

Energy of Graph

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ABSTRACT

By given the adjacency matrix, laplacian matrix of a graph we can find the set of eigenvalues of graph in order to discussed about the energy of graph and laplacian energy of graph. (i.e. the sum of eigenvalues of adjacency matrix and laplacian matrix of a graph is called the energy of graph) and the laplacian energy of graph is greater or equal to zero for any graph and is greater than zero for every connected graph with more or two vertices (i.e. the last eigenvalues of laplacian matrix is zero), according to several theorems about the energy of graph and the laplacian energy of graph that are described in this work; I discussed about energy of graph, laplacian energy of graph and comparing them here.

Keywords- Degree matrix, laplacian matrix, Adjacency matrix, spectrum of graph, energy of graph, Laplacian energy of graph.

I. INTRODUCTION

Let $G(n, m)$ be a graph with vertices set $v(G) = (v_1, v_2, v_3, \dots, v_n)$ then the laplacian matrix of $G(n, m)$ denoted by $L(G) = D - A$, where D and A are degree and adjacency matrices respectively

$$\Rightarrow \text{The } (i, j)^{\text{th}} \text{ entry of } L(G) = \begin{cases} d_i & \text{if } i = j \\ -1 & \text{if } i \neq j \\ 0 & \text{otherwise} \end{cases} \text{ and}$$

$L(G)$ is positive semi definite matrix, all eigenvalues of $L(G) \geq 0$ (that is $L(G)$ does not have negative eigenvalue, if $G(n, m)$ is connected then it has one zero eigenvalue, if it has K components then it has K zero eigenvalue) in other word, let the set $\{\mu_1, \mu_2, \mu_3, \dots, \mu_n\}$ be the spectrum set of $L(G)$ then $\{\mu_1 \geq \mu_2 \geq \mu_3 \geq \dots \mu_{n-1} \geq \mu_n = 0\}$

Let $G(n, m)$ be a graph with vertices set $v(G) = (v_1, v_2, v_3, \dots, v_n)$ then the adjacency matrix of $G(n, m)$ denoted by $A = [a_{ij}]$ is $n \times n$ (square matrix and symmetric matrix) were $a_{ij} = \begin{cases} 1 & i \neq j \\ 0 & \text{otherwise} \end{cases}$.

Note: in this paper $G(n, m)$ is simple and undirected graph.

Definition 1: let A be adjacency matrix of connected graph $G(n, m)$ with spectrum set $(\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n)$, then $\sum_{i=1}^n |\lambda_i|$ is called energy of $G(n, m)$ (that is the sum of absolute value of eigenvalues of adjacency matrix A of $G(n, m)$)

Definition 2: let $L(G)$ be laplacian matrix of connected graph $G(n, m)$ with m edges and n vertices and set of eigenvalues $\mu_1, \mu_2, \mu_3, \dots, \mu_{n-1}, \mu_n = 0$ then the



laplacian energy of $G(n, m)$ denoted by

$$LE(G) = \sum_i^n \mu_i = \sum_i^{n-1} \mu_i \quad (\text{that is})$$

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

Theorem: let $G(n, m)$ be any connected graph with $n \geq 2$ vertices, then we have the following

$$LE(G) \geq 6n - 8 \quad (1) \text{ where } (n \in \mathbb{N})$$

In (1) Equality holds if only if $G(n, m)$ is the path P_n on n vertices

If $G(n, m)$ is connected with $n \geq 2$ vertices such that $LE(G) = 6n - 8$, then $G(n, m)$ must be the path P_n on n vertices.

Proof: I want to show that $d_n = d(v_n) = 1$ (that is $G(n, m)$ is a path)

By contradiction

Assume that $G(n, m)$ is not a path P_n on $d_n \geq 2$, by assumption v_n is adjacent to v_{n-1} and $v_{n-2} \in v(H)$

We have $LE(G) \geq 6n - 14$ so we can write $LE(G) \geq LE(G) + 2d_H(v_{n-2}) + 2d_H(n-1) + 10$

$$\text{And } d_H(n-2), d_H(v_{n-1}) \geq 1$$

$\Rightarrow LE(g) = 6n - 8 \geq 6n - 14 + 14 = 6n$ Which is contradiction, hence $d_n = d(v_n)$ cannot be other than 1 $\Rightarrow d_n = d(v_n) = 1$ and $G(n, m)$ is a path.

Note: if H is (not necessarily) sub graph of finite graph $G(n, m)$ then $\mu_i(G) \geq \mu_i(H)$ for $(i = 1, 2, 3, \dots, |H|)$

Conversely: by notation we can write $LE(G) = LE(F) = LE(H) + 2d_{n-1}(H) + 4 = 6n - 8$

$$\Rightarrow 2d_{n-1}(H) = 6n - 12 - LE(H) \leq 6n - 12 - (6n - 14) = 2$$

$$\Rightarrow d_{n-1}(H) = 1$$

\Rightarrow

$$LE(G) = 6n - 8 - 4 - 2 = 6n - 14 = 6(n-1) = 8$$

$\Rightarrow H$ Is a path p_{n-1} and $(n-1)$ is the end vertex of path $\Rightarrow G(n, m)$ is a path P_n .

Corollary: above theorem (laplacian energy of graph) can help us to know whether the graph is path or not

Theorem: let $G(n, m)$ be any graph with n vertices $(n \in \mathbb{N})$, vertices degree $(d_1, d_2, d_3, \dots, d_n)$ and set of

eigenvalues $(\mu_1, \mu_2, \mu_3, \dots, \mu_{n-1}, \mu_n = 0)$, we have

$$LE(G) = \sum_i^n (d_i^2 + d_i) \quad (1)$$

Proof: by rule of vertices I can write

$$\sum_i^n \mu_i = \sum_i^n d_i \quad (2)$$

$$\sum_{i < j} \mu_i \mu_j = \sum_{i < j} d_i d_j - \sum_{i < j} a_{ij}^2 \quad (3)$$

Since we have $a_{ij}^2 = a_{ij}$ for every $i < j$ we can write

$$\begin{aligned} \sum_{i \neq j} \mu_i \mu_j &= 2 \sum_{i < j} \mu_i \mu_j = \sum_{i \neq j} d_i d_j - \sum_{i \neq j} a_{ij} \\ &= \sum_{i \neq j} d_i d_j - \sum_{i=1}^n d_i \end{aligned}$$

There fore

$$\begin{aligned} LE(G) &= \sum_i^n \mu_i^2 = \left(\sum_i^n \mu_i \right)^2 - \sum_{i \neq j} \mu_i \mu_j \\ &= \left(\sum_i^n d_i \right)^2 - \left(\sum_{i \neq j} d_i d_j - \sum_{i=1}^n d_i \right) \\ &= \sum_{i=1}^n d_i^2 + \sum_{i=1}^n d_i = \sum_{i=1}^n (d_i^2 + d_i) \end{aligned}$$

Corollary: let $G(n, m)$ any graph, then $LE(G)$ is an even integers or zero (here zero considered as even integers).

Lemma: let $G(n, m)$ be r , regular graph then the laplacian energy and energy of graph is equal (that is $LE(G) = E(G)$)

Proof: suppose $G(n, m)$ is r regular graph then

$$r - \frac{2m}{n}$$

$$\mu_i - \frac{2m}{n} = -\lambda_{n-i+1} \quad (i = 1, 2, 3, \dots, n) \text{ By definition}$$

2 we can write $LE(G) = E(G)$.

Proposition:

(1): let $G(n, m)$ be a tree with n vertices in which P be pendent vertices such that $2 \leq P \leq n-1$ then

$$LE(G) < E(G) + 2P \left(1 - \frac{2}{n} \right)$$

(2): let $G(n, m)$ be a unicycle graph with n vertices in which P be pendent vertices such that $0 \leq P \leq n-3$, then $LE(G) \leq E(G) + 2P$, equality holds if and only if $P = 0$, Department of mathematics, south china normal university (2010)

Proof (1): suppose G is a tree on n vertices and P are pendent vertices then $\alpha(G) = \sum_{u \in v(G)} \left| d_u - \frac{2(n-1)}{n} \right| = \left[\frac{2(n-1)}{n} - 1 \right] P + \sum_{\substack{u \in v(G) \\ d_u \geq 2}} \left[d_u - \frac{2(n-1)}{n} \right]$

$$\sum_{u \in v(G)} d_u - 2P - \frac{2(n-1)}{n}(n-2P) = \frac{2P(n-2)}{n}$$

Note: (lemma let $G(n, m)$ a graph then $LE(G) \leq E(G) + \alpha(G)$ (1))

By above note we can say that $LE(G) < E(G) + 2P(1 - \frac{2}{n})$

Proof (2): let $G(m, n)$ be a unicycle graph with n vertices in which P be pendent vertices then we can write

$$\begin{aligned} \alpha(G) &= \sum_{u \in v(G)} |d_n - 2| = P + \sum_{\substack{u \in v(G) \\ d_n \geq 2}} (d_n - 2) \\ &= \sum_{u \in v(G)} d_n - 2(n - P) = 2P \end{aligned}$$

By above notation the result follows

Bound on $E(G)$

Theorem: let $G(n, m)$ be a graph with n vertices and m edges and A be the adjacency matrix of $G(n, m)$ then for $2m \geq n$ we have the upper bound below, Li.Xueliang Shi Youngtang Gutman Ivan (2012)

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

Proof: let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_n$ be the spectrum of $G(n, m)$, then $\lambda_1 \geq 0$ and trace $A^2 = \sum_{i=1}^n \lambda_i^2 = 2m \Rightarrow \sum_{i=2}^n \lambda_i^2 = 2m - \lambda_1^2$
Now we have

$$\begin{aligned} E(G) &= \sum_{i=1}^n |\lambda_i| = \lambda_1 + \sum_{i=2}^n |\lambda_i| \leq \lambda_1 + \sqrt{(n-1) \sum_{i=2}^n \lambda_i^2} \\ \Rightarrow E(G) &\leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)} \quad (1) \end{aligned}$$

Now consider the function bellow

$$\begin{aligned} f(x) &= x + \sqrt{(n-1)(2m-x)}, x \leq \sqrt{2m} \\ f'(x) &= 1 + \frac{-2x(n-1)}{2\sqrt{(n-1)(2m-x^2)}} \\ \Rightarrow f'(x) \leq 0 &\Leftrightarrow 1 \leq \frac{x\sqrt{n-1}}{\sqrt{2m-x^2}} \Leftrightarrow \sqrt{(2m-x^2)} \\ &\leq x\sqrt{n-1} \\ \Leftrightarrow 2m-x^2 &\leq x^2(n-1) \Leftrightarrow \frac{2m}{n} \leq x^2 \end{aligned}$$

Thus f is decreasing function on interval $\sqrt{\frac{2m}{n}} \leq x \leq \sqrt{2m}$ and we have $\frac{2m}{n} \leq \lambda_1$

$\Rightarrow \sqrt{\frac{2m}{n}} \leq \frac{2m}{n} \leq \lambda_1 \leq \sqrt{2m}$, as f is decreasing function and $f(\lambda_1) \leq f(\frac{2m}{n})$

$$\Rightarrow E(G) \leq f(\lambda_1) \leq f\left(\frac{2m}{n}\right) \quad \text{by(1)}$$

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

Note: equality holds if graph $G(n, m)$ is complete graph K_n .

Proof: consider complete graph K_n , it has eigenvalues $(n-1)$ and (-1) with multiplicities 1 and $(n-1)$ respectively, in K_n we have

$$\frac{2m}{n} = \frac{n(n-1)}{n} = n-1 \quad (2)$$

By (1) and (2) we can write bellow

$$\begin{aligned} RHS &= \frac{2m}{n} + \sqrt{(n-1) \left[2m - \left(\frac{2m}{n}\right)^2 \right]} \\ &= (n-1) + \sqrt{(n-1)[n(n-1) - (n-1)^2]} \\ &= (n-1) + (n-1)\sqrt{1} = 2(n-1)(3) \end{aligned}$$

$LHS = E(G) = \sum_{i=1}^n |\lambda_i| = (n-1) + |-1| + |-1| + \dots + |-1| = (n-1) + (n-1) = 2(n-1)(4)$ (-1 has multiplicities $(n-1)$), by (3),(4) the result follows.

Theorem: let $G(n, m)$ be a graph in which $2m \leq n$, then $E(G) \leq 2m$ (it happen when $G(n, m)$ has isolated vertices and it is not for generally)

Proof: in $G(n, m)$ total degree = $2m \Rightarrow n - 2m$ vertices must be of degree zero (that is: these vertices is isolated)

Let H be the sub graph of $G(n, m)$ obtained by deleting $n - 2m$ isolated vertices $\Rightarrow H$ has m edges and $2m$ vertices, also $E(G) = E(H)$ (because isolated vertices correspond to zero eigenvalue)

By above theorem we have

$$\begin{aligned} E(H) &\leq \frac{2m}{2m} + \sqrt{(2m-1) \left[2m - \left(\frac{2m}{2m}\right)^2 \right]} \\ &= 1 + \sqrt{(2m-1)(2m-1)} \\ &= 2m \\ E(G) &\leq E(H) \leq 2m \Rightarrow E(G) \leq 2m \end{aligned}$$

Bound on $LE(G)$:

Theorem: Let $G(n, m)$ be any graph, then $LE(G) \leq \sqrt{2Mn}$, where $M = m + \frac{1}{2} \sum_{i=1}^n (d_i - \frac{2m}{n})^2$, equality holds if and only if $G(n, m)$ is regular of degree zero or consists of α copies of complete graph of order K and $(K-2)\alpha$ isolated vertices for $(\alpha \geq 1, K \geq 2)$

Proof: consider the sum

$$s = \sum_{i=1}^n \sum_{j=1}^n (|\mu_i| - |\mu_j|)^2 \geq 0$$

$$\Rightarrow s = 2n \sum_{i=1}^n \mu_i^2 - 2 \left(\sum_{i=1}^n |\mu_i| \right) \left(\sum_{j=1}^n |\mu_j| \right)$$

$$= 4nM - 2LE(G) \geq 0$$

$$\Rightarrow LE(G) \leq \sqrt{2Mn}$$

Theorem: let $G(n, m)$ be any graph then we have

$$2\sqrt{M} \leq LE(G) \leq \sqrt{2Mn} \quad (1) \text{ where}$$

$$M = m + \frac{1}{2} \sum_{i=1}^n \left(d_i - \frac{2m}{n} \right)^2, \text{ the equality holds (}$$

$LE(G) = 2\sqrt{M}$) if and only if $G(n, m)$ is $K_{n/2, n/2}$, the inequality holds for graph without isolated vertices, for such graph equality ($LE(G) = 2M$) holds if and only if $G(n, m)$ is regular graph of degree 1

Proof: first I want to prove the left hand side of (1)

$$\text{Consider } \gamma_i = \mu_i - \frac{2m}{n}, \sum_{i=1}^n \gamma_i = 0, \sum_{i=1}^n \gamma_i^2, M = m + \frac{1}{2} \sum_{i=1}^n \left(d_i - \frac{2m}{n} \right)^2 \quad (2)$$

$$\text{By (2) we have } \left(\sum_{i=1}^n \gamma_i \right)^2 = 0, M > 0 \Rightarrow 2M = -2 \sum_{i < j} \gamma_i \gamma_j = 2 \left| \sum_{i < j} \gamma_i \gamma_j \right| \Rightarrow 2M \leq 2 \sum_{i < j} |\gamma_i| |\gamma_j| \quad (3)$$

$$\text{By (2) we can write } LE(G)^2 = 2M + 2 \sum_{i < j} |\gamma_i| |\gamma_j| \quad (4)$$

$$\text{By (3), (4) we can write } LE(G) \geq 2\sqrt{M}$$

In (2) equality holds for graph $G(n, m)$ with two vertices, so we assume that $n \geq 3$ and also equality holds if and only if there is at most one positive value and one negative value of γ_i , that is $\gamma_1 > 0, \gamma_2 = \gamma_3 = \dots = \gamma_{n-1} = 0, \gamma_n = -\frac{2m}{n} < 0$ (5)

$$\text{From (5) and condition } n \geq 3 \text{ follows that } \mu_{n-1} = \frac{2m}{n}$$

Note: the conditions (5) are not satisfied by complete graph with more than two vertices, for which $\mu_{n-1} = n \neq \frac{2m}{n}$.

If $G(n, m)$ is not complete graph than $\delta \geq \mu_{n-1}$ (δ is the minimum vertex degree of $G(n, m)$) on the other words $\delta \geq \frac{2m}{n}$ implies that $G(n, m)$ is regular graph and by lemma (1) and ($2\sqrt{m} \leq E(G) \leq 2m$), If G has no isolated vertices, then the equality $E(G) = 2\sqrt{m}$ holds if and only if $G(n, m)$ is complete bipartite graph, if $G(n, m)$ has no isolated vertices then the equality

$E(G) = 2m$ holds if and only if $G(n, m)$ is regular of degree one)

Proof: now I want to proof the right side of inequality that is given on the above theorem

Let $G(n, m)$ be a graph with m edges and no isolated vertices, such that $n \leq 2m$

$$\text{We have } LE(G) \leq \sqrt{2Mn} \Rightarrow LE(G) \leq \sqrt{2Mn} \leq \sqrt{2M(2m)} = 2\sqrt{Mm} \quad (\text{because } M \geq m \Rightarrow \sqrt{Mm} \leq M)$$

Inequalities happened in the above reasoning change to equalities, if $G(n, m)$ is regular graph of degree one, also $LE(G) = 2M$ hold for regular graph of degree one and for all graphs $M = m, n = 2m$ cannot hold at same time, there for equality $LE(G) = 2M$ holds only for regular graph of degree one, Ivan Guttmann [2006]

Theorem: let $G(n, m)$ be a graph of order n and m edges and vertices degree $d_1, d_2, d_3, \dots, d_n$, then $LE(G) \leq E(G) + 2 \sum_{i=1}^{\sigma} \left(d_i - \frac{2m}{n} \right)$ (1) where σ the largest positive integer is satisfying ($\mu_{\sigma} \geq \frac{2m}{n}$)

Proof: for any ($1 \leq K \leq n$) we have $\sum_{i=1}^K \lambda_i(-A(G)) = -\sum_{i=1}^K \lambda_{n-i+1}$ where $\lambda_i(-A(G))$ is the i^{th} largest eigenvalue of $(-A(G))$, then we can

$$\text{write } \sum_{i=1}^K \mu_i \leq \sum_{i=1}^K d_i - \sum_{i=1}^K \lambda_{n-i+1}$$

By definition of energy of graph, we have

$$E(G) = \sum_{i=1}^n |\lambda_i| = 2 \sum_{\lambda_i \geq 0} \lambda_i = -2 \sum_{\lambda_i \leq 0} \lambda_i$$

$$= 2 \max \left\{ - \sum_{i=1}^K \lambda_{n-i+1} : 1 \leq K \leq n-1 \right\} \geq -2 \sum_{i=1}^K \lambda_{n-i+1} : 1 \leq K \leq n-1$$

From above for any K we can have

$$2 \sum_{i=1}^K \mu_i \leq 2 \sum_{i=1}^K d_i + E(G)$$

Since σ is the largest positive integer satisfying ($\mu_{\sigma} \geq \frac{2m}{n}$), we can have

$$2 \sum_{i=1}^{\sigma} \mu_i - \frac{4m\sigma}{n} \leq 2 \sum_{i=1}^{\sigma} d_i + E(G) - \frac{4m\sigma}{n}$$

Note: lemma: let $G(n, m)$ be a graph of order n and m then

$$LE(G) = 2s_{\sigma}(G) - \frac{4m\sigma}{n} = \max\left\{2s_i(G) - \frac{4mi}{n}\right\}$$

From above result and lemma, the result follows, Seyed Ahmad Mojallal [2016]

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