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Research Article

General Zagreb adjacency matrix

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Abstract

Let $A(G)$ and $D(G)$ be the adjacency matrix and the degree diagonal matrix of a graph G, respectively. For any real number α, the general Zagreb adjacency matrix of G is defined as $Z_\alpha(G) = D^\alpha(G)+A(G)$. In this paper, the positive semidefiniteness, spectral moment, coefficients of characteristic polynomials, and energy of the general Zagreb adjacency matrix are studied. The obtained results extend the corresponding results concerning the signless Laplacian matrix, the vertex Zagreb adjacency matrix, and the forgotten adjacency matrix.

Keywords: Zagreb adjacency matrix; positive semidefinite matrix; spectral moment; energy of a graph.

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1. Introduction

Let G be a simple graph with the vertex set $V(G)$ and edge set $E(G)$. For $v_i \in V(G)$, d_i or $d(v_i)$ denotes the degree of the vertex v_i in G. Recently, in order to extend the spectral theory of classical graph matrices such as adjacency matrix, signless Laplacian matrix and distance matrix, many scholars have devoted themselves to the study of the generalization of graph matrices, and proposed many new graph matrices including the generalised adjacency matrix [4], the universal adjacency matrix [6], A_α-matrix [10], and the generalized distance matrix [2]. Inspired by these studies, we propose the general Zagreb adjacency matrix of a graph G as follows:

$$Z_\alpha(G) = D^\alpha(G) + A(G), \quad \alpha \in \mathbb{R},$$

where $A(G)$ and $D(G)$ are the adjacency matrix and the degree diagonal matrix of G, respectively. The general Zagreb adjacency matrix gives several existing matrices as special cases:

1. $Z_0(G) = D^0(G) + A(G) = I + A(G)$, where I is identity matrix;
2. $Z_1(G) = D(G) + A(G)$ is the signless Laplacian matrix [3];
3. $Z_2(G) = D^2(G) + A(G)$ is the vertex Zagreb adjacency matrix [7];
4. $Z_3(G) = D^3(G) + A(G)$ is the forgotten adjacency matrix [7];
5. $Z_\alpha(G) = r^\alpha I + A(G)$ when G is r-regular.

Let $z_1, z_2, \ldots, z_n$ be the eigenvalues of the general Zagreb adjacency matrix of a graph G with n vertices. The general Zagreb adjacency energy of G is defined as

$$E_\alpha(G) = \sum_{i=1}^{n} \left| z_i - \frac{M_\alpha}{n} \right|, \quad \alpha \in \mathbb{R},$$

where $M_\alpha = \sum_{v_i \in V(G)} d_i^\alpha$ is called the first general Zagreb index [8].

In this paper, some spectral properties of the general Zagreb adjacency matrix are reported. The obtained results extend the corresponding results concerning the signless Laplacian matrix, the vertex Zagreb adjacency matrix, and the forgotten adjacency matrix.

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2. Preliminaries

For an integer k, the k-th spectral moment of a graph is defined as the sum over the k-th powers of all eigenvalues of the adjacency matrix. Let λ_i and $tr(A)$ be the ith eigenvalue and trace of the adjacency matrix A, respectively. Denote by P_n and C_n the path and the cycle, respectively, on n vertices. For a graph G with n vertices and m edges, it holds that

$$\sum_{i=1}^{n}\lambda_i^2 = tr(A^2) = 2m, \quad \sum_{i=1}^{n}\lambda_i^3 = tr(A^3) = 6|C_3|, \quad \sum_{i=1}^{n}\lambda_i^4 = tr(A^4) = 8|C_4| + 4|P_3| + 2m,$$

where $|C_3|$ and $|C_4|$ are the number of triangles and quadrangles of G, respectively. In 1998, Bollobás and Erdős [1] defined the general Randić index as:

$$R_\alpha = R_\alpha(G) = \sum_{v_iv_j\in E(G)} (d_id_j)^\alpha,$$

where α is an arbitrary real number.

Lemma 2.1 (see [11]). *Let $M = (m_{ij})$ be a matrix with the characteristic polynomial*

$$\Phi(M) = \det(xI - M) = x^n + \sum_{i=1}^{n} a_ix^{n-i}.$$

Let $s_k = tr(M^k)$. Then the coefficients of $\Phi(M)$ satisfy the following equations:

$$a_1 = -s_1, \quad ka_k = -s_k - a_1s_{k-1} - a_2s_{k-2} - \cdots - a_{k-1}s_1, \quad (k = 2, 3, \ldots, n).$$

Lemma 2.2 (see [5]). *Let $a = (a_1, a_2, \ldots, a_n)$, $b = (b_1, b_2, \ldots, b_n)$ be sequences of real numbers and $s = (s_1, s_2, \ldots, s_n)$, $t = (t_1, t_2, \ldots, t_n)$ be nonnegative. If $\beta, \gamma > 0$ and $\eta \in \mathbb{R}$ such that $\eta^2 \le \beta\gamma$, then*

$$\beta\sum_{i=1}^{n} t_i \sum_{i=1}^{n} a_i^2s_i + \gamma\sum_{i=1}^{n} s_i \sum_{i=1}^{n} b_i^2t_i \ge 2\eta\sum_{i=1}^{n} a_is_i \sum_{i=1}^{n} b_it_i.$$

3. The positive semidefiniteness of the general Zagreb adjacency matrix

Theorem 3.1. *Let G be a connected graph with n vertices. If $\alpha > \beta$, then*

$$z_k(Z_\alpha) > z_k(Z_\beta)$$

for $k = 1, 2, \ldots, n$.

Proof. By Weyl's inequality, we have

$$z_k(Z_\alpha) - z_k(Z_\beta) \ge z_{\min}(D^\alpha - D^\beta) > 0.$$

This completes the proof. □

Corollary 3.1. *If $\alpha = 1$, and G is a graph, then $Z_\alpha(G)$ is positive semidefinite. If $\alpha > 1$, and G is a graph with no isolated vertices, then $Z_\alpha(G)$ is positive definite.*

Proof. It is well known that the signless Laplacian matrix $Z_1(G)$ is positive semidefinite. If $\alpha > 1$, and G is a graph with no isolated vertices, then by Theorem 3.1 one has

$$z_{\min}(Z_\alpha(G)) > z_{\min}(Z_1(G)) \ge 0.$$

Thus $Z_\alpha(G)$ is positive definite for $\alpha > 1$. □

Theorem 3.2. *Let G be a connected bipartite graph. Then $Z_\alpha(G)$ is positive semidefinite if and only if $\alpha \ge 1$.*

Proof. Since a connected graph G is bipartite if and only if $z_{\min}(Z_1(G)) = 0$, by Theorem 3.1, we have that $Z_\alpha(G)$ is positive semidefinite if and only if $\alpha \ge 1$. □

Theorem 3.3. *Let G be a graph with n vertices, m edges and chromatic number χ. Then*

$$z_{\min}(Z_\alpha(G)) \le \frac{(\chi - 1)M_\alpha - 2m}{n(\chi - 1)}.$$

Proof. Let $V_1, V_2, \ldots, V_\chi$ be the color classes of G. For an integer k, $1 \le k \le \chi$, define a vector $X = (x_1, x_2, \ldots, x_n)$ by

$$x_i = \begin{cases} \chi - 1, & \text{if } v_i \in V_k; \\ -1, & \text{otherwise.} \end{cases}$$

By the Rayleigh-Ritz theorem, one has

$$z_{\min}(Z_\alpha(G))||X||^2 \le XZ_\alpha(G)X^T = \sum_{v_i \in V(G)} d_i^\alpha x_i^2 + 2 \sum_{v_iv_j \in E(G)} x_i x_j.$$

On the one hand, for $||X||^2$ it holds that

$$||X||^2 = (\chi-1)^2|V_k| + (n - |V_k|) = \chi(\chi-2)|V_k| + n.$$

But,

$$\begin{aligned} \sum_{v_i \in V(G)} d_i^\alpha x_i^2 + 2 \sum_{v_iv_j \in E(G)} x_i x_j &= \sum_{v_i \in V(G)\setminus V_k} d_i^\alpha + \sum_{v_i \in V_k} (\chi-1)^2 d_i^\alpha - 2(\chi-1) \sum_{v_i \in V_k} d_i + 2\left(m - \sum_{v_i \in V_k} d_i\right) \\ &= M_\alpha + \sum_{v_i \in V_k} \chi(\chi-2) d_i^\alpha + 2\left(m - \chi \sum_{v_i \in V_k} d_i\right). \end{aligned}$$

Therefore,

$$z_{\min}(Z_\alpha(G))\big[\chi(\chi-2)|V_k| + n\big] \le M_\alpha + \sum_{v_i \in V_k} \chi(\chi-2) d_i^\alpha + 2\left(m - \chi \sum_{v_i \in V_k} d_i\right).$$

Adding the above inequalities for all $k \in \{1, 2, \ldots, \chi\}$, one arrives at

$$z_{\min}(Z_\alpha(G)) \sum_{k=1}^{\chi} [\chi(\chi-2)|V_k| + n] \le \sum_{k=1}^{\chi} \left[M_\alpha + \sum_{v_i \in V_k} \chi(\chi-2) d_i^\alpha + 2\left(m - \chi \sum_{v_i \in V_k} d_i\right)\right],$$

which gives,

$$n\chi(\chi-1) z_{\min}(Z_\alpha(G)) \le \chi M_\alpha + \chi(\chi-2) M_\alpha + 2m\chi - 4m\chi,$$

that is,

$$z_{\min}(Z_\alpha(G)) \le \frac{(\chi-1)M_\alpha - 2m}{n(\chi-1)}.$$

This completes the proof. □

Remark 3.1. *Lima et al.* [9] *showed that if G is a graph with n vertices, m edges and chromatic number χ, then*

$$z_{\min}(Z_1(G)) \le \frac{2m(\chi-2)}{n(\chi-1)}.$$

Theorem 3.3 asserts that this bound can be extended to all matrices Z_α.

Corollary 3.2. *If $M_\alpha < \frac{2m}{\chi-1}$, and G is a graph, then $Z_\alpha(G)$ is not positive semidefinite.*

Question 3.1. *Given a graph G, find the smallest α for which $Z_\alpha(G)$ is positive semidefinite.*

4. The spectral moment of the general Zagreb adjacency matrix

Theorem 4.1. *Let G be a graph with n vertices and m edges. Then*

$$\begin{aligned} \sum_{i=1}^{n} z_i &= tr(Z_\alpha) = M_\alpha, \\ \sum_{i=1}^{n} z_i^2 &= tr(Z_\alpha^2) = M_{2\alpha} + 2m, \\ \sum_{i=1}^{n} z_i^3 &= tr(Z_\alpha^3) = M_{3\alpha} + 3M_{\alpha+1} + 6|C_3|, \\ \sum_{i=1}^{n} z_i^4 &= tr(Z_\alpha^4) = M_{4\alpha} + 4M_{2\alpha+1} + 8\sum_{i=1}^{n} t_G(v_i) d_i^\alpha + 4R_\alpha + 8|C_4| + 4|P_3| + 2m, \end{aligned}$$

where $t_G(v_i)$ is the number of triangles containing the vertex v_i of G.

Proof. By definition, the diagonal elements of Z_α are equal to d_i^α. Thus, the trace of Z_α is M_α. Next, we calculate the trace of Z_α^2. Since $tr(BC) = tr(CB)$ and $tr(D^\alpha A) = 0$, one has

$$\begin{aligned} tr(Z_\alpha^2) &= tr(D^{2\alpha}) + tr(D^\alpha A) + tr(AD^\alpha) + tr(A^2) \\ &= tr(D^{2\alpha}) + 2tr(D^\alpha A) + tr(A^2) \\ &= M_{2\alpha} + 2m. \end{aligned}$$

Since $tr(BC) = tr(CB)$ and $tr(D^{2\alpha}A) = 0$, it holds that

$$\begin{aligned} tr(Z_\alpha^3) &= tr(D^{3\alpha}) + tr(D^{2\alpha}A) + tr(D^\alpha AD^\alpha) + tr(D^\alpha A^2) + tr(AD^{2\alpha}) + tr(AD^\alpha A) + tr(A^2D^\alpha) + tr(A^3) \\ &= tr(D^{3\alpha}) + 3tr(D^{2\alpha}A) + 3tr(D^\alpha A^2) + tr(A^3) \\ &= M_{3\alpha} + 3M_{\alpha+1} + 6|C_3|. \end{aligned}$$

Since $tr(BC) = tr(CB)$ and $tr(D^{3\alpha}A) = 0$, one has

$$\begin{aligned} tr(Z_\alpha^4) &= tr(D^{4\alpha}) + tr(D^{3\alpha}A) + tr(D^{2\alpha}AD^\alpha) + tr(D^{2\alpha}A^2) + tr(D^\alpha AD^{2\alpha}) + tr(D^\alpha AD^\alpha A) + tr(D^\alpha A^2D^\alpha) + tr(D^\alpha A^3) \\ &\quad + tr(AD^{3\alpha}) + tr(AD^{2\alpha}A) + tr(AD^\alpha AD^\alpha) + tr(AD^\alpha A^2) + tr(A^2D^{2\alpha}) + tr(A^2D^\alpha A) + tr(A^3D^\alpha) + tr(A^4) \\ &= tr(D^{4\alpha}) + 4tr(D^{3\alpha}A) + 4tr(D^{2\alpha}A^2) + 4tr(D^\alpha A^3) + 2tr(D^\alpha AD^\alpha A) + tr(A^4) \\ &= M_{4\alpha} + 4M_{2\alpha+1} + 8\sum_{i=1}^n t_G(v_i)d_i^\alpha + 4R_\alpha + 8|C_4| + 4|P_3| + 2m. \end{aligned}$$

This completes the proof. □

Corollary 4.1. *Let G be a graph with n vertices and m edges. Then the first four coefficients a_1, a_2, a_3, a_4 of characteristic polynomials of the general Zagreb adjacency matrix are given as follows:*

$$\begin{aligned} a_1 &= -M_\alpha, \\ a_2 &= \frac{M_\alpha^2 - M_{2\alpha}}{2} - m, \\ a_3 &= M_\alpha\left(\frac{M_{2\alpha}}{2} - \frac{M_\alpha^2}{6} + m\right) - \frac{1}{3}M_{3\alpha} - M_{\alpha+1} - 2|C_3|, \\ a_4 &= M_\alpha\left[\frac{M_{3\alpha}}{3} + M_{\alpha+1} + 2|C_3| - M_\alpha\left(\frac{M_{2\alpha}}{8} - \frac{M_\alpha^2}{24} + \frac{m}{4}\right)\right] - \frac{M_{4\alpha}}{4} - M_{2\alpha+1} - 2\sum_{i=1}^n t_G(v_i)d_i^\alpha - R_\alpha - 2|C_4| - |P_3| - \frac{m}{2} \\ &\quad -(M_{2\alpha} + 2m)\left(\frac{M_\alpha^2 - M_{2\alpha}}{8} - \frac{m}{4}\right). \end{aligned}$$

Proof. From Lemma 2.1 and Theorem 4.1, the results follow. □

Corollary 4.2. *Let G be a graph with n vertices and m edges. Then*

$$\begin{aligned} \Gamma_2 &= \sum_{i=1}^n \left|z_i - \frac{M_\alpha}{n}\right|^2 = M_{2\alpha} - \frac{M_\alpha^2}{n} + 2m, \\ \Gamma_4 &= \sum_{i=1}^n \left|z_i - \frac{M_\alpha}{n}\right|^4 \\ &= M_{4\alpha} + 4M_{2\alpha+1} + 8\sum_{i=1}^n t_G(v_i)d_i^\alpha + 4R_\alpha + 8|C_4| + 4|P_3| + 2m - \frac{4M_\alpha}{n}\Big(M_{3\alpha} + 3M_{\alpha+1} + 6|C_3|\Big) \\ &\quad + \frac{6M_\alpha^2}{n^2}\Big(M_{2\alpha} + 2m\Big) - \frac{3M_\alpha^4}{n^3}. \end{aligned}$$

Proof. The result follows from Theorem 4.1. □

5. Bounds on the general Zagreb adjacency energy of a graph

Theorem 5.1. *Let G be a graph with n vertices and m edges. Then*

$$\sqrt{2\left(M_{2\alpha}+2m-\frac{M_\alpha^2}{n}\right)} \le E_\alpha(G) \le \sqrt{n\left(M_{2\alpha}+2m-\frac{M_\alpha^2}{n}\right)}.$$

Proof. By the Cauchy-Schwarz inequality, we have

$$E_\alpha(G)=\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right| \le \sqrt{n\Gamma_2}=\sqrt{n\left(M_{2\alpha}+2m-\frac{M_\alpha^2}{n}\right)}.$$

From the definition of the general Zagreb adjacency energy, it follows that

$$\begin{aligned}
E_\alpha^2(G) &= \left(\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|\right)^2\\
&= \sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|^2+2\sum_{i<j}\left|z_i-\frac{M_\alpha}{n}\right|\left|z_j-\frac{M_\alpha}{n}\right|\\
&\ge \Gamma_2+2\left|\sum_{i<j}\left(z_i-\frac{M_\alpha}{n}\right)\left(z_j-\frac{M_\alpha}{n}\right)\right|\\
&= \Gamma_2+2\left|\sum_{i<j}\left(z_iz_j-\frac{M_\alpha}{n}(z_i+z_j)+\frac{M_\alpha^2}{n^2}\right)\right|\\
&= \Gamma_2+2\left|a_2-\frac{M_\alpha^2}{n}(n-1)+\frac{M_\alpha^2}{n^2}\cdot\frac{n(n-1)}{2}\right|\\
&= \Gamma_2+2\left|a_2-\frac{(n-1)M_\alpha^2}{2n}\right|\\
&= M_{2\alpha}-\frac{M_\alpha^2}{n}+2m+2\left|\frac{M_\alpha^2-M_{2\alpha}}{2}-m-\frac{(n-1)M_\alpha^2}{2n}\right|\\
&= 2\left(M_{2\alpha}+2m-\frac{M_\alpha^2}{n}\right).
\end{aligned}$$

Thus,

$$E_\alpha(G)\ge\sqrt{2\left(M_{2\alpha}+2m-\frac{M_\alpha^2}{n}\right)}.$$

This completes the proof. □

Theorem 5.2. *Let G be a graph with n vertices. If $\beta,\gamma>0$ and $\eta\in\mathbb{R}$ such that $\eta^2\le\beta\gamma$, then*

$$\sqrt{\frac{\Gamma_2^3}{\Gamma_4}} \le E_\alpha(G) \le \frac{n}{2\eta}\left(\beta+\gamma\frac{\Gamma_4}{\Gamma_2}\right).$$

Proof. Taking $a_i=\left|z_i-\frac{M_\alpha}{n}\right|^{\frac{2}{3}}$, $b_i=\left|z_i-\frac{M_\alpha}{n}\right|^{\frac{4}{3}}$, $p=\frac{3}{2}$ and $q=3$ in the Hölder inequality

$$\sum_{i=1}^{n}a_ib_i\le\left(\sum_{i=1}^{n}a_i^p\right)^{\frac{1}{p}}\left(\sum_{i=1}^{n}b_i^q\right)^{\frac{1}{q}}$$

gives

$$\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|^2=\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|^{\frac{2}{3}}\left(\left|z_i-\frac{M_\alpha}{n}\right|^4\right)^{\frac{1}{3}}\le\left(\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|\right)^{\frac{2}{3}}\left(\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|^4\right)^{\frac{1}{3}},$$

that is,

$$E_\alpha(G)\ge\left(\frac{\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|^2}{\left(\sum_{i=1}^{n}\left|z_i-\frac{M_\alpha}{n}\right|^4\right)^{\frac{1}{3}}}\right)^{\frac{3}{2}}=\sqrt{\frac{\Gamma_2^3}{\Gamma_4}}.$$

Setting $s_i = t_i = 1$, $a_i = \left|z_i - \frac{M_\alpha}{n}\right|$ and $b_i = \left|z_i - \frac{M_\alpha}{n}\right|^2$ in Lemma 2.2, yields

$$\beta n \sum_{i=1}^{n} \left|z_i - \frac{M_\alpha}{n}\right|^2 + \gamma n \sum_{i=1}^{n} \left|z_i - \frac{M_\alpha}{n}\right|^4 \geq 2\eta \sum_{i=1}^{n} \left|z_i - \frac{M_\alpha}{n}\right| \sum_{i=1}^{n} \left|z_i - \frac{M_\alpha}{n}\right|^2,$$

that is,

$$E_\alpha(G) \leq \frac{n}{2\eta}\left(\beta + \gamma \frac{\Gamma_4}{\Gamma_2}\right).$$

Combining the above arguments completes the proof. □

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