

Algebraic Method for Characteristic Edge-Zagreb and Laplacian Polynomials of Graphs

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Abstract

Polynomials corresponding to graphs and their roots have many applications including the energy defined algebraically by means of the adjacency matrix which is defined as a $0 - 1$ matrix according to the neighbouring relations of vertices. In literature, many notions depend on the adjacency matrix and the characteristic polynomial of the adjacency matrix is used in the definition of the energy of the graph. Recently, some other matrices are used in obtaining characteristic polynomial. In this work, two important matrices, edge-Zagreb and Laplacian, are used to study the characteristic polynomial by means of rather unusual algebraic way of using elementary subgraphs

1 Introduction

^{1 2} Let G be a graph with vertex set $V(G) = \{v_1, \dots, v_n\}$ and edge set $E(G) = \{e_1, \dots, e_n\}$. The degree of a vertex v is denoted by $d(v)$. If there is an edge e between two vertices v_i and v_j , then these vertices are called adjacent and this situation is shown as $e = v_i v_j$. Also in this case, e is said to be incident to the vertices v_i and v_j . A subgraph of a graph G is a graph H such that $V(H) \subseteq V(G)$, $E(H) \subseteq E(G)$. If $V(H) = V(G)$, then H is called a spanning subgraph of G . A component of G is a maximal connected subgraph of G . If the graph has no multiple edges and

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nor loops, then it is called simple. In this paper, all considered graphs are simple.

Recently people are intensively interested in graph theory to make easier some real life difficulties. Instead of running out of time, manpower, money, we can use graph theoretical methods. Graph theory increasingly used not only for mathematical research but also in theoretical physics, operational research, electrical engineering, organic chemistry, and so forth. Other branches of science take advantages of graph theory. Here we study properties of graphs by means of some corresponding matrices. A lot of matrices are defined with respect to any given graph. The best known matrix is vertex adjacency matrix, which briefly will be called as the adjacency matrix. In addition to adjacency matrix, there are edge adjacency, edge-Zagreb adjacency, Laplacian adjacency and incidence matrices, etc. These matrices are as important as the adjacency matrix and they play a substantial role in several research areas related to several other types of graph energy. For example, the intermolecular energy of a chemical compound which is the sum of the absolute values of the eigenvalues of the adjacency matrix can be obtained by mathematical calculations by means of a graph that is modelling corresponding chemical compound, see [3, 4, 6, 10].

The spectral graph theory takes care of spectral properties of a given graph G by studying matrices, eigenvalues, eigenvectors for G . E. Hückel is the first man that defined the energy of a graph while searching for a method to obtain approximate solutions of Schrödinger equation for a class of organic molecules. In Physics and Chemistry, this equation has a significant inherently constitute a sub-area of graph theory. In chemistry, we make use of graphs very often. Hence calculation of the energy of any molecule has high importance in Chemical Graph Theory.

Mathematically, it is shown that the energy of a graph G which is used in modelling a molecule is defined as the sum of absolute values of all eigenvalues of the adjacency matrix $A(G)$ of G which is an $n \times n$ matrix $A = [a_{ij}]$ defined by

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

The rest of the paper is designed as follows: Similarly to the adjacency matrix, in the second section, we give the definition of edge-Zagreb adjacency matrix and find some spectral properties of it. The idea of edge adjacency similarly to the classical vertex adjacency is studied in [13]. In [12], sum-edge characteristic polynomials of graphs have been obtained. In [15], the authors studied the edge-Zagreb spectral radius and edge-Zagreb energy of graphs in a different manner than the way we follow here. Also in the third section, we recall the definition of Laplacian adjacency matrix and calculate the spectral properties as in Section 2. Some results on Laplacian energy was obtained in [7]. For subdivision graphs with a fixed given chromatic number, the maximal energy was determined in [8].

2 Edge-Zagreb adjacency matrices, determinants and characteristic polynomials

In this part, we study the edge-Zagreb adjacency matrices, their determinants and edge-Zagreb characteristic polynomials. During the calculations, we use permutations that are used in the determinant definition.

Here we start with the definition of edge-Zagreb adjacency matrix of a graph G .

Definition 2.1. [9] [14] Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$ that have n and m elements, respectively. The edge-Zagreb adjacency matrix $ZM(G) = [z_{ij}]_{n \times n}$ of G is defined by

$$z_{ij} = \begin{cases} d(v_i)d(v_j), & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0, & \text{otherwise} \end{cases}.$$

Let M be any matrix with dimension $n \times n$. The characteristic polynomial of M is equal to $|xI - M|$. Analogously, the edge-Zagreb characteristic polynomial of a graph G is equal to $|xI - ZM(G)|$. We denote it with $P_G^{ez}(x)$.

We call a subgraph as an elementary subgraph if every component of it is either an edge or a cycle, [1]. An elementary subgraph is called a spanning elementary subgraph if the set of vertices of the subgraph is the same with the vertex set of the graph G itself. $c_-(H)$ and $c_0(H)$ are defined as the number of components in a subgraph H that are edges and cycles, respectively.

Definition 2.2. [5] Let $A = [a_{ij}]_{n \times n}$ be a matrix. The determinant of the matrix A is defined by

$$|A| = \sum (\pm) a_{1\sigma_1} a_{2\sigma_2} \cdots a_{n\sigma_n}$$

where the summation is taken over all permutations $\sigma_1, \sigma_2, \dots, \sigma_n$ of the set $S = \{1, 2, \dots, n\}$. Since we calculate this summation for all permutations and S has $n!$ permutations, $|A|$ has $n!$ terms. Let us express the formula for edge-Zagreb adjacency matrix:

Let $ZM(G) = [z_{ij}]_{n \times n}$ be the edge-Zagreb adjacency matrix of G as above.

$$|ZM(G)| = \sum \text{sgn}(\sigma) z_{1\sigma(1)} z_{2\sigma(2)} \cdots z_{n\sigma(n)}$$

where the summation is over all permutations of the set S . $\text{sgn}(\sigma)$ is $+1$, -1 if σ is even permutation, if σ is odd permutation, respectively. It is denoted by $\text{sgn}(\sigma) = (-1)^r$, r is the number of transpositions that σ has them, when σ is written as a product of transpositions.

We can now give the following result which can be proven similarly by a method given in [2]. We define v_i and v_j as two adjacent vertices in a cycle component of corresponding spanning elementary subgraph of G . Also, we define u_i and u_j as two adjacent vertices in an edge components of corresponding spanning elementary subgraph of G .

Theorem 2.1. Let G be any graph with vertex set $V(G) = \{v_1, \dots, v_n\}$ and edge set $E(G)$. Let $ZM(G)$ be the edge-Zagreb adjacency matrix of G . Then

$$|ZM(G)| = \sum (-1)^{n-c_-(H)-c_o(H)} 2^{c_o(H)} \prod_{\substack{i,j=1 \\ j>i}}^n [d(u_i)d(u_j)]^2 \prod_{\substack{i,j=1 \\ j>i}}^n [d(v_i)d(v_j)]$$

where the summation is taken over all spanning elementary subgraphs H of G .

When calculating the latter product in Theorem 2.1 corresponding to cycle components, we consider only one of the edges $v_i v_j$ and $v_j v_i$ because of Definition 2.2. Also if either one of the cycle components or edge components does not exist in the spanning elementary subgraph, we exclude the corresponding product in the statement of Theorem 2.1. We consider both of the edges $u_i u_j$ and $u_j u_i$ by using Definition 2.2 and therefore the square appears in the first product corresponding to edge components.

Proof. We know that

$$|ZM(G)| = \sum \operatorname{sgn}(\sigma) z_{1\sigma(1)} z_{2\sigma(2)} \cdots z_{n\sigma(n)}$$

by the Definition 2.2. Let us deal with the term $z_{1\sigma(1)} z_{2\sigma(2)} \cdots z_{n\sigma(n)}$ that is nonzero as other terms are zero due to the non-adjacency, or they do not correspond to any spanning elementary subgraphs because of the deficiency of some vertex. Since the components of spanning elementary subgraphs are allowed to be either an edge or a cycle, some of these terms correspond to 2-dimensional cycles that are edges and some of these terms correspond to k -cycles. In the $|ZM(G)|$, every nonzero term results from any spanning elementary subgraph H of G . Let us assume that $z_{1\sigma(1)} z_{2\sigma(2)} \cdots z_{n\sigma(n)}$ corresponds to a spanning elementary subgraph H of G , then by the definition of $ZM(G)$ we know that entries are the products of the degrees of vertices, and as every permutation can be written in terms of transpositions, we get

$$\sum \prod_{\substack{i,j=1 \\ j>i}}^n [d(u_i)d(u_j)]^2 \prod_{\substack{i,j=1 \\ j>i}}^n [d(v_i)d(v_j)].$$

It is clear that every cycle can be linked to cyclic permutations in two different ways, giving a contribution $2^{c_o(H)}$ to the required determinant.

Since any cycle can be written as a product of transpositions and as any edge has the form (ij) , we have $\operatorname{sgn}(\sigma) = (-1)^{n-c_-(H)-c_o(H)}$. As a result, we have

$$|ZM(G)| = \sum (-1)^{n-c_-(H)-c_o(H)} 2^{c_o(H)} \prod_{\substack{i,j=1 \\ j>i}}^n [d(u_i)d(u_j)]^2 \prod_{\substack{i,j=1 \\ j>i}}^n [d(v_i)d(v_j)].$$

□

The following result will be needed:

Theorem 2.2. [11] Let A be a square matrix of dimension n . Let the characteristic polynomial of A be $P(x) = x^n + c_1x^{n-1} + c_2x^{n-2} + \dots + c_n$. Then $c_k = (-1)^k \sum (\text{all } k \times k \text{ principal minors})$.

We can now give the formula for the coefficients of the edge-Zagreb characteristic polynomial of any graph G . Let us denote the edge-Zagreb characteristic polynomial of G by $P_G^{ez}(x) = x^n + c_1x^{n-1} + c_2x^{n-2} + \dots + c_n$. Then we have

Theorem 2.3. Let G be any graph of order n and let $P_G^{ez}(x)$ be the edge-Zagreb characteristic polynomial of G as above. Then the coefficients of this characteristic polynomial are given by

$$c_k = \sum (-1)^{c_-(H) + c_o(H)} 2^{c_o(H)} \prod_{\substack{i,j=1 \\ j>i}}^n [d(u_i)d(u_j)]^2 \prod_{\substack{i,j=1 \\ j>i}}^n [d(v_i)d(v_j)].$$

Here the summation is taken over all elementary subgraphs H of G with k vertices.

Note that v_i, v_j, u_i , and u_j are defined as in Theorem 2.1, but instead of the statement spanning elementary subgraph, here we have elementary subgraph.

Proof. By Theorem 2.2, $c_k = (-1)^k \sum (\text{all } k \times k \text{ principal minors})$ and by Theorem 2.1, we get

$$c_k = (-1)^k \sum (-1)^{k-c_-(H)-c_o(H)} 2^{c_o(H)} \prod_{\substack{i,j=1 \\ j>i}}^n [d(u_i)d(u_j)]^2 \prod_{\substack{i,j=1 \\ j>i}}^n [d(v_i)d(v_j)]$$

and hence

$$c_k = \sum (-1)^{c_-(H) + c_o(H)} 2^{c_o(H)} \prod_{\substack{i,j=1 \\ j>i}}^n [d(u_i)d(u_j)]^2 \prod_{\substack{i,j=1 \\ j>i}}^n [d(v_i)d(v_j)],$$

where the summation is taken over all elementary subgraphs H of G with k vertices. \square

We can now prove the following result by means of [1].

Theorem 2.4. Let us take any graph G with $|V(G)| = n$. Let $P_G^{ez}(x)$ be as above. Assume that $c_1 = c_3 = \dots = c_{2t+1} = 0$. Then there is no odd cycle with $2j + 1$ edges where $j = 1, 2, \dots, t$. Also, let G be any regular graph and let the number of $2t + 3$ cycles in G be $\alpha(G)$. So we get

$$\alpha(G) = \frac{-c_{2t+3}}{2 \prod_{\substack{i,j=1 \\ j>i}}^n [d(w_i)d(w_j)]}.$$

In the above formula, vertices w_i, w_j are adjacent in one of the elementary or spanning elementary (if $2t + 3 = n$) subgraphs with $2t + 3$ vertices.

Proof. Let us take a graph G . Any elementary or spanning elementary subgraph of G has odd number of vertices if and only if it has at least a cycle with odd vertices. By the hypothesis $c_1 = c_3 = c_5 = \dots = c_{2t+1} = 0$, it is clear that there is no odd cycle with $2j + 1$ edges where $j = 1, 2, \dots, t$ in G . So each component of any elementary or spanning elementary subgraph with $2t + 3$ vertices of G cannot be an edge and has to be a $(2t + 3)$ -cycle. If we add regularity condition to G , then by Theorem 2.3, we find that every elementary or spanning elementary subgraph of G with $2t + 3$ vertices contributes the same number to c_{2t+3} . Moreover, the elementary or spanning elementary subgraphs consist of merely cycle components and we have the required result. \square

3 Laplacian adjacency matrices, determinants and characteristic polynomials

In this section, we are interested in Laplacian adjacency matrices and we establish some methods for finding determinant and characteristic polynomial as in the second section.

First of all, we give the definition of the Laplacian adjacency matrix of a graph G .

Let G be a graph with the vertex set $V(G) = \{u_1, u_2, \dots, u_n\}$ and edge set $E(G)$. We shall denote the Laplacian adjacency matrix by $L(G) = [l_{ij}]_{n \times n}$ which is given by

$$l_{ij} = \begin{cases} -1, & \text{if the vertices } u_i \text{ and } u_j \text{ are adjacent} \\ d(u_i), & \text{if } i = j \\ 0, & \text{otherwise.} \end{cases}$$

Secondly, the characteristic polynomial of the Laplacian adjacency matrix is $|xI - L(G)|$ and it will be denoted by $P_G^L(x)$.

Let r be the sum of the numbers of the vertices that belong to cycles that exist in the corresponding elementary or spanning elementary subgraph of G . Now we are ready to give a theorem for calculation of the determinant of Laplacian adjacency matrix of a graph G . Note that we earlier defined elementary and spanning elementary subgraphs of G . In the next two results, we also allow a new type of component in the form of a vertex in addition to those which are edges or cycles. If there is no such component in the form of a vertex, say u_i , then we omit the product in Theorem 3.1:

Theorem 3.1. *Let G be a graph with the vertex set $V(G) = \{u_1, u_2, \dots, u_n\}$ and $E(G)$. Let the Laplacian adjacency matrix of G be $L(G)$. Then*

$$|L(G)| = (-1)^r \sum (-1)^{n-c-(H)-c_o(H)} 2^{c_o(H)} \prod_{i=1}^n d(u_i)$$

where the summation is taken over all spanning elementary subgraphs H .

Proof. Let G be a graph with n vertices. By the definition of the Laplacian adjacency matrix of G and by the proof of Theorem 2.1, we have $(-1)^r \sum (-1)^{n-c_-(H)-c_o(H)} 2^{c_o(H)}$ and also considering the different entries between the Laplacian adjacency matrix and the edge-Zagreb adjacency matrix, we get by the proof of Theorem 2.1, $\prod_{i=1}^n d(u_i)$. As a result, we have

$$|L(G)| = (-1)^r \sum (-1)^{n-c_-(H)-c_o(H)} 2^{c_o(H)} \prod_{i=1}^n d(u_i)$$

□

We can give a formula for Laplacian characteristic polynomial of a graph G .

Theorem 3.2. Let G be any graph of order n and let $P_G^l(x)$ be Laplacian characteristic polynomial of G as above.

$$c_k = (-1)^r \sum (-1)^{c_-(H)+c_o(H)} 2^{c_o(H)} \prod_{i=1}^n d(u_i).$$

Here the summation is over all elementary subgraphs H with k vertices.

Note that u_i is defined as in Theorem 3.1 but we replace the statement that is spanning elementary subgraph with elementary subgraph.

Proof. By Theorem 2.2, $c_k = (-1)^k \sum (\text{all } k \times k \text{ principal minors})$. Also by Theorem 3.1, we have

$$c_k = (-1)^k (-1)^r \sum (-1)^{k-c_-(H)-c_o(H)} 2^{c_o(H)} \prod_{i=1}^n d(u_i).$$

Consequently, we get

$$c_k = (-1)^r \sum (-1)^{c_-(H)+c_o(H)} 2^{c_o(H)} \prod_{i=1}^n d(u_i).$$

□

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