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On Modified Maximum Degree Energy of Graph and HDR Energy of Graph

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Abstract: The spectral graph theory explores connections between combinatorial features of graphs and algebraic properties of associated matrices. In this paper, we introduce modified maximum degree matrix $M_M(\zeta)$ of a simple graph ζ and obtain a bound for eigenvalues of $M_M(\zeta)$. We also introduce modified maximum degree energy $E_{M_M}(\zeta)$ of a graph ζ and obtain bounds for $E_{M_M}(\zeta)$.

Key Words: Modified maximum degree matrix, modified maximum degree energy, eigenvalues, energy of a graph.

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§1. Introduction

The spectral graph theory plays an important role in analyzing the matrices of graphs with the help of matrix theory and linear algebra. Now, spectral graph theory has attracted the attention of both pure and applied mathematicians whose benefit lies far from the spectral graph theory, which may be surprised because graph energy is a special kind of matrix norm. They will then recognize that the concept of graph energy (under different names) is encountered in several seemingly unrelated areas of their own expertise.

The eigenvalues are closely related to almost all major invariants of a graph, linking one extremal property to another, they play a central role in the fundamental understanding of graph. In 1978, I. Gutman related the Graph energy and total π-electron energy in a molecular graph; it was defined as, the sum of absolute values of the eigenvalues of the associated adjacency matrix of a graph ζ. Later, many matrices were defined based on distance and adjacency among the vertices, degree of the vertices involved in forming the graph structure like: Zagreb matrix [5], Randic matrix [10], distance matrix [1], Seidel matrix [2], Laplacian matrix [6], Seidel Laplacian matrix [9], signless Laplacian matrix [3], Seidel signless Laplacian matrix [8], degree sum matrix [7], etc.

In the study of spectral graph theory, we use the spectra of certain matrix associated with the graph, such as the adjacency matrix, the Laplacian matrix and other related matrices. Some useful information about the graph can be obtained from the spectra of these various matrices.

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Throughout the paper, we consider a simple graph ζ, that is nonempty, finite, having no loops, no multiple and directed edges. Let $V(\zeta) = \{\delta_1, \delta_2, \cdots, \delta_{|V(\zeta)|}\}$. The adjacency matrix $A(\zeta)$ of the graph ζ is a square matrix of order $|V(\zeta)|$ whose (i, j)- entry is equal to unity if the vertices δ_i and δ_j are adjacent and is equal to zero otherwise. The eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_{|V(\zeta)|}$ of $A(\zeta)$, assumed in non-increasing order, are the eigenvalues of the graph ζ. As we defined before the energy of ζ is

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

The concept of graph energy arose in chemistry. An interesting quantity in Huckel theory is the sum of the energies of all the electrons in a molecule, the so-called total $\pi-$electron energy.

In this article, we introduce modified maximum degree Matrix $M_M(\zeta)$ of a simple graph ζ and obtain a bound for eigenvalues of $M_M(\zeta)$. We also introduce modified maximum degree energy $E_{M_M}(\zeta)$ of a graph ζ and obtain bounds for $E_{M_M}(\zeta)$. Also we define the concept of HDR energy of graph with some interesting results.

§2. Modified Maximum Degree Matrix of a Graph

Definition 2.1 *Let ζ be a simple graph with vertices $\delta_1, \delta_2, \cdots, \delta_{|V(\zeta)|}$ and let d_i be the degree of δ_i, $i = 1, 2, \cdots, |V(\zeta)|$. Define,*

$$b_{ij} = \begin{cases} max\{d_{\delta_i}, d_{\delta_j}\} + 1, & \text{if } \delta_i \text{ and } \delta_j \text{ are adjacent,;} \\ 0, & \text{otherwise.} \end{cases}$$

Then, the $|V(\zeta)| \times |V(\zeta)|$ matrix $M_M(\zeta) = [b_{ij}]$ is called the modified maximum degree matrix of graph ζ.

The characteristic polynomial of modified maximum degree matrix $M_M(\zeta)$ is defined by

$$\begin{aligned}\psi(\zeta; \lambda) &= Det(\lambda I - M_M(\zeta)) \\ &= \lambda^{|V(\zeta)|} + a_1\ \lambda^{|V(\zeta)|-1} + a_2\ \lambda^{|V(\zeta)|-2} + ... + a_{|V(\zeta)|},\end{aligned}$$

where I is the unit matrix of order $|V(\zeta)|$. The roots $\lambda_1, \lambda_2, \cdots, \lambda_{|V(\zeta)|}$ assumed in non-increasing order are the modified maximum degree eigenvalues of ζ. The modified maximum degree energy of a graph ζ is defined as

$$E_{M_M}(\zeta) = \sum_{i=1}^{|V(\zeta)|} |\lambda_i|.$$

Since $M_M(\zeta)$ is a real symmetric matrix with zero trace, these modified maximum degree eigenvalues are real numbers with sum equal to zero. Thus $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_{|V(\zeta)|}$ and

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{|V(\zeta)|} = 0.$$

Example 2.2 The modified maximum degree matrix of the graph ζ_1 in Figure 1 is

$$M_M(\zeta_1) = \begin{bmatrix} 0 & 3 & 0 & 3 \\ 3 & 0 & 3 & 0 \\ 0 & 3 & 0 & 3 \\ 3 & 0 & 3 & 0 \end{bmatrix}.$$

The characteristic polynomial of the modified maximum degree matrix $M_M(\zeta)$ is

$$\begin{aligned}
\psi(\zeta_1;\lambda) &= Det(\lambda I - M_M(\zeta_1)) \\
&= \begin{bmatrix} \lambda & -3 & 0 & -3 \\ -3 & \lambda & -3 & 0 \\ 0 & -3 & \lambda & -3 \\ -3 & 0 & -3 & \lambda \end{bmatrix} \\
&= \lambda \begin{bmatrix} \lambda & -3 & 0 \\ -3 & \lambda & -3 \\ 0 & -3 & \lambda \end{bmatrix} + 3 \begin{bmatrix} -3 & -3 & 0 \\ 0 & \lambda & -3 \\ -3 & -3 & \lambda \end{bmatrix} + 0 \begin{bmatrix} -3 & \lambda & 0 \\ 0 & -3 & -3 \\ -3 & 0 & \lambda \end{bmatrix} \\
&\quad + 3 \begin{bmatrix} -3 & \lambda & -3 \\ 0 & -3 & \lambda \\ -3 & 0 & -3 \end{bmatrix} \\
&= \lambda\Big(\lambda(\lambda^2-9) + 3(-3\lambda - 0) + 0\Big) \\
&\quad + 3\Big(-3(\lambda^2-9) + 3(0-9) + 0\Big) \\
&\quad + 3\Big(-3(9-0) - \lambda(0+3\lambda) - 3(0-9)\Big) \\
&= \lambda^4 - 36\lambda^2
\end{aligned}$$

and the modified maximum degree eigenvalues of ζ_1 are

$$\lambda_1 = 0,\ \ \lambda_2 = 0,\ \ \lambda_3 = 6,\ \ \lambda_4 = -6.$$

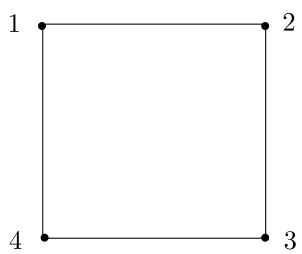

Figure 1. The graph ζ_1

Definition 2.3 *$d_{hr}(v) = |\{u, v \in V(\zeta) | d(u, v) = \lceil \frac{R}{2} \rceil\}|$ and $d(u, v)$ is the distance between the vertices u and v in $V(\zeta)$ and R is the radius of graph ζ.*

Definition 2.4 *Let ζ be a simple graph with n vertices $v_1, v_2, ..., v_n$ and let $d_{hr}i$ be the degree of v_i, $i = 1, 2, ..n$ defined*

$$d_{hr}ij = max\{d_{hr}i, d_{hr}j\}$$

if the $v_{hr}i, v_{hr}j$ adjacent and 0 otherwise. Then the $n \times n$ matrix $H(\zeta) = [d_{hr}ij]$ is called maximum HDR degree matrix of ζ. The characteristic polynomial of the maximum degree matrix $H(\zeta)$ is defined by

$$\begin{aligned} \alpha(\zeta; \epsilon) &= \det(\epsilon I - H(\zeta)) \\ &= \epsilon^n + a_1\epsilon^{n-1} + a_2\epsilon^{n-2} + \cdots + a_n, \end{aligned}$$

where I is the unit matrix of order n.

§3. Some Bounds of Modified Maximum Degree Energy

We now give the explicit expression for the coefficient a_i of $\lambda^{|V(\zeta)|-i}$ $(i = 1, 2, 3, \cdots, |V(\zeta)|)$ in the modified characteristic polynomial of the maximum degree matrix $M_M(\zeta)$. It is clear that $a_0 = 1$ and $a_1 = trace \;\; M_M(\zeta) = 0$. We have

$$a_2 = \sum_{1 \le L \le J \le |V(\zeta)|} \begin{vmatrix} 0 & \delta_{LJ} + 1 \\ \delta_{JL} + 1 & 0 \end{vmatrix}$$

and

$$\begin{vmatrix} 0 & d_{LJ} + 1 \\ d_{JL} + 1 & 0 \end{vmatrix} = \begin{cases} -(max\{d_J + 1, d_L + 1\})^2, & \text{if } \delta_J \text{ and } \delta_L \text{ are adjacent;} \\ 0, & \text{otherwise.} \end{cases}$$

Thus,

$$\begin{aligned} a_2 &= -\sum_{k=1}^{|V(\zeta)|} (r_k + z_k)(d_k + 1)^2 \\ &= -\sum_{k=1}^{|V(\zeta)|} (r_k + z_k)(d(\delta_k) + 1)^2 \end{aligned}$$

where $r_k =$ the number of vertices in the neighborhood of δ_k whose degrees are less than $d(\delta_k)$ and $z_k =$ the number of vertices δ_j $j > k$ in the neighborhood of δ_k whose degrees are equal to

$d(\delta_k)$.

$$a_3 = (-1)^{-3} \sum_{1 \le L \le J \le h \le |V(\zeta)|} \begin{vmatrix} d_{LL}+1 & d_{LJ}+1 & d_{Lh}+1 \\ d_{JL}+1 & d_{JJ}+1 & d_{Jh}+1 \\ d_{hL}+1 & d_{hJ}+1 & d_{hh}+1 \end{vmatrix}$$

$$= -2 \sum_{1 \le L \le J \le h \le |V(\zeta)|} (d_{LJ}+1)(d_{Jh}+1)(d_{hL}+1)$$

$$= -2 \sum_{d(\delta_L) \le d(\delta_J) \le d(\delta_h)} (d(\delta_h)+1)^2 (d(\delta_J)+1)$$

Example 3.1 For the graph ζ_1 in Figure 1, the coefficient a_2 of λ^2 in the characteristic polynomial of the modified maximum degree matrix $M_M(\zeta_1)$ is equal to

$$\begin{aligned} a_2 &= -\sum_{k=1}^{4} (r_k + z_k)(d(\delta_k)+1)^2 \\ &= -\Big((0+2)(2+1)^2 + (0+1)(2+1)^2 + (0+1)(2+1)^2 + (0+0)(2+1)^2\Big) = -36. \end{aligned}$$

Theorem 3.2 *If $\lambda_1, \lambda_2, \cdots, \lambda_{|V(\zeta)|}$ are the modified maximum degree eigenvalues of a graph ζ, then*

$$\sum_{i=1}^{|V(\zeta)|} \lambda_i^2 = -2a_2.$$

Proof We have

$$\begin{aligned} \sum_{i=1}^{|V(\zeta)|} \lambda_i^2 &= trace\ \ of\ \ M_M^2(\zeta) = \sum_{i=1}^{|V(\zeta)|} \left(\sum_{j=1}^{|V(\zeta)|} d_{ij} d_{ji} \right) \\ &= 2 \sum_{i=1}^{|V(\zeta)|} (r_i + z_i)(d(\delta_i)+1)^2 = -2a_2. \end{aligned}$$

This completes the proof. $\square$

Theorem 3.3 *Let ζ be a graph. Then,*

$$\sqrt{2 \sum_{i=1}^{|V(\zeta)|} (d(\delta_i)+1)^2 + |V(\zeta)|(|V(\zeta)|-1)\beta^{\frac{2}{|V(\zeta)|}}}$$

$$\le E_{M_M}(\zeta) \le \sqrt{2|V(\zeta)| \sum_{i=1}^{|V(\zeta)|} (r_i + z_i)(d(\delta_i)+1)^2}.$$

Proof We have

$$E^2_{M_M}(\zeta) = \left(\sum_{i=1}^{|V(\zeta)|} |\lambda_i|\right)^2 = \sum_{i=1}^{|V(\zeta)|} |\lambda_i|^2 + \sum_{i\neq l} |\lambda_i||\lambda_l|$$
$$\geq 2\sum_{i=1}^{|V(\zeta)|} (r_i + z_i)(d(\delta_i)+1)^2 + |V(\zeta)|(|V(\zeta)-1|)\beta^{\frac{2}{|V(\zeta)|}},$$

where
$$\beta = \prod_{i=1}^{|V(\zeta)|} |\lambda_i|$$

and the last inequality is due to Theorem 3.2, the arithmetic mean, the geometric mean inequality. On employing Holder's inequality, we obtain

$$E_{M_M}(\zeta) = \sum_{i=1}^{|V(\zeta)|} |\lambda_i|$$
$$\leq \sqrt{\sum_{i=1}^{|V(\zeta)|} |\lambda_i|^2}.\ \sqrt{|V(\zeta)|}$$
$$= \sqrt{2|V(\zeta)| \sum_{i=1}^{|V(\zeta)|} (r_i + z_i)(d(\delta_i)+1)^2}$$

This completes the proof. □

Proposition 3.4 *Let ζ be a graph such that $\zeta \cong C_n, K_{n,m}, W_n, F_p$. Then, the maximum HDR degree energy of ζ is same as its maximum first degree energy.*

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