ORIGINAL PAPER

BOUNDS FOR THE ENERGY OF $A(G), L(G)$ USING 2-ADJACENCY

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Abstract. *Let G be a simple connected graph. We redefined adjacency for any two vertices if there is connected two edges between any two vertices i and j. In this case, this vertices are called 2-adjacency and denoted by $i \sim_2 j$. In this study, we redefined the energy of Adjacency matrix $A(G)$ and Laplacian matrix $L(G)$ by using 2-adjacency definition. Also, we found some bounds for the energy of $A(G)$ and $L(G)$ of a graph G, respectively by using 2-adjacency.*

Keywords: *2-adjacency, energy, bound.*

1. INTRODUCTION

Let $G = (V, E)$ be a simple graph with n vertices and m edges having vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \dots, e_m\}$. For $v_i \in V$, the degree of v_i, the set of neighbors of v_i and the average of the degrees of the vertices adjacent to v_i are denoted by d_i, $N_G(v_i)$ and m_i, respectively. Let $D(G)$ be the diagonal matrix of vertex degrees of a graph G. Also, let $A(G)$ be the adjacency matrix of G and $A(G) = (a_{ij})$ be defined as the $n \times n$ matrix (a_{ij}), where

$$(a_{ij})=\begin{cases} 1 & ; \quad v_i\, v_j \in V \\ 0 & ; \quad otherwise. \end{cases}$$

It follows immediately that if G is a simple graph, then $A(G)$ is a symmetric (0,1) matrix where all diagonal elements are zero. We will denote the characteristic polynomial of G by

$$P(G) = det\big(xI - A(G)\big) = \sum_{i=0}^{n} a_i x_i^{n-i}.$$

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Since $A(G)$ is a real symmetric matrix, its eigenvalues must be real and may be ordered as

$$\lambda_1\big(A(G)\big) \geq \lambda_2\big(A(G)\big) \geq \cdots \geq \lambda_n(A(G)).$$

Denoted $\lambda_i\big(A(G)\big)$ simply by $\lambda_i(G)$. The sequence of n eigenvalues is called the spectrum of G.

The largest eigenvalue $\lambda_1(G)$ is often called the spectral radius of G. We now give some known upper bounds for the spectral radius $\lambda_1(G)$.

The energy of the graph G is defined as

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

The Laplacian matrix of a graph G is defined as $L(G) = (l_{ij})$, where

$$l_{ij} = \begin{cases} d_i & ; \quad i = j \\ -1 & ; \quad i \sim j \\ 0 & ; \quad otherwise \end{cases}$$

The Laplacian matrix of G is $L(G) = D(G) - A(G)$. Clearly, $L(G)$ is a real symmetric matrix. From this fact and Gersgorin's theorem, it follows that its eigenvalues are nonnegative real numbers. Moreover, since its rows sum to 0, 0 is the smallest eigenvalue of $L(G)$. We assume that the Laplacian eigenvalues are $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. Especially the largest eigenvalue of $L(G)$ is called Laplacian spectral radius of G, denoted by $\mu(G)$.

The Laplacian energy of a graph G as put forward by Gutman and Zhou is defined as

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

Firstly, we now give some known upper bounds for $E(G)$.

Let G be a simple graph with n vertices and m edges.

1) In 1971, McClelland [10] discovered the first upper bound for $E(G)$ as follows:

$$E(G) \leq \sqrt{2mn} \tag{1}$$

2) If $2m \geq n$, then [6]

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

Moreover, equality holds if and only if G is either $\frac{n}{2}K_2$, K_n or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-\left(\frac{2m}{n}\right)^2}{n-1}}$.

If $2m \leq n$, then

$$E(G) = 2m.$$

Equality holds if and only if G is disjoint union of edges and isolated vertices.

3) If G is a graph with n vertices, m edges and degree sequence $d_1, d_2, \dots, d_n$ then [13]

$$E(G) \leq \sqrt{\frac{\sum_i^n d_i^2}{n}} + \sqrt{(n-1)\left[2m - \frac{\sum_i^n d_i^2}{n}\right]} \tag{3}$$

with equality holds if and only if G is either $\frac{n}{2}K_2$, a complete bipartite graph, a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-\left(\frac{2m}{n}\right)^2}{n-1}}$ or nK_1.

Secondly, many researchers have investigated upper bounds for $LE(G)$ is the following:

Let G be a simple graph with n vertices and m edges.

1) B.J.McClelland's bound [10]:

$$LE(G) \leq \sqrt{2Mn}, \tag{4}$$

where $M = m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i - \frac{2m}{n}\right)^2$.

2) J.H.Koolen, V.Moulton, I.Gutman's bound [7]:

$$LE(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2M - \left(\frac{2m}{n}\right)^2\right]} \tag{5}$$

2. BOUNDS FOR THE ENERGY OF GRAPHS USING 2-ADJACENCY

Let G be a simple connected graph. We redefined adjacency for any two vertices i and j. And then, we called this vertices as 2-adjacency. If this vertices are 2-adjacency, we denoted it by $i \ \sim_2 \ j$.

In this study, we defined 2-adjacency matrix and denoted by $A^{\sim 2}(G)$. We redefined the 2-adjacency energy of the graph G by using 2-adjacency definition. We found an upper bound for the 2-adjacency energy of the graph G. Then we expanded to k-adjacency of two vertices and redefined the k-adjacency matrix and obtained a new bound for the k-adjacency energy of a graph.

Definition 2.1 If there are two connected edges between vertices of the i and j, then this vertices are called 2-adjacent and denoted by $i \ \sim_2 \ j$.

Definition 2.2 The 2-degree of any vertex i in graph is the number of 2-adjacency vertices regarding the vertex i and the 2-degree of a vertex i is denoted by $d_i^{\sim 2}$.

We can define the k-adjacency by generalizing 2-adjacency concept further.

Definition 2.3 If there are k connected edges between vertices of the i and j, then this vertices are called k-adjacency and denoted by $i \sim_k j$.

Definition 2.4 The k- degree of any vertex i in graph is the number of k-adjacency regarding the vertex i and the k-degree of a vertex i is denoted by $d_i^{\sim k}$.

Given a graph $G = (V, E)$ with $|V| = n$ the 2-adjaceny degree matrix $D^{\sim 2}(G)$ for G is a $n \times n$ diagonal matrix defined as:

$$\left(d_{ij}^{\sim 2}\right) = \begin{cases} d_i^{\sim 2} & ; \quad i = j \\ 0 & ; \quad otherwise \end{cases}$$

where the 2-degree $d_i^{\sim 2}$ of a vertex i is the number of 2-adjacency regarding the vertex i.

Given a simple, connected graph G with n vertices, its 2-adjacency matrix $A^{\sim 2}(G) = \left(a_{ij}^{\sim 2}\right)_{n \times n}$ defined as:

$$\left(a_{ij}^{\sim 2}\right) = \begin{cases} 1 & ; \quad i \sim_2 j \\ 0 & ; \quad otherwise \end{cases}$$

Because the 2-adjacency matrix is real, symmetric matrix, its eigenvalues are real and we denoted by

$$0 = \lambda_n^{\sim 2} \leq \cdots \leq \lambda_2^{\sim 2} \leq \lambda_1^{\sim 2}.$$

$\lambda_1^{\sim 2}$ denote the largest eigenvalue of $A^{\sim 2}(G)$.

Definition 2.5 The 2-adjacency energy of the graph G is defined as

$$E^{\sim 2}(G) = \sum_{i=1}^{n} \left|\lambda_i^{\sim 2}\right|$$

Theorem 2.6 If G is a graph with n vertices, m edges and degree sequence $d_1^{\sim 2}, d_2^{\sim 2}, \dots, d_n^{\sim 2}$, then

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

Proof: Among the known lower bounds for λ_1 is the following [14]:

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}}.$$

If you apply for 2-adjacency to this inequality, it is obtained

$$\lambda_1^{\sim 2} \geq \sqrt{\frac{\sum_{i=1}^{n} d_i^{\sim 2}}{n}}$$

By the Cauchy-Schwartz inequality,

$$\sum_{i=2}^{n}\left|\lambda_i^{\sim 2}\right| \leq \sqrt{(n-1)\sum_{i=2}^{n}(\lambda_i^{\sim 2})^2} = \sqrt{(n-1)(2m-(\lambda_1^{\sim 2})^2)}$$

Hence

$$E^{\sim 2}(G) \leq \lambda_1^{\sim 2} + \sqrt{(n-1)(2m-(\lambda_1^{\sim 2})^2)}$$

Note that the function $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{2m/n} \leq x \leq \sqrt{2m}$ and $\sqrt{2m/n} \leq \sqrt{(\sum_{i=1}^{n}(d_i^{\sim 2})^2)/n} \leq \lambda_1^{\sim 2}$, we see that $F(\lambda_1^{\sim 2}) = F\left(\sqrt{(\sum_{i=1}^{n}(d_i^{\sim 2})^2)/n}\right)$.

Since,

$$2m \leq \sum_{i=1}^{n} d_i^{\sim 2} \ ,$$

it is obtained

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

Given a simple, connected graph G with n vertices, its 2-adjacency self-adjacency matrix $A^{\approx}(G) = \left(a_{ij}^{\approx}\right)_{n\times n}$ defined as:

$$\left(a_{ij}^{\approx}\right) = \begin{cases} 2 & ; \quad i \sim_2 j \\ 0 & ; \quad otherwise \end{cases}$$

Because the 2-adjacency self-adjacency matrix is real, symmetric matrix, its eigenvalues are real and we denoted by

$$0 = \lambda_n^{\approx} \leq \cdots \leq \lambda_2^{\approx} \leq \lambda_1^{\approx}.$$

$\lambda_1^{\approx}$ denote the largest eigenvalue of $A^{\approx}(G)$.

Definition 2.7. The 2-adjacency self energy of the graph G is defined as

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

Theorem 2.8 If G is a graph with n vertices, m edges and degree sequence $d_1^{\sim 2}, d_2^{\sim 2}, \ldots, d_n^{\sim 2}$, then

$$E^{\approx}(G) > \sqrt{\frac{(\sum_{i=1}^{n}(d_i^{\sim 2})^2)}{n}} + \sqrt{(n-1)\left(\sum_{i=1}^{n} d_i^{\sim 2} - \frac{\sum_{i=1}^{n}(d_i^{\sim 2})^2}{n}\right)}$$

Conjecture 2.9. Let G be a simple, connected graph. Then

$$E(G) \leq E^{\sim 2}(G) \leq E^{\approx}(G).$$

When we generalize for k-adjacency to find bound, we obtain following result.

Theorem 2.10. If G is a graph with n vertices, m edges and degree sequence $d_1^{\sim k}, d_2^{\sim k}, \dots, d_n^{\sim k}$, then

$$E^{\sim k}(G) \leq \sqrt{\frac{\sum_{i=1}^{n}\left(d_i^{\sim k}\right)^2}{n}} + \sqrt{(n-1)\left(\sum_{i=1}^{n} d_i^{\sim k} - \frac{\sum_{i=1}^{n}\left(d_i^{\sim k}\right)^2}{n}\right)}$$

Specially, if we get k=1, Theorem 2.10 will turn (3).

3. BOUNDS FOR THE LAPLACIAN ENERGY OF GRAPHS USING 2-ADJACENCY

Let G be a simple connected graph. We redefined adjacency for any two vertices i and j. And then we called this vertices as 2-adjacency. If this vertices are 2-adjacency then denoted by $i \sim_2 j$.

In this study, we defined 2-adjacency Laplacian matrix and denoted by $L^{\sim 2}(G)$. We found an upper bound for the energy of $L^{\sim 2}(G)$. Then we expanded to k-adjacency of two vertices and redefined the k-adjacency Laplacian matrix and obtained a new bound for the 2-adjacency Laplacian energy of a graph.

Given a simple, connected graph G with n vertices, its 2-adjacency Laplacian matrix $L^{\sim 2}(G) = \left(l_{ij}^{\sim 2}\right)_{n \times n}$ defined as:

$$\left(l_{ij}^{\sim 2}\right) = \begin{cases} d_i^{\sim 2} & ; \quad i = j \\ -1 & ; \quad i \sim_2 j \\ 0 & ; \quad otherwise \end{cases}$$

where $d_i^{\sim 2}$ is 2-degree of the vertex i.

Because the 2-adjacency Laplacian matrix is real, symmetric matrix, its eigenvalues are real and we denoted by

$$0 = \mu_n^{\sim 2} \leq \cdots \leq \mu_2^{\sim 2} \leq \mu_1^{\sim 2}.$$

$\mu_1^{\sim 2}$ denotes the largest eigenvalue of $L^{\sim 2}(G)$. Also, every row sum and column sum of $L^{\sim 2}$ is zero. There are equality

$$L^{\sim 2}(G) = D^{\sim 2}(G) - A^{\sim 2}(G)$$

for 2-adjacency Laplacian matrix.

Definition 3.1 The 2-adjacency Laplacian energy of the graph G is defined as

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

Theorem 3.2. If $2m \geq n$ and G is a graph on n vertices with m edges, then

$$LE^{\sim 2}(G) < \frac{2m}{n} + \sqrt{(n-1)\left[2M^{\sim 2} - \left(\frac{2m}{n}\right)^2\right]}$$

where $M^{\sim 2} = m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i^{\sim 2} - \frac{2m}{n}\right)^2$.

Proof: We first introduce the auxiliary "eigenvalues" $\gamma_i^{\sim 2}$, $i = 1,2,\dots,n$, defined via

$$\gamma_i^{\sim 2} = \mu_i^{\sim 2} - \frac{2m}{n}.$$

The 2-adjacency Laplacian eigenvalues satisfy the conditions

$$\sum_{i=1}^{n} \gamma_i^{\sim 2} = 0 \ ; \ \sum_{i=1}^{n} (\gamma_i^{\sim 2})^2 = 2M^{\sim 2}$$

where

$$M^{\sim 2} = m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i^{\sim 2} - \frac{2m}{n}\right)^2$$

with $d_i^{\sim 2}$ denoting the 2-degree of the i-th vertex of G.

Since $\sum_{i=1}^{n}(\gamma_i^{\sim 2})^2 = 2M^{\sim 2}$, we have $\sum_{i=2}^{n}(\gamma_i^{\sim 2})^2 = 2M^{\sim 2} - \gamma_1^{\sim 2}$.

Using this together with the Cauchy-Schwartz inequality, we obtain the inequality

$$\sum_{i=2}^{n}\left|\gamma_i^{\sim 2}\right| = \sqrt{(n-1)\sum_{i=2}^{n}(\gamma_i^{\sim 2})^2} = \sqrt{(n-1)\left[2M^{\sim 2} - \left(\frac{2m}{n}\right)^2\right]}$$

Hence

$$LE^{\sim 2}(G) \leq \gamma_1^{\sim 2} + \sqrt{(n-1)\left[2M^{\sim 2} - \left(\frac{2m}{n}\right)^2\right]}$$

Since $\gamma_1^{\sim 2} \geq \frac{2m}{n}$, it is obtained

$$LE^{\sim 2}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2M^{\sim 2} - \left(\frac{2m}{n}\right)^2\right]}.$$

Given a simple, connected graph G with n vertices, its 2-adjacency self-Laplacian matrix $L^{\approx}(G) = \left(l_{ij}^{\approx}\right)_{n\times n}$ defined as:

$$\left(l_{ij}^{\approx}\right) = \begin{cases} d_i^{\sim 2} & ; \quad i = j \\ -2 & ; \quad i \sim_2 j \\ 0 & ; \quad otherwise \end{cases}$$

where $d_i^{\sim 2}$ is 2-degree of the vertex i.

Because the 2-adjacency self-Laplacian matrix is real, symmetric matrix, its eigenvalues are real and we denoted by

$$0 = \mu_n^{\approx} \leq \cdots \leq \mu_2^{\approx} \leq \mu_1^{\approx}.$$

$\mu_1^{\approx}$ denotes the largest eigenvalue of $L^{\approx}(G)$. There are equality

$$L^{\approx}(G) = D^{\sim 2}(G) - A^{\approx}(G)$$

for 2-adjacency self-Laplacian matrix.

Definition 3.3. The 2-adjacency self-Laplacian energy of the graph G is defined as

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

Theorem 3.4. If $2m \geq n$ and G is a graph on n vertices with m edges, then

$$LE^{\approx}(G) > \frac{2m}{n} + \sqrt{(n-1)\left[2M^{\approx} - \left(\frac{2m}{n}\right)^2\right]}$$

where $M^{\approx} = m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i^{\sim 2} - \frac{2m}{n}\right)^2$.

Conjecture 3.5. Let G be a simple, connected graph. Then

$$LE(G) \leq LE^{\sim 2}(G) \leq LE^{\approx}(G).$$

When we generalize for k-adjacency to find bound, we obtain following result.

Corollary 3.6 If $2m \geq n$ and G is a graph on n vertices with m edges, then

$$LE^{\sim k}(G) > \frac{2m}{n} + \sqrt{(n-1)\left[2M^{\sim k} - \left(\frac{2m}{n}\right)^2\right]}$$

where $M^{\sim k} = m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i^{\sim k} - \frac{2m}{n}\right)^2$.

Specially, if we get k=1, Corollary 3.6 will turn (5).

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