Different Graph Energies and Their Relation

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Abstract:

This paper discusses one graph spectral-based invariant, graph energy. First, we define the adjacency, Laplacian, and signless Laplacian matrices associated with the graph. Then, the characteristic equations of these matrices are described. The graph spectra are obtained by solving these adjacency, Laplacian, and signless Laplacian characteristic equations. The roots of these characteristic equations are called eigenvalues of the respective matrices of the graph. The set of eigenvalues of the graph with their multiplicities is known as the spectrum. Subsequently, adjacency, Laplacian, and signless Laplacian spectra are obtained. The graph's energy is the sum of the absolute values of the eigenvalues of the matrix of the respective graphs. Consequently, energy, Laplacian energy, and signless Laplacian energy are obtained and established in their relation in this paper.

Keywords : spectrum, energy, Laplacian energy, signless Laplacian energy

1. Introduction

Let G be a finite, simple and undirected graph with a set of vertex $V(G)$ and a set of edges $E(G)$. Let $|V(G)| = n$ and $|E(G)| = m$. Let $A = [a_{ij}]$ be an adjacency matrix of a graph G with vertices $v_1, v_2, v_3 \cdots v_n$ such that $A(G) = [a_{ij}] = 1$ if v_i is adjacent to v_j and equal to 0 otherwise. The characteristic polynomial of the adjacency matrix $A(G)$ is $\det(\lambda I - A(G))$, where I is the unit matrix of order n and is indicated by $P(G;\lambda)$. The eigenvalues of the graph are defined as the eigenvalues of adjacency matrix A(G), so they are just the root of the equation $P(G;\lambda) = 0$. Since A (G) is real symmetric, all roots are real, i.e., its eigenvalues are real. Denote them $\lambda_1,\ \lambda_2, \ldots\ldots \lambda_n$. The set of eigenvalues of the graph with their multiplicities is known as spectrum [2] of the graph and it is denoted by

$$\text{Spec}(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_n \\ m_1 & m_2 & \cdots & m_n \end{pmatrix}$$

Since $A(G)$ is symmetric therefore eigenvalues are in non-increasing order $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.

Some well-known results on eigenvalues of the adjacency matrix of the graph G are the following

$$\sum_{i=1}^{n} \lambda_i = 0 \ldots\ldots\ldots (1)$$

$$\sum_{i=1}^{n} \lambda_i^2 = 2m \ldots\ldots\ldots (2)$$

Let $D(G) = \text{diag}(d_1, d_2, \cdots, d_n)$ be the diagonal matrix of graph , where $d_i = \deg(v_i)$, for all $i = 1,2,3,\cdots,n$. Then the Laplacian matrix and the signless Laplacian matrix of G can be presented as $L(G) = D(G) - A(G)$ and $L^+(G) = D(G) + A(G)$, respectively. Both matrices are real symmetric positive semi-definite matrices. Therefore, their eigenvalues are nonnegative real numbers. Let $\mu_1, \mu_2, \cdots \mu_n$ be the eigenvalues of $L(G)$. It is known that $\mu_n = 0$ and $\mu_{n-1} > 0$ if and only if G is connected. Then

$$\sum_{i=1}^{n} \mu_i = 2m \dots \dots (3)$$

Moreover, we have

$$\sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n} d_i(d_i + 1) = M_1(G) + 2m \dots \dots \dots (4)$$

Where M_1 is called first Zagreb index of graph G.
Similarly, if $\mu_1^+, \mu_2^+, \cdots \mu_n^+$be the eigenvalues of $L^+(G)$ then it can be easily shown that

$$\sum_{i=1}^{n} \mu_i^+ = 2m \dots \dots \dots (5)$$

One of the chemical applications of spectral graph theory is based on the close correspondence between the graph eigenvalues and molecular orbital energy level of electrons in conjugated hydrocarbons. The total -electron energy was calculated by Erich Huckel in 1930. In light of this relation, Ivan Gutman, in 1978, proposed [4] a mathematical definition of the energy of graphs as shown in equation (6) that the energy of the graph is the sum of the absolute values of the eigenvalues of a graph G and is denoted by, that is

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \dots \dots (6)$$

Equation (6) is the graph spectrum-based quantity. Since $\mu_1, \mu_2, \cdots \mu_n$ be the eigenvalues of $L(G)$ then Laplacian energy of $L(G)$ is denoted by $LE(G)$ and defined by Gutman [6] as

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| \dots \dots (7)$$

Similarly if $\mu_1^+, \mu_2^+, \cdots \mu_n^+$be the eigenvalues of $L^+(G)$ then signless Laplacian energy[1] is defined as

$$LE^+(G) = \sum_{i=1}^{n} \left| \mu_i^+ - \frac{2m}{n} \right| \dots \dots (8)$$

The application of Laplacian energy and signless Laplacian energy is not only on organic chemistry [5] but also on image processing and information theory [10].

2. Preliminaries

Some of the basic properties of energy and Laplacian energy and signless Laplacian energy are discussed here

Lemma 2.1 Let A and B be two real symmetric matrices of order n. Then for $1 \leq k \leq n$,

$$\sum_{i=1}^{k} \lambda(A+B) \leq \sum_{i=1}^{k} \lambda_i(A) + \sum_{i=1}^{k} \lambda_i(B)$$

Proposition 2.1 The spectrum of adjacency matrix $A(G)$,the Laplacian matrix $L(G)$ and signless Laplacian matrix $L^+(G)$ consist entirely of real number

Theorem 2.2 Let G be regular graph where all vertices have degree d. If $\lambda_1,\ \lambda_2, \dots . \lambda_n$ eigenvalues of adjacency matrix of G then eigenvalues of Laplacian matrix are $d-\lambda_1, d-\lambda_2, \dots . . d-\lambda_n$.

Lemma 2.2 Let $\mu_1, \mu_2, \cdots \mu_n$ be the eigenvalues of $L(G)$ of a graph G, then

$$\sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n} d_i(d_i+1) = M_1(G) + 2m$$

where M_1 is called first Zagreb index of graph G.
Corollary 2.1 If $\mu_1, \mu_2, \cdots, \mu_n$ be the Laplacian eigenvalues of a graph G with n vertices and m edges, then

$$\sum_{i=1}^{n} \left(\mu_i - \frac{2m}{n}\right)^2 = 2m + M_1(G) - \frac{4m^2}{n}$$

Proof: We have

$$\begin{aligned}\sum_{i=1}^{n} \left(\mu_i - \frac{2m}{n}\right)^2 &= \sum_{i=1}^{n} \mu_i^2 - \frac{4m}{n}\mu_i + n\left(\frac{2m}{n}\right)^2 \\ &= M_1(G) + 2m - \frac{8m^2}{n} + \frac{4m^2}{n} \\ &= M_1(G) + 2m - \frac{4m^2}{n}\end{aligned}$$

Lemma 2.3 Let G be a graph and let $\sigma(1 \leq \sigma \leq n)$ be the largest positive integer such that

$$LE(G) = 2S_\sigma(G) - \frac{4m\sigma}{n} = \max_{1 \leqq i < n-1} \left\{2S_i(G) - \frac{4mi}{n}\right\}$$

where

$$S_\sigma(G) = \sum_{i=1}^{\sigma} \mu_i$$

3. Hyperenergetic, non-hyperenergetic, borderenergetic and equienergetic graphs

In 1978, Ivan Gutman conjectured that the complete graph K_n has maximum energy. i.e.

$$E(G) \leq E(K_n) \leq 2(n-1)$$

However, that was not true. There are graphs whose energy is larger than the energy of K_n. This gives the concept of hyperenergetic graphs. If $E(G) > 2(n-1)$, then the graph is called hyperenergetic graph, and if $E(G) < 2(n-1)$, the graph is called Non-hyper-energetic graph. A non-complete graph with energy equal to $2n(n-1)$ is called a borderenergetic graph. Two graphs G_1 and G_2 are said to be equienergetic if $E(G_1) = E(G_2)$. The co-spectral graph is obviously equienergetic.

3.1 Relation between $E(G)$ and $LE(G)$

For some classes of non-regular graphs say, $C_6 \cup K_2$, the relation $E(G) = LE(G)$ holds. For complete bipartite graph $K_{p,q}, K_a \cup K_b$ graphs, the graphs $Kb_p(k)$ obtained by deleting the edges from the complete graph K_n, and $Kc_n(k)$ obtained by deleting the $\frac{k(k-1)}{2}$ edges of a complete graph K_k from complete graph K_n, the extremal Hakimi graph (H_n) and Coalscence of $K_n \cdot K_n$, the relation $LE(G) \geq E(G)$ holds. Therefore, Gutman et. al [5] formulate the given conjecture. Gutman proved a conjecture [5] that $LE(G) \geq E(G)$ for all graphs. However, Stevanovic et al.[14] disproved the inequality by giving a single counter-example for an infinite family of graphs G, namely $G \cong KK_n$ for which $n \geq 8$, the reverse inequality holds. Liu and Liu [7] also give the counterexample of the above conjecture. Later, it is proven [11,13] that $LE(G) \geq E(G)$ holds for all bipartite graphs by using the Ky-Fan theorem.

For any square matrix M of order n . if $s_i(M), i = 1,2,\cdots,n$ be its singular values and $x_i(M), i = 1,2\cdots,n$ be its eigenvalues. Then $s_i(m) = |x_i(m)|$ for $i = 1,2,\cdots,n$ Nikiforov[9] obtained that the energy of graph G is equal to the sum of the singular values of its adjacency matrix $A(G)$. According to the above definition if $\mu_1, \mu_2, \cdots \mu_n$ be the eigenvalues of $L(G)$.Then $\mu_1 - \frac{2m}{n}, \mu_2 - \frac{2m}{n}, \cdots \mu_n - \frac{2m}{n}$ are the eigenvalues of

$$L(G) - \frac{2m}{n} I_n \dots\dots\dots (9)$$

Similarly, if $\mu_1^+, \mu_2^+, \cdots \mu_n^+$ be the eigenvalues of $L^+(G)$. Then $\mu_1^+ - \frac{2m}{n}, \mu_2^+ - \frac{2m}{n}, \cdots \mu_n^+ - \frac{2m}{n}$ are the eigenvalues of

$$L^{+}(G)-\frac{2m}{n}I_n \dots \dots (10)$$

where I_n be the unit matrix of order n .

Theorem 3.1 (Ky-Fan Theorem) Let A, B and C be square matrices of order n, such that $A + B = C$., Then

$$\sum_{i=1}^{n} s_i(A)+\sum_{i=1}^{n} s_i(B) \geq \sum_{i=1}^{n} s_i(C)$$

Equality holds iff there exists an orthogonal matrix P, such that PA and PB are both positive semi-definite.

Theorem 3.2 For a graph G with vertex degrees $d_1, d_2, \cdots, d_n$ and average vertex degree $\frac{2m}{n}$,

$$LE(G) \leq E(G)+\sum_{i=1}^{n}\left|d_i-\frac{2m}{n}\right|$$

Proof: We rewrite equation (7) in below matrix form,

$$L-\frac{2m}{n}I_n=\left(D-\frac{2m}{n}\right)I_n-A$$
$$=(-A)+\left(D-\frac{2m}{n}\right)I_n$$

Now applying Ky-Fan theorem 3.1 in above by keeping mind equation (9) we get,

gives the results.

$$\sum_{i=1}^{n} s_i\left(L-\frac{2m}{n}I_n\right) \leq -\sum_{i=1}^{n} s_i(A)+\sum_{i=1}^{n} s_i\left(D-\frac{2m}{n}I_n\right)$$
$$\sum_{i=1}^{n}|\gamma_i| \leq \sum_{i=1}^{n}|\lambda_i|+\sum_{i=1}^{n}\left|d_i-\frac{2m}{n}\right|$$

W.So et.al [13] proved the conjecture is true for all bipartite graphs.
Theorem 3.3 If G is bipartite graph then also $LE(G) \geq E(G)$
Proof: Subtracting equation (3) from (5)

$$L^{+}(G)-L(G)=2A(G)$$

Rewritten above as

$$\left(L^{+}-\frac{2m}{n}I_n\right)-\left(L-\frac{2m}{n}I_n\right)=2A \dots \dots (11)$$

As per theorem (9) $L^+(G)$ and $L(G)$ has same spectra so

$$\sum_{i=1}^{n} s_i\left(L^+ - \frac{2m}{n}I_n\right) = \sum_{i=1}^{n} s_i\left(L - \frac{2m}{n}I_n\right) = \sum_{i=1}^{n} s_i\left[-\left(L - \frac{2m}{n}I_n\right)\right] = LE(G)$$

Applying Ky-Fan theorem in the equation , we have

$$LE(G) \geq E(G)$$

Using Ky Fan, So et al.[12] are also given the relation between energy and Laplacian energy in bipartite graphs as

$$\text{LE}(G) \geq \max\left[E(G), \sum_{i=1}^{n} \left|d_i - \frac{2m}{n}\right|\right] \ldots \ldots (12)$$

Du. et al [3] proved that the conjecture given by Gutman is true for almost all graphs. Until then, characterizing all graphs for which inequality holds or not $LE(G) \geq E(G)$ or $LE(G) \leq E(G)$ is a challenging task. Still, it is an open problem.

4. Relation between $E(G)$ and $LE^+(G)$

P. Wang et al.[15] obtains a relation between energy and signless Laplacian energy for regular graph G

$$E(G) = LE^+(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} \ldots \ldots (13)$$

with equality holds if and only if $G \equiv K_n, \frac{n}{2}K_2$ or $G \equiv S(n,r)$

5. Relation among $E(G), LE(G)$ and $LE^+(G)$

If a graph G is bipartite, then signless Laplacian energy $L^+E(G) = E(G)$.Also if the graph G is regular then $L^+E(G) = LE(G) = E(G)$. Therefore, we must find the relation between energy and Laplacian energy; if a graph G is bipartite, then signless Laplacian energy$L^+E(G) = E(G)$. Also, if the graph G is regular then $L^+E(G) = LE(G) = E(G)$. Therefore, we must find the relation between energy, Laplacian energy, and signless Laplacian energy for non-bipartite nonregular graphs. However, it is an open problem. The relation between them has yet to come for non-bipartite, non-regular graphs.

The relation among $E(G)$, $LE(G)$ and $LE^+(G)$ is presented by Abreu et al.[1] as givev below:

If G is an (n, m) graph. Then

$$|LE^{+}(G) - LE(G)| \leq 2E(G) \dots \dots (14)$$

The equality holds G is null graph
Also, they obtain Also, they obtain

$$LE^{+}(G) + LE(G) \geq \max\left[2E(G), 2\sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right|\right] \dots \dots (15)$$

Moreover, Das and Mojjalal [8] proved the given theorem in their thesis

$$LE^{+}(G) + LE(G) \geq 4E(G) - \frac{4mr}{n} \dots \dots (16)$$

with equality holding iff $G \equiv nK_1$ or $G \equiv K_2 \cup (n-2)K_1$ or $G \equiv K_{n/2,n/2}$. Two equ.(15) and equ.(16) are not comparable. Sometimes equ. (16) is better than equ. (15) but not always.

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