General Zagreb adjacency matrix

Zhen Lin1,2,*

1School of Mathematics and Statistics, The State Key Laboratory of Tibetan Intelligent Information Processing and Application, Qinghai Normal University, Xining, Qinghai, China
2Academy of Plateau Science and Sustainability, People’s Government of Qinghai Province and Beijing Normal University, China

(Received: 27 August 2022. Received in revised form: 10 September 2022. Accepted: 10 September 2022. Published online: 13 September 2022.)

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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 \( \alpha \), 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.

2020 Mathematics Subject Classification: 05C50, 05C07, 05C09.

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], \( A_\alpha \)-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.

*E-mail address: lnlinzhen@163.com
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 $\lambda_i$ and $tr(A)$ be the $i$th 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

$$\sum_{i=1}^{n} \lambda_i^2 = tr(A^2) = 2m,$$

$$\sum_{i=1}^{n} \lambda_i^3 = tr(A^3) = 6|C_3|, \quad \sum_{i=1}^{n} \lambda_i^4 = tr(A^4) = 8|C_4| + 4|P_5| + 2m,$$

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:

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

where $\alpha$ is an arbitrary real number.

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

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

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

$$a_1 = -s_1, \quad k a_k = -s_k - a_1 s_{k-1} - a_2 s_{k-2} - \cdots - a_{k-1} s_1, \quad (k = 2, 3, \ldots, n).$$

**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 $\eta^2 \leq \beta \gamma$, then

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

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

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

This completes the proof. \qed

**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

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

Thus $Z_{\alpha}(G)$ is positive definite for $\alpha > 1$. \qed

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

**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 $\alpha \geq 1$. \qed

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

$$z_{\min}(Z_{\alpha}(G)) \leq \frac{(\chi - 1)M_{\alpha} - 2m}{n(\chi - 1)}.$$
Proof. Let \( V_1, V_2, \ldots, V_\chi \) be the color classes of \( G \). For an integer \( k, 1 \leq k \leq \chi \), 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
\[
z_{\min}(Z_\alpha(G))||X||^2 \leq XZ_\alpha(G)X^T = \sum_{v_i \in V(G)} d_i^\alpha x_i^2 + 2 \sum_{v_i, v_j \in E(G)} x_i x_j.
\]
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,
\[
\sum_{v_i \in V(G)} d_i^\alpha x_i^2 + 2 \sum_{v_i, v_j \in E(G)} x_i x_j = \sum_{v_i \in V(G) \setminus V_k} d_i^\alpha + \sum_{v_i \in V_k} (\chi - 1)^2 d_i^\alpha - 2(\chi - 1) \sum_{v_i \in V_k} d_i + 2 \left( m - \sum_{v_i \in V_k} d_i \right)
\]
\[
= M_\alpha + \sum_{v_i \in V_k} \chi(\chi - 2)d_i^\alpha + 2 \left( m - \chi \sum_{v_i \in V_k} d_i \right).
\]
Therefore,
\[
z_{\min}(Z_\alpha(G)) [\chi(\chi - 2)|V_k| + n] \leq M_\alpha + \sum_{v_i \in V_k} \chi(\chi - 2)d_i^\alpha + 2 \left( m - \chi \sum_{v_i \in V_k} d_i \right).
\]
Adding the above inequalities for all \( k \in \{1, 2, \ldots, \chi\} \), one arrives at
\[
z_{\min}(Z_\alpha(G)) \frac{\sum_{k=1}^\chi [\chi(\chi - 2)|V_k| + n]}{\chi} \leq \sum_{k=1}^\chi \left[ M_\alpha + \sum_{v_i \in V_k} \chi(\chi - 2)d_i^\alpha + 2 \left( m - \chi \sum_{v_i \in V_k} d_i \right) \right],
\]
which gives,
\[
n\chi - 1 \chi z_{\min}(Z_\alpha(G)) \leq \chi M_\alpha + \chi(\chi - 2)M_\alpha + 2m\chi - 4m\chi,
\]
that is,
\[
z_{\min}(Z_\alpha(G)) \leq \frac{(\chi - 1)M_\alpha - 2m}{n(\chi - 1)}.
\]
This completes the proof. \(\square\)

Remark 3.1. Lima et al. [9] showed that if \( G \) is a graph with \( n \) vertices, \( m \) edges and chromatic number \( \chi \), then
\[
z_{\min}(Z_\chi(G)) \leq \frac{2m(\chi - 2)}{n(\chi - 1)}.
\]

Theorem 3.3 asserts that this bound can be extended to all matrices \( Z_\alpha \).

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 \( \alpha \) 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
\[
\sum_{i=1}^n z_i = tr(Z_\alpha) = M_\alpha,
\]
\[
\sum_{i=1}^n z_i^2 = tr(Z_\alpha^2) = M_{2\alpha} + 2m,
\]
\[
\sum_{i=1}^n z_i^3 = tr(Z_\alpha^3) = M_{3\alpha} + 3M_{\alpha+1} + 6|C_3|,
\]
\[
\sum_{i=1}^n z_i^4 = tr(Z_\alpha^4) = M_{4\alpha} + 4M_{2\alpha+1} + 8 \sum_{i=1}^n t_G(v_i)d_i^\alpha + 4R_\alpha + 8|C_4| + 4|P_3| + 2m,
\]
where \( t_G(v_i) \) is the number of triangles containing the vertex \( v_i \) of \( G \).
The result follows from Theorem 4.1. From Lemma 2.1 and Theorem 4.1, the results follow.

Proof. Let Corollary 4.2.

\[ \text{Let } Z = \text{polynomials of the general Zagreb adjacency matrix are given as follows:} \]

This completes the proof. \( \blacksquare \)

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:

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

Proof. From Lemma 2.1 and Theorem 4.1, the results follow. \( \blacksquare \)

Corollary 4.2. Let \( G \) be a graph with \( n \) vertices and \( m \) edges. Then

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

Proof. The result follows from Theorem 4.1. \( \blacksquare \)
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

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

**Proof.** By the Cauchy-Schwarz inequality, we have

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

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

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

Thus,

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

This completes the proof. \( \square \)

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

$$\sqrt{\frac{\Gamma_3}{\Gamma_4}} \leq E_\alpha(G) \leq \frac{n}{2\eta} \left( \beta + \gamma \frac{\Gamma_4}{\Gamma_2} \right).$$

**Proof.** Taking $a_i = \left| z_i - \frac{M_\alpha}{n} \right|^\frac{p}{q}$, $b_i = \left| z_i - \frac{M_\alpha}{n} \right|^\frac{1}{q}$, $p = \frac{3}{2}$ and $q = 3$ in the Hölder inequality

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

gives

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

that is,

$$E_\alpha(G) \geq \left( \frac{\sum_{i=1}^{n} \left| z_i - \frac{M_\alpha}{n} \right|^2}{\left( \sum_{i=1}^{n} \left| z_i - \frac{M_\alpha}{n} \right|^4 \right)^{\frac{1}{4}}} \right)^{\frac{2}{3}} = \sqrt{\frac{\Gamma_3}{\Gamma_4}}.$$
Setting $s_i = t_i = 1, a_i = |z_i - M\alpha n|$ and $b_i = |z_i - M\alpha n|^2$ in Lemma 2.2, yields

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

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.

Acknowledgements

The author would like to thank the anonymous referees very much for valuable suggestions, corrections, and comments, which improved the original version of this paper. This study was supported by the National Natural Science Foundation of China (Grant No. 12071411).

References

[1] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Combin.* 50 (1998) 225–233.
[2] S. Cui, J. He, G. Tian, The generalized distance matrix, *Linear Algebra Appl.* 563 (2019) 1–23.
[3] D. Cvetkovic, Signless Laplacians and line graphs, *Bull. Acad. Serbe Sci. Arts Cl. Sci. Math. Natur. Sci. Math.* 131 (2005) 85–92.
[4] E. R. van Dam, W. H. Haemers, Which graphs are determined by their spectrum?, *Linear Algebra Appl.* 373 (2003) 241–272.
[5] S. S. Dragomir, On Some Inequalities, Caiete Metodico Științifice 13, Timișoara University, Timișoara, 1984.
[6] W. H. Haemers, G. R. Omidi, Universal adjacency matrices with two eigenvalues, *Linear Algebra Appl.* 435 (2011) 2520–2529.
[7] S. M. Hosamani, B. B. Kulkarni, R. G. Boli, V. M. Gadag, QSPR analysis of certain graph theoretical matrices and their corresponding energy, *Appl. Math. Nonlinear Sci.* 2 (2017) 131–150.
[8] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* 54 (2005) 195–208.
[9] L. S. de Lima, C. S. Oliveira, N. M. M. de Abreu, V. Nikiforov, The smallest eigenvalue of the signless Laplacian, *Linear Algebra Appl.* 435 (2011) 2570–2584.
[10] V. Nikiforov, Merging the $A$- and $Q$-spectral theories, *Appl. Anal. Discrete Math.* 11 (2017) 81–107.
[11] V. V. Prasolov, *Problems and Theorems in Linear Algebra*, American Mathematical Society, Cambridge, 1994.