + a_\Delta = n - a_1$, see [7]. The realization with maximum cycle length is called as the fundamental realization. For more information and further properties of the omega invariant, see [1, 4, 5, 6, 8, 11, 12, 13].

So, the possible cycle lengths of the connected unicyclic graph realizations of a given degree sequence with $\Omega(D) = 0$ are between 1 and $n - a_1$. We shall denote the unicyclic graph having k vertices by U_k in a unicyclic graph. In the case where the cycle length is maximum, all non-pendant vertices lie on the unique cycle. As an example, consider the following degree sequence $D = \{1^{(11)}, 2^{(2)}, 3^{(3)}, 4^{(1)}, 5^{(2)}\}$. The fundamental graph realization is U_8 which is the first graph in Fig. 1. In the same figure, one can see one realization of D having 7, 6, 5, 4, 3, 2 and 1 cycles. These realizations are denoted by U_7, U_6, U_5, U_4, U_3, U_2, U_1.

Now we have the signature of the leading term of the characteristic polynomial of a unicyclic graph:

Theorem 2.2. *Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ be a realizable degree sequence with $a_1 + a_2 + \cdots + a_\Delta = n$ and its realizations be the graphs $G_1, G_2, \cdots$. Then, the first*

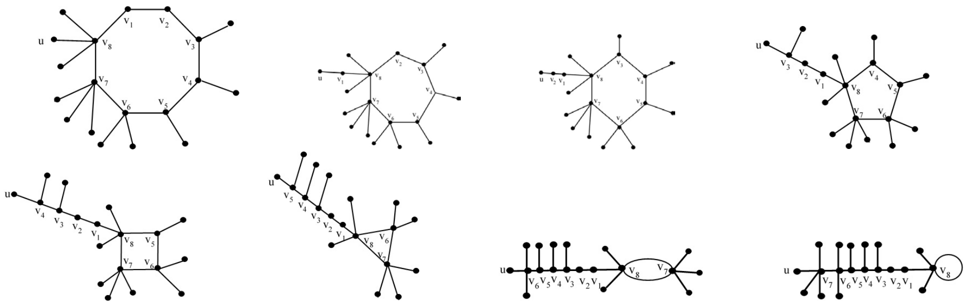

Figure 1: Fundamental realizations of $D = \{1^{(11)}, 2^{(2)}, 3^{(3)}, 4^{(1)}, 5^{(2)}\}$

term in the characteristic polynomial of a realization of D *is*

positive	*if* n *is even*
negative	*if* n *is odd.*

Therefore the first term of the characteristic polynomial of a unicyclic graph is x^n if n is even and $-x^n$ if n is odd.

Proof. From the definition of the characteristic polynomial, all entries in the main diagonal of the matrix $A(G) - \lambda I$ are $-\lambda$. This proves the sign of the leading term. Also as the adjacency matrix is of dimension n, the leading term should contain n-th power of λ which completes the proof. □

In general, the characteristic polynomial of a unicyclic graph G of order n starts with $\pm x^n$ and there is no unique formula for the remaining terms. There are some well-known formulae for some classes of graphs. The only certain thing is that there is no term of order $n-1$. The second term is normally the term of order $n-1$, but here, for the characteristic polynomial of a unicyclic graph, we have $a_{n-1} = 0$.

Theorem 2.3. *The second non-zero term in the characteristic polynomial of any unicyclic realization of* D *is* $a_{n-2}x^{n-2}$.

Therefore the first two terms of the characteristic polynomial of G are $\pm x^n \mp a_{n-2}x^{n-2}$. The lower order terms follow no rule. For some graphs such as complete bipartite graphs $K_{r,s}$, there are only two terms, namely $x^{r+s} - rsx^{r+s-2}$.

Recall that the number of edges in the complete bipartite graph $K_{r,s}$ is rs which is the coefficient of x^{n-2}. This is true in fact for all unicyclic graphs:

Conjecture 2.1. *The coefficient of x^{n-2} in the characteristic polynomial of a unicyclic graph is equal to the number of edges in the graph, that is*

$$a_{n-2} = \begin{pmatrix} n \\ 2 \end{pmatrix}.$$

Finally, we obtain a formula for one of the most popular unicyclic graph classes called the tadpole graphs. A tadpole graph $T_{r,s}$ is a graph obtained by adjoining a path P_s to a cycle graph C_r. In Fig. 2, the tadpole graph for $r = 4$ and $s = 2$.

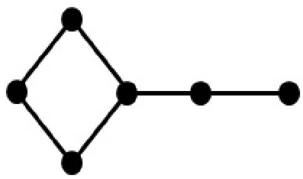

Figure 2: Tadpole graph $T_{4,2}$

Theorem 2.4. *The characteristic polynomial of the tadpole graph $T_{r,1}$, $r \geq 3$, satisfies the following relation:*

$$P(T_{r,1})(\lambda) = \lambda P(C_r)(\lambda) - P(P_{r-1}).$$

Proof. The characteristic polynomial of the tadpole graph $T_{r,1}$ is obtained by the determinant

$$P(T_{r,1})(\lambda) = \begin{bmatrix} -\lambda & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 \\ 1 & -\lambda & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\lambda & 1 & \cdots & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & -\lambda & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -\lambda & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -\lambda & 1 \\ 0 & 1 & 1 & 0 & 1 & \cdots & 0 & 0 & 1 & -\lambda \end{bmatrix}.$$

This is an $(r + 1) \times (r + 1)$ matrix. We now calculate this determinant according to the last column as follows:

$$P(T_{r,1})(\lambda) = (-\lambda)(-1)^{2r+2} \begin{bmatrix} -\lambda & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 1 & -\lambda & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & -\lambda & 1 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & -\lambda & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -\lambda & 1 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -\lambda \end{bmatrix} +$$

$$(-1)^{2r+1} \begin{bmatrix} -\lambda & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -\lambda & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & -\lambda & 1 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -\lambda & 0 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 \end{bmatrix}.$$

Here the first $r \times r$ determinant corresponds to the characteristic polynomial of $P(C_r)$ and the second $r \times r$ determinant can be calculated according to the last column giving the characteristic polynomial of the path graph P_{r-1} completing the proof. □

3 Summary and conclusions

In this work, we obtained several properties of the characteristic polynomials corresponding to all unicyclic graphs having the same degree sequence using the concept of $\Omega(G)$. We also tried to find some of the general terms for the characteristic polynomials of these graphs.

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