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Department of Applied Mathematics
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Master Thesis

圖的阿爾發指標之研究

The Alpha-Index of a Graph

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摘　要

給定 $0 \leq \alpha \leq 1$，一個圖 G 的 A_α-矩陣定義爲 $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$，其中 $A(G)$ 和 $D(G)$ 分別是 G 的鄰接矩陣和度數矩陣。 $A_\alpha(G)$ 的最大特徵值稱爲 G 的阿爾發指標。在本論文中，我們探討當 α 較小時，在 $\mathcal{G}(n,m)$（即點數爲 n 且邊數爲 m 的圖的集合）中，哪個圖擁有最大的阿爾發指標。我們證明，如果 $2m = c(c-1)+2t$，其中 c 和 t 滿足 $1 \leq t \leq c-1$，並且 α 滿足 $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$，那麼在 $\mathcal{G}(n,m)$ 中，只有圖 G_0 擁有最大的阿爾發指標。圖 G_0 是從點數爲 c 的完全圖 K_c 中通過添加一個新頂點 v、添加 t 條邊（每條邊都連接 v 和 K_c 中的一個頂點）、以及添加 $n-c-1$ 個孤立頂點所得到的圖。

關鍵字：譜半徑，阿爾發矩陣，阿爾發指標，矩陣分割

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Abstract

Given $0 \leq \alpha \leq 1$, the A_α-matrix of a graph G is the matrix defined by $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$, where $A(G)$ and $D(G)$ are the adjacency matrix and the degree matrix of G, respectively. The largest eigenvalue of $A_\alpha(G)$ is called the α-index of G. In this thesis, we focus on determining the graph with the maximum α-index among $\mathcal{G}(n,m)$, the set of graphs of order n and size m, for small values of α. We prove that if $2m = c(c-1) + 2t$ with $1 \leq t \leq c-1$, and $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$, then G_0 is the only graph with the maximum α-index among $\mathcal{G}(n,m)$. Here, G_0 is the graph obtained from the complete graph K_c of order c by adding a new vertex v, adding t edges, each incident on v and a vertex in K_c, and adding $n-c-1$ isolated vertices.

Keywords: spectral radius, A_α-matrix, α-index, matrix partition

Contents

Chapter 1. Introduction

All graphs considered in this thesis are finite, undirected, and simple. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The cardinalities of $V(G)$ and $E(G)$ are called the *order* and the *size* of G, respectively. The *degree* of a vertex v is the number of edges incident to v. If $V(G) = \{v_1, v_2, \ldots, v_n\}$, then the *adjacency matrix* of G is defined as an $n \times n$ matrix whose (i, j)-entry is 1 if v_i and v_j are adjacent and 0 otherwise. The *degree matrix* of G is a diagonal matrix whose (i, i)-entry is equal to the degree of v_i.

In 2017, Nikiforov [5] introduced the study of the A_α-*matrix* of G, defined by $A_\alpha(G) = \alpha D(G)+(1-\alpha)A(G)$ for $0 \leq \alpha \leq 1$. This matrix generalizes adjacency and degree matrices, providing a flexible tool for spectral graph analysis. The α-*index* of G, denoted by $\rho_\alpha(G)$ is the largest eigenvalue of $A_\alpha(G)$. We will discuss some details in Chapter 2.

The problem of determining the graph with the maximal α-index among graphs of a given condition has attracted considerable interest. In 2017, Nikiforov [6] solved this problem for trees of order n and $0 \leq \alpha \leq 1$. In 2022, Zhai, Lin, and Zhao [8] solved the case where $\alpha = \frac{1}{2}$, for graphs of order n and size $m = n + k$ with $4 \leq k \leq n - 3$. In 2023, Chang and Tam [1] generalized this result to all $\alpha \in [\frac{1}{2}, 1)$.

In this thesis, we focus on the problem of determining the maximal α-index for graphs of a given order and size for small values of α. The case of $\alpha = 0$ was solved by Rowlinson in 1987 [7], who proved the following theorem.

Theorem 1.1. *[7] If $2m = c(c-1) + 2t$, where $1 \leq t \leq c - 1$ and G is a graph with the maximal index among all the graphs in $\mathcal{G}(n, m)$, then $G = G_0$.*

Here, $\mathcal{G}(n, m)$ denotes the set of all graphs with order n and size m, and G_0 is the graph in $\mathcal{G}(n, m)$ obtained from a complete graph K_c of order c by adding a vertex v and t edges, each incident on v and a vertex in K_c, and adding $n - c - 1$ isolated vertices. We will discuss more details of the graph G_0 in Section 4.1.

Since $\rho_\alpha(G)$ is a continuous function in α, it makes sense that the result of Theorem 1.1 might also work for small values of α. In this thesis, we extend Rowlinson's result to the α-index for $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$:

Theorem 1.2. *If* $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$, $2m = c(c-1) + 2t$, *where* $1 \leq t \leq c-1$ *and* G *is a graph with the maximal* α*-index among all the graphs in* $\mathcal{G}(n, m)$, *then* $G = G_0$.

The thesis is organized as follows: In Chapter 2, we provide the necessary background on graph theory and spectral graph theory. Key concepts and theorems, including the Perron-Frobenius theorem, are introduced to set the stage for the subsequent chapters. In Chapter 3, we explore the properties of the A_α-matrix, establishing upper bounds for the spectral radius. In Chapter 4, we focus on the maximal α-index problem for graphs with a given order and size when α is small and prove Theorem 1.2.

Chapter 2. Preliminaries

2.1 Perron-Frobenius Theorem

Let C be a real square matrix. The *spectral radius* of C is defined by

$$\rho(C) := \max\{|\lambda| : \lambda \text{ is an eigenvalue of } C\}.$$

We denote the largest real eigenvalue of C by $\rho_r(C)$. If C has no real eigenvalue, define $\rho_r(C) = \infty$. Note that if C is symmetric, then $\rho(C) = \rho_r(C)$. A square matrix C is said to be *reducible* if there is a permutation matrix P such that

$$PCP^{-1} = \begin{pmatrix} C_{11} & 0 \\ C_{12} & C_{22} \end{pmatrix},$$

where C_{11} and C_{22} are square matrices. A matrix is said to be *irreducible* if it is not reducible. The well-known Perron-Frobenius theorem plays an important role in spectral theory. Here we state a few parts of the theorem that we need in this thesis.

Theorem 2.1. *[4, Page553] If C is a nonnegative square matrix, then the following (i)–(v) hold.*

(i) The spectral radius $\rho(C)$ is an eigenvalue of C.

(ii) There exist a nonnegative left eigenvector x and a nonnegative right eigenvector y corresponding to $\rho(C)$. If C is irreducible, then x and y can be chosen to be positive.

(iii) If C is irreducible, the eigenvalue $\rho(C)$ is simple (has algebraic multiplicity one).

(iv) If there exists a positive column vector v and a nonnegative number λ such that $Cv \leq \lambda v$, then $\rho(C) \leq \lambda$.

(v) If there exists a positive column vector v and a nonnegative number λ such that $Cv \geq \lambda v$, then $\rho(C) \geq \lambda$.

The above nonnegative right eigenvector of length 1 corresponding to $\rho(C)$ is called the *Perron vector* of C. A well-known consequence of the Perron-Frobenius theorem is stated as follows.

Lemma 2.2. *[4, Page553] If $C = (c_{ij})$ and $C' = (c'_{ij})$ are square matrices of the same size, and $0 \leq C \leq C'$, which means $0 \leq c_{ij} \leq c'_{ij}$ for all i, j, then $\rho(C) \leq \rho(C')$. Moreover, if C' is irreducible, then $\rho(C) = \rho(C')$ if and only if $C = C'$.*

The following is a well-known property for symmetric matrices.

Lemma 2.3. *[4, Page234] If C is a real symmetric matrix and v is a column vector of length 1, then $\rho(C) \geq v^T Cv$, with equality holds if and only if v is an eigenvector of $\rho(C)$.*

2.2 The A_α-matrix of a graph

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Let $A(G)$ be the adjacency matrix and $D(G)$ the diagonal matrix of the degrees of G. For $0 \leq \alpha \leq 1$, the A_α-*matrix* of G is the matrix defined by $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$. Note that $A_\alpha(G)$ and $A(G)$ have the same i-th row-sum r_i. The spectral radius of $A_\alpha(G)$ is called the α-*index* of G, and is denoted by $\rho_\alpha(G)$. Note that the α-index of G is independent to the order of the vertex set of G, and for $0 \leq \alpha < 1$, the A_α-*matrix* of G is irreducible if and only if G is connected.

Example 2.4. Consider a path graph $G = P_3$, which is one of the simplest forms of a graph. After a suitable arrangement of the vertex set, the adjacency matrix and the diagonal matrix of the degrees of G are

$$A(G) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad D(G) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

For $\alpha = 0.5$, the A_α matrix is computed as:

$$A_{0.5}(G) = 0.5 \times D(G) + (1-0.5) \times A(G) = \begin{pmatrix} 0.5 & 0.5 & 0 \\ 0.5 & 1 & 0.5 \\ 0 & 0.5 & 0.5 \end{pmatrix}.$$

The matrices $A(G)$ and $A_\alpha(G)$ have the same row-sums $r_1 = 1$, $r_2 = 2$ and $r_3 = 1$. Since $A_\alpha(G)$ has three eigenvalues: 0, 0.5, and 1.5, the α-index of G is $\rho_\alpha(G) = 1.5$.

2.3 Spectral bounds from matrix partitions

Let $\Pi = \{\pi_1, \ldots, \pi_\ell\}$ be a partition of the set $[n] := \{1, 2, \ldots, n\}$ and let $C = (c_{ij})$ be an $n \times n$ matrix. Define an $\ell \times \ell$ matrix $\Pi(C) := (p_{ab})$, which is called the *quotient matrix* of C with respect to Π, to be the matrix whose (a, b)- entry is

$$p_{ab} = \frac{1}{|\pi_a|} \sum_{i \in \pi_a} \sum_{j \in \pi_b} c_{ij}.$$

If $p_{ab} = \sum_{j \in \pi_b} c_{ij}$ for every $1 \le a, b \le \ell$, $i \in \pi_a$, then the partition Π of $[n]$ is also called an *equitable partition* of C.

Example 2.5. Given the matrix

$$C = \begin{pmatrix} 1 & 3 & 0 & 1 & 1 & 0 \\ 2 & 2 & 0 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 4 & 4 & 0 \\ 1 & 1 & 0 & 3 & 3 & 2 \\ 0 & 2 & 0 & 2 & 5 & 1 \end{pmatrix}$$

Let $\Pi_1 = \{\{1, 2\}, \{3\}, \{4, 5, 6\}\}$ and $\Pi_2 = \{\{1, 2\}, \{3, 4\}, \{5, 6\}\}$ be two partitions of $[6]$. Then the corresponding quotient matrices are

$$\Pi_1(C) = \begin{pmatrix} 4 & 0 & 2 \\ 0 & 2 & 1 \\ 2 & 0 & 8 \end{pmatrix}, \quad \Pi_2(C) = \begin{pmatrix} 4 & 0.5 & 1.5 \\ 1 & 3 & 3 \\ 2 & 2.5 & 5.5 \end{pmatrix}.$$

In this case, the partition Π_1 is an equitable partition of C.

A vector $(x_1, x_2, \ldots, x_n)$ is called *rooted* if $x_i \ge x_n \ge 0$ for $1 \le i \le n - 1$. An $n \times n$ matrix M is called *rooted* if there is a constant d such that the first $n - 1$ columns and the row-sum vector of $M + dI_n$ are rooted. Note that the entries in the diagonal and the last column of a rooted matrix M are not necessarily nonnegative. Here we use $\rho_r(M)$ instead of $\rho(M)$ to denote the largest real eigenvalue of M. It is difficult to compute the α-index of a graph of large order since it is hard to find the eigenvalues of a matrix of large size. The following lemmas related to a quotient matrix from some partition of a matrix will help us simplifying a large A_α-*matrix* and estimate the α-index of a large order graph G.

Lemma 2.6. *[3] If $M = (m_{ij})$ is an $n \times n$ rooted matrix, then $\rho_r(M)$ exists and M has a rooted eigenvector x for $\rho_r(M)$. Moreover, for any eigenvalue λ with a rooted eigenvector $x = (x_1, x_2, \ldots, x_n)^T$ of M, the following (i), (ii) hold.*

(i) If the row vector $(m_{n1}, m_{n2}, \ldots, m_{n(n-1)})$ is positive, then x is positive.

(ii) If x is positive and the row-sum $r_i > r_n$ for some $1 \leq i \leq n-1$, then $x_i > x_n$.

Lemma 2.7. *[3] If M is an $n \times n$ rooted matrix and $\Pi = \{\pi_1, \ldots, \pi_\ell\}$ is an equitable partition of M^T with $\pi_\ell = \{n\}$, then $\rho_r(M) = \rho_r(\Pi(M^T))$.*

Lemma 2.8. *[3] Let $M = (m_{ab})$ be an $\ell \times \ell$ rooted matrix. If $C = (c_{ij})$ is an $n \times n$ nonnegative matrix and there exists a partition $\Pi = (\pi_1, \pi_2, \ldots, \pi_\ell)$ of $[n]$ such that*

$$\max_{i \in \pi_a} \sum_{j \in \pi_b} c_{ij} \leq m_{ab} \quad \textit{and} \quad \max_{i \in \pi_a} \sum_{j=1}^{n} c_{ij} \leq \sum_{c=1}^{\ell} m_{ac}$$

for $1 \leq a \leq \ell$ and $1 \leq b \leq \ell - 1$, then $\rho(C) \leq \rho_r(M)$. Moreover, if C is irreducible, $x = (x_1, \ldots, x_\ell)$ is a rooted eigenvector of M for $\rho_r(M)$, then $\rho(C) = \rho_r(M)$ if and only if the following (i), (ii) hold.

(i) If $x > 0$, then $\sum_{j=1}^{n} c_{ij} = \sum_{c=1}^{\ell} m_{ac}$ for $1 \leq a \leq \ell$ and $i \in \pi_a$.

(ii) $\sum_{j \in \pi_b} c_{ij} = m_{ab}$ for $1 \leq a \leq \ell, 1 \leq b \leq \ell - 1, i \in \pi_a$ with $x_b > x_\ell$.

Chapter 3. A_α-index of graphs with given order and size

Recall that $\mathcal{G}(n, m)$ is the set of all graphs with order n and size m. Let $\rho_\alpha(n, m)$ denote the maximum α-index among the graphs in $\mathcal{G}(n, m)$.

3.1 The shape of $G \in \mathcal{G}(n, m)$ with $\rho_\alpha(G) = \rho_\alpha(n, m)$

We give some lemmas to restrict the shape of graphs in $\mathcal{G}(n, m)$ with α-index $\rho_\alpha(n, m)$.

Lemma 3.1. *Let $0 \le \alpha \le 1$. If $G \in \mathcal{G}(n, m)$ attains the maximum α-index, then G is connected except for isolated vertices.*

Proof. Let $G \in \mathcal{G}(n, m)$ be a graph such that $\rho_\alpha(G) = \rho_\alpha(n, m)$, and H is a component of G such that $\rho_\alpha(G) = \rho_\alpha(H)$. On the contrary, suppose there is an edge not in H. This happens only if there are at least two vertices not in H. Add a new isolated vertex x to H to form a graph H_1, and add an edge incident on x and the vertex in H with the largest degree to form a graph H_2. Then $A_\alpha(H) = A_\alpha(H_1) < A_\alpha(H_2)$. If $\alpha \neq 1$, then $A_\alpha(H_2)$ is irreducible and $\rho_\alpha(H) < \rho_\alpha(H_2)$ by Lemma 2.2. If $\alpha = 1$ then $\rho_0(H) = \rho_0(H_2) - 1$. Notice that $\rho_\alpha(H_2) \le \rho(H_3) \le \rho_\alpha(n, m)$, where $H_3 \in \mathcal{G}(n, m)$ is obtained from H_2 by adding more vertices and edges to H_2 if necessary. Putting together, $\rho_\alpha(n, m) = \rho_\alpha(G) = \rho_\alpha(H) < \rho_\alpha(H_2) \le \rho_\alpha(n, m)$, a contradiction. $\square$

Let $\mathcal{G}^*(n, m)$ be the set of graphs whose vertex set $\{v_1, \ldots, v_n\}$ can be arranged so that if $v_iv_j \in E(G)$, then $v_iv_k \in E(G)$ for $1 \le k \le j$ and $k \neq i$. If $G \in \mathcal{G}^*(n, m)$, we always arrange the vertex set of G in this way.

Lemma 3.2. *Let $0 \le \alpha \le 1$. If $G \in \mathcal{G}(n, m)$ satisfies $\rho_\alpha(G) = \rho_\alpha(n, m)$, then $G \in \mathcal{G}^*(n, m)$.*

Proof. Let $G \in \mathcal{G}(n,m)$ with $\rho_\alpha(G) = \rho_\alpha(n,m)$. By Lemma 3.1, G is connected except for $n-\ell$ isolated vertices. Let the vertex set $\{v_1,\dots,v_n\}$ of G be arranged such that the eigenvector of $A_\alpha(G)$ is $x = (x_1,\dots,x_n)^T$ with $x_1 \geq \cdots \geq x_\ell$ is Perron vector of the largest connected component of G and $x_{\ell+1} = \cdots = x_n = 0$. On the contrary, suppose there exist $1 \leq i \leq \ell$ and $1 \leq k \leq j$ with $k \neq i$ such that $v_iv_j \in E(G)$ and $v_iv_k \notin E(G)$. Let $G' \in \mathcal{G}(n,m)$ be the graph obtained from G by deleting v_iv_j and adding v_iv_k. Then $x^TA_\alpha(G)x = \rho_\alpha(G)$ by definition, and $x^TA_\alpha(G')x \leq \rho_\alpha(G')$ by Lemma 2.3. Thus

$$\rho_\alpha(G') - \rho_\alpha(G) \geq x^T(A_\alpha(G') - A_\alpha(G))x = (1-\alpha)(2x_ix_k - 2x_ix_j) + \alpha(x_k^2 - x_j^2) \geq 0.$$

Since $\rho_\alpha(G) = \rho_\alpha(n,m)$, we have $\rho_\alpha(G') = \rho_\alpha(G)$, implying $\rho_\alpha(G')x = A_\alpha(G')x$, and

$$\rho_\alpha(G')x_k = (A_\alpha(G')x)_k = (\rho_\alpha(G)x)_k + \alpha x_k + (1-\alpha)x_i \geq \rho_\alpha(G)x + k + x_i > \rho_\alpha(G')x_k,$$

a contradiction. Hence $G \in \mathcal{G}^*(n,m)$. □

3.2 Upper bounds of α-indices

The following is a known upper bound of α-indices for $G \in \mathcal{G}(n,m)$ with given a maximum degree $\Delta(G)$ and minimum degree $\delta(G)$.

Lemma 3.3. *[2] Let $0 \leq \alpha < 1$. If $G \in \mathcal{G}(n,m)$ is connected with maximum degree Δ and minimum degree δ, then*

$$\rho_\alpha(G) \leq \frac{\alpha\Delta + (1-\alpha)(\delta-1) + \sqrt{(\alpha\Delta + (1-\alpha)(\delta-1))^2 + 4(1-\alpha)(2m-(n-1)\delta)}}{2}.$$

Moreover, the equality holds if and only if G is regular, or $\alpha = 0$ and every vertex in G has degree $n-1$ or δ.

We shall investigate other upper bounds of α-indices by employing Lemma 2.8. Throughout this section, fix a graph $G \in \mathcal{G}^*(n,m)$ and $0 \leq \alpha \leq 1$. Let $(r_1, r_2, \dots, r_n)$ denote the row-sum vector of the adjacency matrix $A(G)$. Find an integer $d \in [n-1]$ such that $s := r_{d+1} \leq d$. Such d exists since $d = n-1$ is a choice. Let $\Pi = \{\{1\},\{2\},\dots,\{d\},\{d+1,d+2,\dots,n\}\}$ be a partition of $[n]$ into $d+1$ classes. Applying Lemma 2.8 with the above Π, $\ell = d+1$, the

$(d+1)\times(d+1)$ matrix

$$M = \left(\begin{array}{c|c|c} \begin{matrix} (1-\alpha)J_{s\times s} \\ +(\alpha(r_1+1)-1)I_s \end{matrix} & (1-\alpha)J_{s\times(d-s)} & \begin{matrix} r_1-\alpha r_1-(1-\alpha)(d-1) \\ \vdots \\ r_s-\alpha r_1-(1-\alpha)(d-1) \end{matrix} \\ \hline (1-\alpha)J_{(d-s)\times s} & \begin{matrix} (1-\alpha)J_{(d-s)\times(d-s)} \\ +(\alpha(r_{s+1}+1)-1)I_{d-s} \end{matrix} & \begin{matrix} r_{s+1}-\alpha r_{s+1}-(1-\alpha)(d-1) \\ \vdots \\ r_d-\alpha r_{s+1}-(1-\alpha)(d-1) \end{matrix} \\ \hline 1-\alpha \ \cdots \ 1-\alpha & 0 \ \cdots \ 0 & \alpha s \end{array}\right) \tag{3.1}$$

and $C = A_\alpha$, where I_s is the $s\times s$ identity matrix and $J_{s\times t}$ is the $s\times t$ all one's matrix, we have the following lemma.

Lemma 3.4. $\rho_\alpha(G) \le \rho_r(M)$.

To find $\rho_r(M)$, we consider the partition $\Pi_1 = \{\{1,2,\ldots,s\},\{s+1,\ldots,d\},\{d+1\}\}$ of $[d+1]$ into two classes if $s=d$ or $s=0$ and into three classes if $0<s<d$. We shall consider only $0<s<d$ and the case $s=d$ or $s=0$ is more easily. Observe that Π_1 is an equitable partition of M^T. By Lemma 2.7, we have $\rho_r(M)=\rho_r(\Pi_1(M^T))$, and

$$\Pi_1(M^T) = \begin{pmatrix} (1-\alpha)(s-1)+\alpha r_1 & (1-\alpha)(d-s) & 1-\alpha \\ s(1-\alpha) & (1-\alpha)(d-s-1)+\alpha r_{s+1} & 0 \\ a_\alpha & b_\alpha & \alpha s \end{pmatrix}, \tag{3.2}$$

where

$$a_\alpha := \sum_{i=1}^{s}(r_i-\alpha r_1-(1-\alpha)(d-1)),\ b_\alpha := \sum_{i=s+1}^{d}(r_i-\alpha r_{s+1}-(1-\alpha)(d-1)). \tag{3.3}$$

Notice that when $\alpha=1$, we have

$$\Pi_1(M^T) = \begin{pmatrix} r_1 & 0 & 0 \\ 0 & r_{s+1} & 0 \\ a_1 & b_1 & s \end{pmatrix}, \tag{3.4}$$

and $\rho_r(\Pi_1(M^T)) = r_1$. By Lemma 3.4 and Lemma 2.7, we have the following Theorem.

Theorem 3.5. $\rho_\alpha(G) \le \rho_r(\Pi_1(M^T))$.

3.3 Graphs with $\rho_\alpha(G) = \rho_r(\Pi_1(M^T))$

Let $G \in \mathcal{G}^*(n, m)$ and M be the matrix in (3.1) obtained from G. We will investigate the neccessary and sufficient conditions on G when the equality $\rho_\alpha(G) = \rho_r(\Pi_1(M^T))$ holds, where $\Pi_1 = \{\{1, 2, \ldots, s\}, \{s + 1, \ldots, d\}, \{d + 1\}\}$, $0 < s < r_{d+1} < d$, and $\Pi_1(M^T)$ is in (3.2). Let $(r_1, r_2, \ldots, r_n)$ denote the row-sum vector of $A_\alpha(G)$.

Theorem 3.6. *If $\alpha = 1$, then $\rho_\alpha(G) = \rho_r(\Pi_1(M^T))$ holds for any $G \in \mathcal{G}^*(n, m)$.*

Proof. If $\alpha = 1$, then $A_\alpha(G)$ is a diagonal matrix whose (i, i)-entry is r_i for all $0 \le i \le n$. Thus $\rho_\alpha(G) = r_1$. By (3.4) we have $\rho_r(\Pi_1(M^T)) = r_1$. Hence, $\rho_\alpha(G) = \rho_r(\Pi_1(M^T))$. $\square$

Now, consider the case $0 \le \alpha < 1$. Since the number of vertices in the only nontrivial component of G is $r_1 + 1$, $A_\alpha(G)[r_1 + 1]$ is irreducible and $\rho_\alpha(G) = \rho(A_\alpha(G)[r_1 + 1])$, where $A_\alpha(G)[r_1 + 1]$ is the principle submatrix of $A_\alpha(G)$ restricted to the first $r_1 + 1$ rows and columns. Note that M is equal to the matrix in (3.1) obtained from $A_\alpha(G)[r_1 + 1]$ with $\Pi = \{\{1\}, \{2\}, \ldots, \{d\}, \{d + 1, d + 2, \ldots, r_1 + 1\}\}$. We will find out the necessary and sufficient condition of $\rho(A_\alpha(G)[r_1 + 1]) = \rho_r(M)$ by Lemma 2.6 and Lemma 2.8. Let $x = (x_1, x_2, \ldots, x_{d+1})^T$ be a rooted eigenvector of M, which exists by Lemma 2.6. To apply Lemma 2.6(ii) and Lemma 2.8(i) in our later proof, we provide the following lemma to show that $x > 0$.

Lemma 3.7. *If $0 \le \alpha < 1$, $s > 0$ and $u = (u_1, \ldots, u_{d+1})^T$ is a rooted eigenvector of M, then $u > 0$.*

Proof. Let $u = (u_1, \ldots, u_{d+1})$ be a rooted eigenvector of M. Suppose $u_{d+1} = 0$, then

$$0 = u_{d+1} = \alpha s u_{d+1} + (1 - \alpha) \sum_{i=1}^{s} u_i.$$

This implies $u_1 = \cdots = u_s = 0$, so

$$0 = u_1 = \alpha r_1 u_1 + (1 - \alpha) \sum_{i=2}^{d+1} u_i.$$

Hence, $u_i = 0$ for all $1 \le i \le d + 1$. This is a contradiction. So $u_{d+1} > 0$ and $u > 0$ since u is rooted. $\square$

Theorem 3.8. *If $0 \leq \alpha < 1$ and $0 < s < d$, then $\rho_\alpha(G) = \rho_r(\Pi_1(M^T))$ if and only if one of the following holds.*

(i) $r_1 = \cdots = r_s$ *and* $r_i = s$ *for all* $s+1 \leq i \leq r_1+1$.

(ii) $r_1 = \cdots = r_s$, $r_{s+1} = \cdots = r_d = d-1$ *and* $r_i = s$ *for all* $d+1 \leq i \leq r_1+1$

Proof. Since $\rho_\alpha(G) = \rho(A_\alpha(G)[r_1+1])$ and $\rho_r(M) = \rho_r(\Pi_1(M^T))$, it is sufficient to show that $\rho(A_\alpha(G)[r_1+1]) = \rho_r(M)$ if and only if one of (i) or (ii) holds. To prove the necessity, assume $\rho(A_\alpha(G)[r_1+1]) = \rho_r(M)$. Applying Lemma 2.8(i), we have $r_i = r_{d+1} = s$ for all $i \in \Pi_{d+1} = \{d+1, d+2, \ldots r_1+1\}$. Since $A_\alpha(G)[r_1+1]$ is symmetric, we have $r_1 = \cdots = r_s$. There are two cases.

Case 1: $r_{s+1} = s$.

Then $r_i = s$ for all $s+1 \leq i \leq d$. Thus $r_1 = \cdots r_s$ and $r_i = s$ for all $s+1 \leq i \leq r_1+1$, (i) holds.

Case 2: $r_{s+1} > s$.

Then $x_{s+1} > x_{d+1}$ by Lemma 2.6(ii). Applying Lemma 2.8(ii), since $\Pi_i = \{i\}$ for $1 \leq i \leq d$, we have $a_{i(s+1)} = m_{i(s+1)} = 1-\alpha$ for $1 \leq i \leq d$, $i \neq s+1$. This implies $r_{s+1} = d-1$. The symmetry of $A_\alpha(G)$ then implies $r_i > s$ and thus $x_i > x_{d+1}$ for all $s+2 \leq i \leq d$ by Lemma 2.6(ii). Applying Lemma 2.8(ii) again, we have $a_{ij} = m_{ij}$ for all $s+1 \leq i,j \leq d$. In particular, $\alpha r_i = a_{ii} = m_{ii} = \alpha r_{s+1} = \alpha(d-1)$ for all $s+1 \leq i \leq d$. Thus $r_1 = \cdots r_s$, $r_{s+1} = \cdots = r_d = d-1$ and $r_i = s$ for all $d+1 \leq i \leq r_1+1$, (ii) holds.

To prove the sufficiency, first assume that (i) holds. Then

$$A_\alpha(G)[r_1+1] = \left(\begin{array}{c|c} \begin{array}{r}(1-\alpha)J_{s\times s}\\ +(\alpha(r_1+1)-1)I_s\end{array} & (1-\alpha)J_{s\times(r_1+1-s)} \\ \hline (1-\alpha)J_{(r_1+1-s)\times s} & \alpha s I_{r_1+1-s}\end{array}\right),$$

$$M = \left(\begin{array}{c|c|c} \begin{array}{r}(1-\alpha)J_{s\times s}\\ +(\alpha(r_1+1)-1)I_s\end{array} & (1-\alpha)J_{s\times(d-s)} & \begin{array}{c}(1-\alpha)(r_1-d+1)\\ \vdots \\ (1-\alpha)(r_1-d+1)\end{array} \\ \hline (1-\alpha)J_{(d-s)\times s} & \begin{array}{r}(1-\alpha)J_{(d-s)\times(d-s)}\\ +(\alpha(s+1)-1)I_{d-s}\end{array} & \begin{array}{c}(1-\alpha)(s-d+1)\\ \vdots \\ (1-\alpha)(s-d+1)\end{array} \\ \hline 1-\alpha \ \cdots \ 1-\alpha & 0 \ \cdots \ 0 & \alpha s\end{array}\right).$$

Note that in this case $x_{s+1} = \cdots = x_{d+1}$. Thus the conditions (i) and (ii) in Lemma 2.8 both hold, and so we have $\rho(A_\alpha(G)[r_1+1]) = \rho_r(M)$. Assume (ii) holds, then

$$A_\alpha(G)[r_1+1] = \left(\begin{array}{c|c|c} \begin{array}{r}(1-\alpha)J_{s\times s}\\ +(\alpha(r_1+1)-1)I_s\end{array} & (1-\alpha)J_{s\times(d-s)} & (1-\alpha)J_{s\times(r_1+1-d)} \\ \hline (1-\alpha)J_{(d-s)\times s} & \begin{array}{r}(1-\alpha)J_{(d-s)\times(d-s)}\\ +(\alpha d-1)I_{d-s}\end{array} & O_{(d-s)\times(r_1+1-d)} \\ \hline (1-\alpha)J_{(r_1+1-d)\times s} & O_{(r_1+1-d)\times(d-s)} & \alpha s I_{r_1+1-d} \end{array}\right).$$

$$M = \left(\begin{array}{c|c|c} \begin{array}{r}(1-\alpha)J_{s\times s}\\ +(\alpha(r_1+1)-1)I_s\end{array} & (1-\alpha)J_{s\times(d-s)} & \begin{array}{c}(1-\alpha)(r_1-d+1)\\ \vdots \\ (1-\alpha)(r_1-d+1)\end{array} \\ \hline (1-\alpha)J_{(d-s)\times s} & \begin{array}{r}(1-\alpha)J_{(d-s)\times(d-s)}\\ +(\alpha d-1)I_{d-s}\end{array} & \begin{array}{c}0\\ \vdots \\ 0\end{array} \\ \hline 1-\alpha \ \ \cdots \ \ 1-\alpha & 0 \ \ \cdots \ \ 0 & \alpha s \end{array}\right).$$

The conditions (i) and (ii) in Lemma 2.8 also hold in this case. Hence $\rho(A_\alpha(G)[r_1+1]) = \rho_r(M)$. $\square$

Chapter 4. The α-index for small α

In this chapter, assume $G \in \mathcal{G}^*(n,m)$, where $2m = c(c-1) + 2t$ with $1 \le t \le c-1$. Let $(r_1, r_2, \ldots, r_n)$ be the row-sum vector of the adjacency matrix $A(G)$.

Lemma 4.1. $1 \le r_{c+1} \le c-1$.

Proof. If $r_{c+1} \ge c$, then

$$2m = c(c-1) + 2t \le c(c-1) + 2(c-1) < c(c+1) \le \sum_{i=1}^{c+1} r_i \le 2m,$$

a contradiction. If $r_{c+1} = 0$, then $2m = \sum_{i=1}^{n} r_i = \sum_{i=1}^{c} r_i \le c(c-1) < c(c-1)+2t = 2m$, a contradiction. □

By Lemma 4.1, we choose $d = c$ for the construction of the matrix M in (3.1) and $s = r_{c+1}$ to apply $\rho_\alpha(G) \le \rho_r(M)$ in Lemma 3.4

4.1 The graph G_0

Let G_0 be the graph in $\mathcal{G}^*(n,m)$ obtained from the complete graph K_c of order c by adding a new vertex v, adding t edges, each incident on v and a vertex in K_c, and adding $n-c-1$ isolated vertices. Hence G_0 has row-sums $r_1 = \cdots = r_t = c$, $r_{t+1} = \cdots = r_c = c-1$, $r_{c+1} = t$, and $r_{c+2} = \cdots = r_n = 0$. Let $\Pi_1(M_0^T)$ be the matrix in (3.2) obtained from this G_0. By Theorem 3.8(ii) with $d = c$ and $s = t$, we have

$$\rho_\alpha(G_0) = \rho_r(\Pi_1(M_0^T)). \tag{4.1}$$

Given a graph $G \in \mathcal{G}^*(n,m)$, and let $\Pi_1(M^T)$ be the matrix in (3.2) obtain from G. We will investigate the following problem: Whether or not if $G \ne G_0$, then $\rho_r(\Pi_1(M^T)) <$

$\rho_r(\Pi_1(M_0^T))$. If this is true, by theorem 3.5 and (4.1) we have $\rho_\alpha(G) \leq \rho_r(\Pi_1(M^T)) < \rho_r(\Pi_1(M_0^T)) = \rho_\alpha(G_0)$ for $G \neq G_0$.

First, consider the case $\alpha = 1$. Then $\rho_\alpha(G) = r_1 = \rho_r(\Pi_1(M^T))$ by Theorem 3.6 and $\rho_r(\Pi_1(M_0^T)) = \rho_\alpha(G_0) = c$. The statement does not hold in this case. In fact, since $r_{c+1} \geq 1$ by Lemma 4.1 and $A_\alpha(G)$ is symmetric, we have $r_1 \geq c$ and thus $\rho_r(\Pi_1(M^T)) \geq \rho_r(\Pi_1(M_0^T))$ for all $G \neq G_0$.

If $0 \leq \alpha < 1$, since $A_\alpha(K_c) \oplus O_{1\times 1} < A_\alpha(G_0)[c+1] < A_\alpha(K_{c+1})$, by Lemma 2.2 we have $c - 1 < \rho_\alpha(G_0) < c$. To estimate $\rho_\alpha(G_0)$ more accurately, we apply Lemma 3.3 to the only nontrivial component of G_0, which has order $c+1$, size $\frac{c(c-1)+2t}{2}$. The maximum degree Δ and the minimum degree δ of this graph is equal to c and t, respectively. Hence

$$\begin{aligned}
\rho_\alpha(G_0) \leq & \frac{\alpha c + (1-\alpha)(t-1) + \sqrt{(\alpha c + (1-\alpha)(t-1))^2 + 4(1-\alpha)(c(c-1) + 2t - ct))}}{2} \\
= & \frac{\alpha c + (1-\alpha)(t-1) + \sqrt{(\alpha c + (1-\alpha)(2c-t+1))^2 - 8(1-\alpha)(c-t)}}{2}.
\end{aligned}$$

And we have

$$\begin{aligned}
c - \rho_\alpha(G_0) \geq & \frac{\alpha c + (1-\alpha)(2c-t+1) - \sqrt{(\alpha c + (1-\alpha)(2c-t+1))^2 - 8(1-\alpha)(c-t)}}{2} \\
= & \frac{8(1-\alpha)(c-t)}{2(\alpha c + (1-\alpha)(2c-t+1) + \sqrt{(\alpha c + (1-\alpha)(2c-t+1))^2 - 8(1-\alpha)(c-t)})} \\
\geq & \frac{8(1-\alpha)(c-t)}{4(\alpha c + (1-\alpha)(2c-t+1))} \\
\geq & \frac{(1-\alpha)(c-t)}{c}. \qquad (4.2)
\end{aligned}$$

4.2 The shape of the characteristic polynomial of $\Pi_1(M^T)$

Let $\Pi_1(M^T)$ be the matrix in (3.2) obtained from G. The characteristic polynomial of $\Pi_1(M^T)$ is given by

$$\begin{aligned}
f_G(x) =&\det(xI - \Pi_1(M^T))\\
=&\det\begin{pmatrix} x-(1-\alpha)(s-1)-\alpha r_1 & (1-\alpha)(c-s) & 1-\alpha \\ s(1-\alpha) & x-(1-\alpha)(c-s-1)-\alpha r_{s+1} & 0 \\ a_\alpha & b_\alpha & x-\alpha s \end{pmatrix}\\
=&x^3 - ((c-2)(1-\alpha)+\alpha(s+r_1+r_{s+1}))x^2\\
&+(\alpha(1-\alpha)s(c-2)+\alpha^2 s(r_1+r_{s+1})+\alpha(1-\alpha)(c-s-1)r_1\\
&+\alpha(1-\alpha)(s-1)r_{s+1}+\alpha^2 r_1 r_{s+1} - a_\alpha(1-\alpha)-(1-\alpha)^2(c-1))x\\
&+a_\alpha(1-\alpha)((1-\alpha)(c-s-1)+\alpha r_{s+1})+\alpha(1-\alpha)^2 s^2(c-s)\\
&-(1-\alpha)^2 s b_\alpha - \alpha s(\alpha(1-\alpha)(c-s-1)r_1+\alpha(1-\alpha)(s-1)r_{s+1}\\
&+\alpha^2 r_1 r_{s+1}+(1-\alpha)^2(s-1)(c-s-1)). \qquad (4.3)
\end{aligned}$$

In this section, we will prove that if $0 \leq \alpha \leq \frac{c-1}{8m}$, then $f_G(x)$ is increasing in the interval $(c-1,\infty)$. First, we need some inequalities. Referring to the notation in (3.3),

$$a_\alpha \leq \sum_{i=1}^{s}(1-\alpha)(r_i-c+1) = (1-\alpha)a_0,$$

and

$$b_\alpha \leq \sum_{i=s+1}^{c}(1-\alpha)(r_i-c+1) = (1-\alpha)b_0.$$

Since $A_\alpha(G)$ is symmetric and $s = r_{c+1}$, all row-sums $r_1, r_2, \ldots, r_s \geq c$. This means that a_0 represents the number of off-diagonal entries with value $(1-\alpha)$ between the $(c+1)$-th column and the n-th column of $A_\alpha(G)$. The symmetry of $A_\alpha(G)$ implies $a_0 = \sum_{i=c+1}^{n} r_i$. Thus we have

$$2a_0 + b_0 = \sum_{i=1}^{c}(r_i-c+1) + \sum_{i=c+1}^{n} r_i = 2m - c(c-1) = 2t. \qquad (4.4)$$

Since $r_i \geq s$ for $s+1 \leq i \leq c$, $t \leq c-1$, and $s \leq 1$, the value a_0 has a bound

$$\begin{aligned} a_0 =& \frac{2t - b_0}{2} = \frac{2t + \sum_{i=s+1}^{c}(c-1-r_i)}{2} \\ \leq& \frac{2(c-1) + (c-s)(c-s-1)}{2} \leq \frac{c(c-1)}{2}. \end{aligned} \tag{4.5}$$

The following Lemma helps us to study the shape of $f_G(x)$ for small α.

Lemma 4.2. *If* $0 \leq \alpha \leq \frac{c-1}{8m}$*, then* $f_G(x)$ *is increasing in the interval* $(c-1, \infty)$.

Proof. To show that $f_G(x)$ is increasing in $(c-1, \infty)$, we check the derivative $f'(x) > 0$ for $x > c-1$. We do this by providing the following two inequalities.

1. $f'_G(x) > f'_G(c-1)$ for $x > c-1$.

2. $f'_G(c-1) \geq 0$.

Since $r_1 + r_{s+1} + s \leq 2m$, for $x > c-1$ we have

$$\begin{aligned} & f'_G(x) - f'_G(c-1) \\ & = 3(x^2 - (c-1)^2) - 2(x-c+1)((c-2)(1-\alpha) + \alpha(s + r_1 + r_{s+1})) \\ & \geq 3(x+c-1)(x-c+1) - 2(x-c+1)(c-2+\alpha(2-c+2m)) \\ & \geq (3x + 3(c-1) - (c-2) - \frac{c-1}{4})(x-(c-1)) > 0. \end{aligned}$$

Since $s \leq c-1$, $1-\alpha \leq 1$ and $a_0 \leq \frac{c(c-1)}{2}$, $f'_G(c-1)$ can be estimate by

$$\begin{aligned} f'_G(c-1) =& 3(c-1)^2 - 2(c-1)(c-2+\alpha(s-c+2+r_1+r_{s+1})) \\ & + \alpha(1-\alpha)s(c-2) + \alpha^2 s(r_1 + r_{s+1}) + \alpha(1-\alpha)(c-s-1)r_1 \\ & + \alpha(1-\alpha)(s-1)r_{s+1} + \alpha^2 r_1 r_{s+1} - a_\alpha(1-\alpha) - (1-\alpha)^2(c-1) \\ \geq& (c+1)(c-1) - a_\alpha(1-\alpha) - (1-\alpha)^2(c-1) - (c-1)2\alpha(1+r_1+r_{s+1}) \\ \geq& (c+1)(c-1) - (1-\alpha)^2(a_0 + c - 1) - (c-1)\frac{c-1}{4m}(2m) \\ \geq& c(c-1) - a_0 - \frac{(c-1)^2}{2} \geq c(c-1) - \frac{c(c-1)}{2} - \frac{(c-1)^2}{2} > 0. \end{aligned}$$

□

Since $\rho_r(\Pi_1(M^T))$ is the largest root of f_G and $\rho_\alpha(G_0) > c-1$, by Lemma 4.2, if $0 \leq \alpha \leq \frac{c-1}{8m}$ and $f_G(\rho_\alpha(G_0)) > 0$, then $\rho_\alpha(G_0) > \rho_r(\Pi_1(M^T))$.

4.3 The case $G \neq G_0$ and $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$

In this section, assume $G \neq G_0$ and $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$. We will show $f_G(\rho_\alpha(G_0)) > 0$. The following lemma enhances Lemma 4.1.

Lemma 4.3. $1 \leq s \leq c-2$.

Proof. If $s = c-1$, then $c(c-1) + 2t = 2m \geq \sum_{i=1}^{c+1} r_i \geq c(c-1) + 2(c-1)$, implying $t = c-1$, and $r_1 = r_2 \cdots r_{c-1} = c, r_c = r_{c+1} = c-1, r_{c+2} = \cdots = r_n = 0$, a contradiction to $G \neq G_0$. □

Let $\Pi_1(M_0^T)$ be the matrices in (3.2) obtained from G_0. Denote $\rho_\alpha(G_0)$ easily by ρ for convenience. Let $f_{G_0}(x)$ be the characteristic polynomial of $\Pi_1(M_0^T)$. Then by (4.3),

$$\begin{aligned}
f_{G_0}(x) =& x^3 + (-\alpha c - \alpha t - \alpha - c + 2)x^2 \\
&+ (\alpha^2 ct + \alpha^2 t + \alpha c^2 + \alpha ct - \alpha t - \alpha - c - t + 1)x \\
&- \alpha^2 c^2 t + \alpha^2 ct - 2\alpha^2 t^2 - \alpha ct + 3\alpha t^2 + \alpha t + ct - t^2 - t,
\end{aligned}$$

and ρ is the largest root of $f_{G_0}(x)$ by (4.1). The value of $f_G(\rho)$ can be computed as

$$\begin{aligned}
f_G(\rho) =& f_G(\rho) - f_{G_0}(\rho) \\
& \alpha^3 \left(cr_1 s + cs - r_1 r_{s+1} s - r_1 s^2 - r_1 s + r_{s+1} s^2 - r_{s+1} s - s\right) \\
& + \alpha^2 \big(a_\alpha c - a_\alpha r_{s+1} - a_\alpha s - a_\alpha - b_\alpha s + c^2 t - cr_1 s - cr_1 \rho \\
& \quad -cs\rho - 2cs - ct\rho - ct - c\rho + r_1 r_{s+1}\rho + r_1 s^2 + 2r_1 s\rho + r_1 s \\
& \quad +r_1\rho - r_{s+1}s^2 + r_{s+1}s + r_{s+1}\rho + 2s\rho + 2s + 2t^2 - t\rho + \rho\big) \\
& + \alpha \big(-2a_\alpha c + a_\alpha r_{s+1} + 2a_\alpha s + a_\alpha \rho + 2a_\alpha + 2b_\alpha s - c^2\rho + cr_1\rho \\
& \quad +cs\rho + cs - ct\rho + ct + 2c\rho^2 + 2c\rho - r_1 s\rho - r_1\rho^2 - r_1\rho + r_{s+1}s\rho \\
& \quad -r_{s+1}\rho^2 - r_{s+1}\rho - s\rho^2 - 2s\rho - s - 3t^2 + t\rho^2 + t\rho - t - \rho^2 - \rho\big) \\
& + a_\alpha c - a_\alpha s - a_\alpha \rho - a_\alpha - b_\alpha s - ct + t^2 + t\rho + t. \qquad (4.6)
\end{aligned}$$

We first compute (4.6) for some special cases in the following two lemmas.

Lemma 4.4. *If* $c = 3$ *and* $s = t$*, then* $f_G(\rho) > 0$.

Proof. In this case, by Lemma 4.3, we have $s = 1$, and thus $t = 1$. The A_α-matrix of G_0 is

$$A_\alpha(G_0) = \begin{pmatrix} 3\alpha & 1-\alpha & 1-\alpha & 1-\alpha \\ 1-\alpha & 2\alpha & 1-\alpha & 0 \\ 1-\alpha & 1-\alpha & 2\alpha & 0 \\ 1-\alpha & 0 & 0 & \alpha \end{pmatrix} \oplus O_{(n-4)\times(n-4)}.$$

Since $G \neq G_0$, $2m = c(c-1) + 2t = 8$, and $r_4 = s = 1$, the row sum of $A_\alpha(G)$ should be $r_1 = 4, r_2 = r_3 = r_4 = r_5 = 1$, and $r_6 = \cdots = r_n = 0$. Thus,

$$a_\alpha = \sum_{i=1}^{1}(r_i - \alpha r_1 - (1-\alpha)(c-1)) = 2 - 2\alpha,$$

$$b_\alpha = \sum_{i=2}^{3}(r_i - \alpha r_{c-1} - (1-\alpha)(c-1)) = -2 + 2\alpha.$$

By (4.2), we have $3 - \rho \geq \frac{(1-\alpha)(c-t)}{c} = \frac{2(1-\alpha)}{3}$. Since $\alpha \leq \frac{1}{c(c+1)(t+2)} = \frac{1}{36}$ and $2 < \rho < 3$, by (4.6), we have

$$\begin{aligned} f_G(\rho) =& \alpha^2(-4\rho + 8) + \alpha(3\rho - 9) + 3 - \rho \\ >& - 4\alpha^2 - 3\alpha + 3 - \rho \\ \geq& - \frac{1}{324} - \frac{1}{12} + \frac{35}{54} > 0. \end{aligned}$$

□

Lemma 4.5. *If $s = t + 1$ and $r_{c+2} = 0$, then $f_G(\rho) > 0$.*

Proof. By Lemma 4.3, $1 \leq s \leq c - 2$. There are two cases.

Case 1: $s = t + 1 = c - 2$.

In this case, $r_1 = r_2 = \cdots = r_{c-2} = c, r_{c-1} = r_c = r_{c+1} = c - 2$,

$$a_\alpha = \sum_{i=1}^{c-2}(r_i - \alpha r_1 - (1-\alpha)(c-1)) = (1-\alpha)(c-2),$$

$$b_\alpha = \sum_{i=c-1}^{c}(r_i - \alpha r_{c-1} - (1-\alpha)(c-1)) = -2(1-\alpha).$$

Hence by (4.6)

$$f_G(\rho) = (c-\rho)(1-2\alpha) > 0.$$

Case 2: $s = t+1 \le c-3$.

In this case, $r_1 = \cdots = r_{t+1} = c, r_{t+2} = \cdots = r_{c-2} = c-1, r_{c-1} = r_c = c-2$,

$$a_\alpha = \sum_{i=1}^{t+1}(r_i - \alpha r_1 - (1-\alpha)(c-1)) = (1-\alpha)(t+1),$$

$$b_\alpha = \sum_{i=t+2}^{c}(r_i - \alpha r_{t+2} - (1-\alpha)(c-1)) = -2.$$

Hence by (4.6)

$$f_G(\rho) = \alpha^2(-c^2 + c\rho + c - 2t + \rho) + \alpha(c\rho - c + 2t - \rho^2 - \rho) + c - \rho.$$

Since $c-1 \le \rho \le c$ and $c - \rho \ge \frac{(1-\alpha)(c-t)}{c}$, we have

$$\begin{aligned} f_G(\rho) >& \alpha^2(-2t + c - 1) + \alpha(2t - 3c) + \frac{(1-\alpha)(c-t)}{c} \\ =& \alpha^2(c-1) + \alpha(1-\alpha)2t - \alpha(2c-t) + \frac{c-t}{c} \\ >& -2\alpha c + \frac{1}{c} \ge \frac{(c+1)(t+2) - 2c}{c(c+1)(t+2)} > 0 \end{aligned}$$

□

We change some variables to simplified (4.6) for other cases. Let $p = c - r_{s+1} - 1$, $q = \rho + 1 - c$, $u = r_1 - c + 1$. Then $a_\alpha = a_0 - \alpha s u, b_\alpha = b_0 + \alpha(c-s)p$, and $f_G(\rho)$ can be rewrite as $f_G(\rho) = g + h$, where

$$g = t^2 - s(a_0 + b_0) - (a_0 - t)q - \alpha(r_1\rho(s+q) + 2t^2 - 2s(a_0 + b_0)). \qquad (4.7)$$

and

$$\begin{aligned} h =&\alpha^2 \left(t^2 - s(a_0+b_0) + a_0 p + scq + sp(r_1+c) + (su\rho - t) - p\rho(r_1+1)\right.\\ &\left.-s^2(p+u) - t(\rho + qc - t - 1))\right)\\ &+ \alpha\left(qa_0 + q\rho(c-s) + qs(u-1) + p\rho + p(\rho^2 - a_0 - sc) + s^2(p+u)\right.\\ &\left.+r_{s+1}s\rho + t(c + q\rho - t - 1)\right). \end{aligned} \tag{4.8}$$

For the remaining cases, we will prove $f_G(\rho) > 0$ by showing $g > 0$ and $h > 0$.

Lemma 4.6. $h > 0$.

Proof. Because $s + a_0 + b_0 \leq 2a_0 + b_0 = 2t$, we have $s(a_0 + b_0) \leq t^2$. Since $p \geq 0$, $0 < q < 1$, $u \geq 1$ and $a_0 \geq s \geq 1$,

$$\begin{aligned} h >&\alpha(p\rho + p(\rho^2 - a_0 - sc) + r_{s+1}s\rho - \alpha p\rho(r_1+1))\\ &+ \alpha(1-\alpha)(s^2(p+u) + t(c + q\rho - t - 1))\\ >&\alpha(p\rho + p(\rho^2 - a_0 - sc) + r_{s+1}s\rho - \alpha p\rho(r_1+1)). \end{aligned} \tag{4.9}$$

By (4.5), we have

$$a_0 + sc \leq \frac{2(c-1) + (c-s)(c-s-1) + 2sc}{2} = \frac{(c+2)(c-1) + s(s+1)}{2}. \tag{4.10}$$

By Lemma 4.3, $1 \leq s \leq c-2$. There are two cases.

Case 1: $s \leq c-4$.

In this case, since $c - 1 < \rho$, by (4.10) we have

$$a_0 + sc \leq \frac{(c+2)(c-1) + (c-4)(c-3)}{2} = (c-1)^2 - c + 4 \leq (c-1)^2 < \rho^2.$$

Since $\alpha \leq \frac{1}{c(c+1)} \leq \frac{1}{2m+2} \leq \frac{1}{r_1+1}$, we have $p\rho - \alpha p\rho(r_1+1) \geq 0$. Thus by (4.9),

$$h > \alpha(p(\rho^2 - a_0 - sc) + r_{s+1}s\rho + (p\rho + -\alpha p\rho(r_1+1))) \geq 0.$$

Case 2: $s = c-2$ or $s = c-3$.

In this case, since $c-1<\rho$, by (4.10) we have

$$a_0+sc \le \frac{(c+2)(c-1)+(c-2)(c-1)}{2} = c(c-1) < \rho(\rho+1) = \rho^2+\rho,$$

and $p=c-r_{s+1}-1\le 2$. Since $\alpha \le \frac{1}{c(c+1)} \le \frac{1}{2m+2} \le \frac{1}{2(r_1+1)}$, We have

$$r_{s+1}s\rho - \alpha p\rho(r_1+1) \ge \rho - 2\alpha\rho(r_1+1) \ge 0.$$

Thus by (4.9),

$$h > \alpha(p(\rho^2+\rho-a_0-sc)+(r_{s+1}s\rho-\alpha p\rho(r_1+1))) \ge 0.$$

□

Lemma 4.7. $g>0$ *except for the following two cases.*

(i) $s=t+1$ *and* $r_{c+2}=0$.

(ii) $c=3$ *and* $s=t$.

Proof. Define a function g_1 by

$$g_1(x,y)=t^2-x(2t-y)-(y-t)q-\alpha((y+c-x)c(x+1)+2(t^2-x(2t-y))).$$

Since $2a_0+b_0=2t$, $\rho<c$, and $r_1\le a_0+c-s$, we have

$$\begin{aligned} g =& t^2-s(a_0+b_0)-(a_0-t)q-\alpha(r_1\rho(s+q)+2t^2-2s(a_0+b_0)) \\ \ge& t^2-s(2t-a_0)-(a_0-t)q-\alpha((a_0+c-s)c(s+1)+2(t^2-s(2t-a_0))) \\ =& g_1(s,a_0). \end{aligned}$$

To find out the shape of $g_1(x,y)$ and estimate the value of $g_1(s,a_0)$, we compute the partial derivatives

$$\frac{\partial g_1}{\partial y} = x-q-\alpha(c(x+1)+2x), \tag{4.11}$$

$$\frac{\partial^2 g_1}{\partial x \partial y} = 1-\alpha(c+2) \ge 1-\alpha(c+2) > 0. \tag{4.12}$$

It follows from (4.12) that $\frac{\partial g_1}{\partial y}$ is increasing with respect to x. Since $s \geq 1$ and , for all y we have

$$\begin{aligned}
\frac{\partial g_1}{\partial y}(s,y) \geq & \frac{\partial g_1}{\partial y}(1,y) = 1 - q - \alpha(2c+2) \\
\geq & \frac{(1-\alpha)(c-t)}{c} - \alpha(2c+2) \\
\geq & \frac{c-t}{c} - \frac{2c+3}{c(c+1)(t+2)} \quad (4.13)\\
= & \frac{c}{c(c+1)(t+2)} > 0 \quad (4.14)
\end{aligned}$$

Case 1: $s < t$.

Let $g_2(x)$ be a function defined by

$$g_2(x) = x^2 + xq - \alpha(c^2(t-x+1) + 2x^2).$$

Since $q > 0, \alpha \leq \frac{1}{3c(c+1)}$, for $x \geq 1$ we have

$$g_2'(x) = 2x + q - \alpha(c^2 + 4x) > \frac{6c(c+1)x - c^2 - 4x}{3c(c+1)} > 0. \quad (4.15)$$

Since $a_0 \geq s, t - s \geq 1$ in this case, by (4.14) and (4.15) we have

$$\begin{aligned}
g_1(s, a_0) \geq & g_1(s,s) \\
= & (t-s)^2 + (t-s)q - \alpha(c^2(s+1) + 2(t-s)^2) \\
= & g_2(t-s) \geq g_2(1) = 1 + q - \alpha(c^2 t + 2) \\
\geq & 1 - \frac{c^2 t + 2}{c(c+1)(t+2)} > 0.
\end{aligned}$$

Case 2: $s \geq t + 2$.

Since $q < 1$ and $\alpha \leq \frac{1}{c(c+1)(t+2)} < \frac{1}{4}$, for $x \leq -2$ we have

$$g_2'(x) = 2x + q - \alpha(c^2 + 4x) < x - 4\alpha x < 0. \quad (4.16)$$

Since $a_0 \geq s, t-s \leq -2$, by (4.14) and (4.16) we have

$$\begin{aligned} g_1(s,a_0) \geq & g_1(s,s) \\ =&(t-s)^2+(t-s)q-\alpha(c^2(s+1)+2(t-s)^2) \\ =&g_2(t-s) \geq g_2(-2)=4-2q-\alpha(c^2(t+3)+8) \\ \geq& 2-\frac{c^2(t+3)+8}{c(c+1)(t+2)}>0. \end{aligned}$$

Case 3: $s=t$ and $c \neq 3$.

By Lemma 4.3, $c \geq 4$ in this case. Let $g_3(x)$ be a function defined by

$$g_3(x)=x-1+\frac{(1-\alpha)(c-x)}{c}-\alpha(c(c+1)(x+1)+2x).$$

Since $\alpha \leq \frac{1}{3c(c+1)}$, we have

$$\begin{aligned} g_3'(x)=&1-\frac{1}{c}+\alpha\frac{1}{c}-\alpha(c(c+1)+2) \\ >&\frac{c-1}{c}-\frac{c(c+1)+2}{3c(c+1)} \\ =&\frac{2c^2-c-5}{3c(c+1)}>0. \end{aligned} \tag{4.17}$$

Since $s=a_0=t$ implies $G=G_0$, a contradiction, we have $a_0 \geq t+1$ in this case. $1-q=c-\rho \leq \frac{(1-\alpha)(c-t)}{c}$ by (4.2), hence by (4.14) and (4.17) we have

$$\begin{aligned} g_1(s,a_0)=&g_1(t,a_0) \geq g_1(t,t+1) \\ =&t-q-\alpha(c(c+1)(t+1)+2t) \\ \geq& g_3(t) \geq g_3(1) \geq \frac{c-1}{c}-\alpha(2c(c+1)+2+\frac{c-1}{c}) \\ \geq&\frac{3(c-1)(c+1)-2c(c+1)-3}{3c(c+1)} \\ \geq&\frac{c^2-2c-6}{3c(c+1)}>0. \end{aligned}$$

Case 4: $s=t+1$ and $r_{c+2} \geq 1$.

Let $g_4(x)$ be a function defined by

$$g_4(x)=x+\frac{2(1-\alpha)(c-x)}{c}-\alpha(c(c+1)(x+2)+2x+4).$$

Since $\alpha \leq \frac{1}{3c(c+1)}$, we have

$$\begin{aligned} g_4'(x) =& 1 - \frac{2}{c} + \alpha\frac{2}{c} - \alpha(c(c+1)+2) \\ >& \frac{3(c-2)(c+1) - c(c+1) - 2}{3c(c+1)} \\ =& \frac{2c^2 - 4c - 8}{3c(c+1)} > 0. \end{aligned} \tag{4.18}$$

Since in this case $a_0 = \sum_{i=c+1}^{n} \geq t+2$, and by (4.2) $1 - q = c - \rho \leq \frac{(1-\alpha)(c-t)}{c}$, by (4.14) and (4.18) we have

$$\begin{aligned} g_1(s, a_0) =& g_1(t+1, a_0) \geq g_1(t+1, t+2) \\ =& x + 2 - 2q - \alpha((c+1)c(t+2) + 2t + 4) \\ \geq& g_4(t) \geq g_4(1) = 1 + \frac{2(1-\alpha)(c-1)}{c} - \alpha(3c(c+1)+6) \\ \geq& \frac{3c(c+1) + 6(c-1)(c+1) - 3c(c+1) - 8}{3c(c+1)} \\ \geq& \frac{6(c-1)(c+1) - 8}{3c(c+1)} > 0. \end{aligned}$$

□

Combining Lemma 4.4, Lemma 4.5, Lemma 4.6, and Lemma 4.7, we conclude the following lemma.

Lemma 4.8. *If $G \neq G_0$ and $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$, then $f_G(\rho) > 0$.*

4.4 The proof of Theorem 1.2

Let G be a graph in $\mathcal{G}(n,m)$ with $\rho_\alpha(G) = \rho_\alpha(n,m)$. By Lemma 3.2, we might assume $G \in \mathcal{G}^*(n,m)$. On the contrary, suppose $G \neq G_0$. Let $(r_1, r_2, \ldots, r_n)$ be the row-sum vector of $A_\alpha(G)$, and choose $d = c$ and $s = r_{c+1}$. By Lemma 4.3, $1 \leq s \leq c-2$. This implies $c \geq 3$. Let M be the matrix defined in (3.1). By Theorem 3.5, we have $\rho_\alpha(G) \leq \rho_r(\Pi_1(M^T))$, where $\Pi_1 = \{\{1, 2, \ldots, s\}, \{s+1, \ldots, c\}, \{c+1\}\}$ of $[c+1]$. Let $f_G(x)$ be the characteristic polynomial of $\Pi_1(M^T)$. Since $0 \leq \alpha \leq \frac{1}{c(c+1)(t+2)}$, by Lemma 4.8 we have $f_G(\rho_\alpha(G_0)) > 0$. Since for $c \geq 3$,

$$\alpha \leq \frac{1}{3c(c+1)} \leq \frac{1}{6m} \leq \frac{c-1}{8m},$$

the function $f_G(x)$ is increasing in the interval $(c-1, \infty)$ by Lemma 4.2. Since $\rho_\alpha(G_0) > c-1$ and $\rho_r(\Pi_1(M^T))$ is the largest root of $f_G(x)$, we have $\rho_r(\Pi_1(M^T)) < \rho_\alpha(G_0)$. Hence, $\rho_\alpha(G) < \rho_\alpha(G_0) \leq \rho_\alpha(n, m)$, a contradiction. Hence, $G = G_0$. $\square$

References

[1] T.-C. Chang and B.-S. Tam. Graphs of fixed order and size with maximal A_α-index. *Linear Algebra and its Applications*, 673:69–100, 2023.

[2] Y.-J. Cheng, L. Kao, and C.-W. Weng. Corrigendum of a Theorem on New Upper Bounds for the α-Indices. Comment on Lenes et al. New Bounds for the α-Indices of Graphs. *Mathematics*, 10(15):2619, 2022.

[3] Y.-J. Cheng and C.-W. Weng. A matrix realization of spectral bounds. arXiv preprint arXiv:2307.03880, 2023.

[4] R. A. Horn and C. R. Johnson. *Matrix Analysis*. Cambridge University Press, 2nd edition, 2013.

[5] V. Nikiforov. Merging the A- and Q-spectral Theories. *Applicable Analysis and Discrete Mathematics*, 11(1):81–107, 2017.

[6] V. Nikiforov, G. Pastén, O. Rojo, and R. L. Soto. On the A_α-spectra of trees. *Linear Algebra and its Applications*, 520:286–305, 2017.

[7] P. Rowlinson. On the maximal index of graphs with a prescribed number of edges. *Linear Algebra and its Applications*, 110:43–53, 1987.

[8] M.-Q. Zhai, H.-Q. Lin, and Y.-H. Zhao. Maximize the Q-index of graphs with fixed order and size. *Discrete Mathematics*, 345(1), 2022.