On the First Eigenvalue of Bipartite Graphs

Amitava Bhattacharya

School of Mathematics
Tata Institute of Fundamental Research
Homi Bhabha Road, Colaba, Mumbai 400005, INDIA

amitava@math.tifr.res.in

Shmuel Friedland*

Department of Mathematics, Statistics, and Computer Science
University of Illinois at Chicago
Chicago, Illinois 60607-7045, USA

friedlan@uic.edu

Uri N. Peled

Department of Mathematics, Statistics, and Computer Science
University of Illinois at Chicago
Chicago, Illinois 60607-7045, USA

uripeled@uic.edu

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Abstract

In this paper we study the maximum value of the largest eigenvalue for simple bipartite graphs, where the number of edges is given and the number of vertices on each side of the bipartition is given. We state a conjectured solution, which is an analog of the Brualdi-Hoffman conjecture for general graphs, and prove the conjecture in some special cases.

Key words. Bipartite graph, maximal eigenvalue, Brualdi-Hoffman conjecture, degree, sequences, chain graphs.

1 Introduction

The purpose of this paper is to study the maximum value of the maximum eigenvalue of certain classes of bipartite graphs. These problems are analogous to the problems

*Visiting Professor, Fall 2007 - Winter 2008, Berlin Mathematical School, Berlin, Germany considered in the literature for general graphs and $0-1$ matrices [1, 2, 3, 5, 8]. We describe briefly the main problems and results obtained in this paper.

We consider only finite simple undirected graphs bipartite graphs G. Let $G = (V \cup W, E)$, where $V = \{v_1, \ldots, v_m\}, W = \{w_1, \ldots, w_n\}$ are the two set of vertices of G. We view the undirected edges E of G as a subset of $V \times W$. Denote by $\deg v_i, \deg w_j$ the degrees of the vertices v_i, w_j respectively. Let $D(G) = \{d_1(G) \geqslant d_2(G) \geqslant \cdots \geqslant d_m(G)\}$ be the rearranged set of the degrees $\deg v_1, \ldots, \deg v_m$. Note that $e(G) = \sum_{i=1}^m \deg v_i$ is the number of edges in G. Denote by $\lambda_{\max}(G)$ the maximal eigenvalue of G. Denote by G_{ni} the induced subgraph of G consisting of nonisolated vertices of G. Note that $e(G) = e(G_{\mathrm{ni}}), \lambda_{\max}(G) = \lambda_{\max}(G_{\mathrm{ni}})$. It is straightforward to show, see Proposition 2.1, that

$$\lambda_{\max}(G) \leqslant \sqrt{e(G)}. \tag{1.1}$$

Furthermore the equality holds if and only if G_{ni} is a complete bipartite graph. In what follows we assume that $G = G_{\mathrm{ni}}$, unless stated otherwise.

The majority of this paper is devoted to refinements of (1.1) for noncomplete bipartite graphs. We now state the basic problem that this paper deal with. Denote by $K_{p,q} = (V \cup W, E)$ the complete bipartite graph where $\#V = p, \#W = q, E = V \times W$. We assume here the normalization $1 \leq p \leqslant q$. Let e be a positive integer satisfying $e \leqslant pq$. Denote by $\mathcal{K}(p, q, e)$ the family of subgraphs of $K_{p,q}$ with e edges and with no isolated vertices and *which are not complete bipartite graphs.*

Problem 1.1. *Let $2 \leqslant p \leqslant q, 1 < e < pq$ be integers. Characterize the graphs which solve the maximal problem*

$$\max_{G \in \mathcal{K}(p,q,e)} \lambda_{max}(G). \tag{1.2}$$

We conjecture below an analog of the Brualdi-Hoffman conjecture for nonbipartite graphs [1], which was proved by Rowlinson [5]. See [3, 8] for the proof of partial cases of this conjecture.

Conjecture 1.2. *Under the assumptions of Problem 1.1 an extremal graph that solves the maximal problem (1.2) is obtained from a complete bipartite graph by adding one vertex and a corresponding number of edges.*

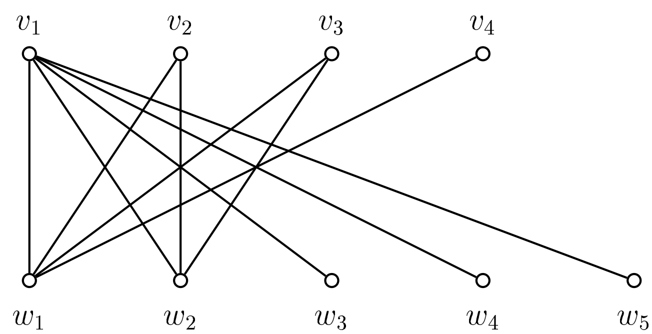
Our first result toward the solution of Problem 1.1 is of interest by itself. Let $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$ be a set of positive integers, and let $\mathscr{B}_D$ be the class of bipartite graphs G with no isolated vertices, where $D(G) = D$. We show that $\max_{G \in \mathscr{B}_D} \lambda_{\max}(G)$ is achieved for a unique graph, up to isomorphism, which is the chain graph [9], or the difference graph [7], corresponding to D. (See §2.) It follows that an extremal graph solving the Problem 1.1 is a chain graph.

Our main result, Theorem 8.1, shows that Conjecture 1.2 holds in the following cases. Fix $r \geqslant 2$ and assume that $e \equiv r-1 \mod r$. Assume that $l = \lfloor \frac{e}{r} \rfloor \geqslant r$. Let $p \in [r, l+1]$ and $q \in [l+1, l+1+\frac{l}{r-1}]$. So $K_{p,q}$ has more than e edges. Then the maximum (1.2) is achieved if and only if G is isomorphic to the following chain graph $G_{r,l+1}$. $G_{r,l+1}$ obtained from $K_{r-1,l+1} = (V \cup W, E)$ by adding an additional vertex v_r to the set V, and connecting v_r to the vertices $w_1, \ldots, w_l$ in W.

We now list briefly the contents of the paper. §2 is a preliminary section in which we recall some known results on bipartite graphs and related results on nonnegative matrices. In §3 we show that the maximum eigenvalue of a bipartite graph increases if we replace it by the corresponding chain graph. §4 gives upper estimates on the maximum eigenvalue of chain graphs. In §5 we discuss a minimal problem related to the sharp estimate of chain graphs with two different degrees. §6 discuses a special case of the above minimal problem over the integers. In §7 we introduce C-matrices, which can be viewed as continuous analogs of the square of the adjacency matrix of chain graphs. In §8 we prove Theorem 8.1.

2 Preliminaries

Figure 1: The chain graph G_D for $D = \{5, 2, 2, 1\}$.



We now set up some notation and review basic results. Denote by $\mathbb{R}^{m\times n}$ the set of $m \times n$ matrices with real entries. We view $A \in \mathbb{R}^{m\times n}$ as $A = (A_{i,j})_{i,j=1}^{m,n}$. Let $G = (V \cup W, E)$ be a bipartite graph with $V = \{v_1, \ldots, v_m\}, W = \{w_1, \ldots, w_n\}$, possibly with isolated vertices. We arrange the vertices $V \cup W$ in the order $v_1, \ldots, v_m, w_1, \ldots, w_n$. Then the adjacency matrix B of G is of the form

$$B = \begin{pmatrix} 0 & A \\ A^\top & 0 \end{pmatrix}, \tag{2.1}$$

where A is an $m \times n$ matrix of 0's and 1's. We call A the *representation matrix* of the bipartite graph G. Note that $i - th$ row sum of A is $\deg v_i$ and the $j - th$ column sum of A is $\deg w_j$. The graph G can be specified by specifying the matrix A. Then G does not have isolated vertices if and only if A does not have zero rows and columns.

Given $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$, a set of positive integers, we construct from D the following graph $G_D \in \mathscr{B}_D$, well-known as a chain graph [9] or a difference graph [7]. The vertices of G_D are partitioned into $\{v_1, \ldots, v_m\}$ and $\{w_1, \ldots, w_n\}$, $n = d_1$, and the neighbors of v_i are $w_1, w_2, \ldots, w_{d_i}$. This is illustrated in Figure 1.

We now recall the well known spectral properties of the symmetric matrix $B \in \mathbb{R}^{(m+n)\times(m+n)}$ of the form (2.1), where $A \in \mathbb{R}_{+}^{m\times n}$, i.e. A is $m \times n$ matrix with nonnegative entries. The spectrum of B is real (by the symmetry of B) and symmetric around the origin (because if $(\mathbf{x}, \mathbf{y})$ is an eigenvector for λ, then $(\mathbf{x}, -\mathbf{y})$ is an eigenvector for $-\lambda$). Every real matrix possesses a singular value decomposition (SVD). Specifically, if A is $m \times n$ of rank r, then there exist positive numbers $\sigma_i = \sigma_i(A)$, $i = 1, \ldots, r$ (the singular values of A) and orthogonal matrices U, V of orders m, n such that $A = U\Sigma V^\top$, where $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_r, 0, \ldots)$ is an $m \times n$ matrix having the σ_i along the main diagonal and otherwise zeros. It is possible and usually done to have the σ_i in non-increasing order. For symmetric matrices the singular values are the absolute values of the eigenvalues. The matrix B from (2.1) satisfies $B^2 = \left(\begin{smallmatrix} AA^\top & 0 \\ 0 & A^\top A \end{smallmatrix}\right)$, and so the eigenvalues of B^2 are those of $AA^\top$ together with those of $A^\top A$. Using the SVD for A we see that $AA^\top$ has the m eigenvalues $\sigma_1^2, \ldots, \sigma_r^2, 0, 0, \ldots$ and $A^\top A$ has the n eigenvalues $\sigma_1^2, \ldots, \sigma_r^2, 0, 0, \ldots$. The eigenvalues of B are therefore square roots of these numbers, and by the symmetry of the spectrum of B, the eigenvalues of B are the $m+n$ numbers $\sigma_1, \ldots, \sigma_r, 0, \ldots, 0, -\sigma_r, \ldots, -\sigma_1$. In particular, *the largest eigenvalue of B is $\sigma_1(A)$*. We denote this eigenvalue by $\lambda_{\max}(B) = \sigma_1(A)$. If B is the adjacency matrix of G then $\lambda_{\max}(G) = \lambda_{\max}(B) = \sigma_1(A)$.

For $\mathbf{x} = (x_1, \ldots, x_n)^\top \in \mathbb{R}^n$ we denote by $\|\mathbf{x}\| = \sqrt{\sum_{j=1}^n x_j^2}$, the Euclidean norm of $\mathbf{x}$. For $A \in \mathbb{R}^{m\times n}$ the operator norm of A is given by $\sigma_1(A) = \sqrt{\lambda_{\max}(AA^\top)} = \sqrt{\lambda_{\max}(A^\top A)}$. We can find $\sigma_1(A)$ by the following maximum principle.

$$\sigma_1(A) = \max_{\substack{\mathbf{x}\in\mathbb{R}^m, \|\mathbf{x}\|=1 \\ \mathbf{y}\in\mathbb{R}^n, \|\mathbf{y}\|=1}} \mathbf{x}^\top A\mathbf{y} = \max_{\mathbf{y}\in\mathbb{R}^n, \|\mathbf{y}\|=1} \|A\mathbf{y}\|. \tag{2.2}$$

To see this, consider the SVD $A = U\Sigma V^\top$. Every $\mathbf{x} \in \mathbb{R}^m$ with $\|\mathbf{x}\| = 1$ can be written as $\mathbf{x} = U\mathbf{a}$, $\mathbf{a} = (a_1, \ldots, a_m)^\top$, with $\|\mathbf{a}\| = 1$, and every $\mathbf{y} \in \mathbb{R}^n$ with $\|\mathbf{y}\| = 1$ can be written as $\mathbf{y} = V\mathbf{b}$, $\mathbf{b} = (b_1, \ldots, b_n)^\top$, with $\|\mathbf{b}\| = 1$. Then

$$\begin{aligned} \mathbf{x}^\top A\mathbf{y} = \mathbf{a}^\top U^\top AV\mathbf{b} = \mathbf{a}^\top \Sigma\mathbf{b} = \sum_{i=1}^r a_i b_i \sigma_i \leqslant \sigma_1 \sum_{i=1}^r |a_i b_i| \leqslant \\ \leqslant \sigma_1 \left(\sum_{i=1}^r a_i^2 \sum_{i=1}^r b_i^2\right)^{\frac{1}{2}} \leqslant \sigma_1 \left(\sum_{i=1}^m a_i^2 \sum_{i=1}^n b_i^2\right)^{\frac{1}{2}} = \sigma_1 \|\mathbf{a}\|\|\mathbf{b}\| = \sigma_1. \end{aligned}$$

Equality is achieved when $\mathbf{x}$ is the first column of U and $\mathbf{y}$ is the first column of V, and this proves the first equality of (2.2). The second equality is obtained by observing that for a given $\mathbf{y}$, the maximizing $\mathbf{x}$ is parallel to $A\mathbf{y}$.

Another useful fact that can be derived from the SVD $A = U\Sigma V^\top$ is the following: if $(\mathbf{x}, \mathbf{y})$ is an eigenvector of $\left(\begin{smallmatrix} 0 & A \\ A^\top & 0 \end{smallmatrix}\right)$ belonging to $\sigma_1 > 0$, then $\|\mathbf{x}\| = \|\mathbf{y}\|$. To see this, observe that $A\mathbf{y} = \sigma_1\mathbf{x}$ and $A^\top\mathbf{x} = \sigma_1\mathbf{y}$. Define vectors $\mathbf{a} = U^\top\mathbf{x}$ and $\mathbf{b} = V^\top\mathbf{y}$. Then

$$\begin{aligned} \Sigma\mathbf{b} = \Sigma V^\top\mathbf{y} = U^\top A\mathbf{y} = \sigma_1 U^\top\mathbf{x} = \sigma_1\mathbf{a} \\ \Sigma^\top\mathbf{a} = \Sigma^\top U^\top\mathbf{x} = V^\top A^\top\mathbf{x} = \sigma_1 V^\top\mathbf{y} = \sigma_1\mathbf{b}. \end{aligned}$$

It follows that for all i we have $\sigma_i b_i = \sigma_1 a_i$ and $\sigma_i a_i = \sigma_1 b_i$. Thus $(\sigma_1 + \sigma_i)(b_i - a_i) = 0$. Since $\sigma_1 + \sigma_i > 0$, it follows that $a_i = b_i$ for all i, and so $\mathbf{a} = \mathbf{b}$, i.e., $U^\top \mathbf{x} = V^\top \mathbf{y}$. The orthogonal matrices $U^\top$ and $V^\top$ preserve the norms, and therefore $\|\mathbf{x}\| = \|\mathbf{y}\|$.

Recall the Rayleigh quotient characterization of the largest eigenvalue of a symmetric matric $M \in \mathbb{R}^{m\times m}$: $\lambda_{\max}(M) = \max_{\|\mathbf{x}\|=1} \mathbf{x}^\top M\mathbf{x}$. Every $\mathbf{x}$ achieving the maximum is an eigenvector of M belonging to $\lambda_{\max}(M)$. If the entries of M are non-negative ($M \geqslant 0$), the maximization can be restricted to vectors $\mathbf{x}$ with non-negative entries ($\mathbf{x} \geqslant \mathbf{0}$) because $\mathbf{x}^\top M\mathbf{x} \leqslant |\mathbf{x}|^\top M|\mathbf{x}|$ and $\||\mathbf{x}|\| = \|\mathbf{x}\|$, where $|\mathbf{x}| = (|x_1|, \ldots, |x_m|)^\top$.

Recall that a square non-negative matrix C is said to be irreducible when some power of $I + C$ is positive (has positive entries). Equivalently the digraph induced by C is strongly connected. Thus a symmetric non-negative matrix B is irreducible when the graph induced by B is connected. For a rectangular non-negative matrix A, $AA^\top$ is irreducible if and only if the bipartite graph with adjacency matrix B given by (2.1) is connected.

If a symmetric non-negative matrix B is irreducible, then the Perron-Frobenius theorem implies that the spectral radius of B is a simple root of the characteristic polynomial of B and the corresponding eigenvector can be chosen to be positive. The following result is well known and we bring its proof for completeness.

Proposition 2.1. *$A = (A_{i,j})_{i,j=1}^{m,n} \in \mathbb{R}_+^{m\times n}$ and assume that B is of the form (2.1). Then*

$$\lambda_{max}(B) \leqslant \sqrt{\sum_{i,j=1}^{m,n} A_{i,j}^2}. \tag{2.3}$$

Equality holds if and only if either $A = 0$ or A is a rank one matrix. In particular, if G is a bipartite graph with $e(G) \geqslant 1$ edges then

$$\lambda_{max}(G) \leqslant \sqrt{e(G)}, \tag{2.4}$$

and equality holds if and only if G_{ni} is $K_{p,q}$, where $pq = e(G)$.

Proof. Let r be the rank of A. Recall that the positive eigenvalues of $AA^\top$ are $\sigma_1(A)^2, \ldots, \sigma_r(A)^2$. Hence $\operatorname{trace} AA^\top = \sum_{i,j}^{m,n} A_{i,j}^2 = \sum_{k=1}^r \sigma_k(A)^2 \geqslant \sigma_1(A)^2$. Combine this equality with the equality $\lambda_{\max}(B) = \sigma_1(A)$ to deduce (2.3). Clearly, equality holds if and only if either $r = 0$, i.e. $A = 0$, or $r = 1$.

Assume now that G is a bipartite graph. Let A be the representation matrix of G. Then $\operatorname{trace} AA^\top = e(G)$. Hence (2.3) implies (2.4).

Assume that $G = K_{p,q}$. Then the entries of the representation matrix A consist of all 1. So rank of A is one and $e(K_{p,q}) = pq$, i.e. equality holds in (2.4). Conversely, suppose that $\lambda_{\max}(G) = \sqrt{e(G)}$. Hence $\lambda_{\max}(G_{\mathrm{ni}}) = \sqrt{e(G_{\mathrm{ni}})}$. Let $C \in \mathbb{R}^{p\times q}$ be the representation matrix of G_{ni}. Since $G_{\mathrm{n}i}$ satisfies equality in (2.3) we deduce that C is a rank one matrix. But C is $0-1$ matrix that does not have a zero row or column. Hence all the rows and columns of C must be identical. Hence all the entries of C are 1, i.e. G_{ni} is a complete bipartite graph with $e(G)$ edges. ☐

3 The Optimal Graphs

The aim of this section is to prove the following theorem.

Theorem 3.1. *Let $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$ be a set of positive integers. Then the chain graph G_D is the unique graph in $\mathscr{B}_D$, (up to isomorphism), which solves the maximum problem* $\max_{G \in \mathscr{B}_D} \lambda_{max}(G)$.

Let us call a graph $G \in \mathscr{B}_D$ *optimal* if it solves the maximum problem of the above theorem. Our first goal is to prove that every optimal graph is connected. For that purpose we partially order the finite sets of positive integers as follows.

Definition 3.2. *Let $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$ and $D' = \{d'_1 \geqslant d'_2 \geqslant \cdots \geqslant d'_{m'}\}$ be sets of m and m' positive integers. Then $D > D'$ means that $m \geqslant m'$, and $d_1 \geqslant d'_1$, $d_2 \geqslant d'_2$, $\ldots$, $d_{m'} \geqslant d'_{m'}$, and $D \neq D'$.*

Theorem 3.3. *If $D > D'$, then $\lambda_{max}(G_D) > \lambda_{max}(G_{D'})$.*

Proof. Let A be the $m \times d_1$ matrix of 0's and 1's with row sums $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m$, and columns ordered so that each row is left-justified (1's first, then 0's). Then $B = \left(\begin{smallmatrix} 0 & A \\ A^\top & 0 \end{smallmatrix}\right)$ of order $m + d_1$ is the adjacency matrix of G_D. Let A' and B' be defined similarly for $G_{D'}$.

Let $M = BB^\top$ and $M' = B'B'^\top$. Then M and M' are symmetric non-negative irreducible matrices of orders m and m', and $\lambda_{\max}(G_D) = \lambda_{\max}(M)$, $\lambda_{\max}(G_{M'}) = \lambda_{\max}(M')$.

Case 1: $m = m'$. In this case, by Definition 3.2, at least one of the inequalities $d_1 \geqslant d'_1$, $d_2 \geqslant d'_2, \ldots, d_m \geqslant d'_m$ holds with strict inequality. It follows that $M \geqslant M'$ (i.e., $M - M'$ is a non-negative matrix), and some integer $i \in [1, m]$ satisfies $M_{i,i} > M'_{i,i}$. Therefore every positive vector $\mathbf{y}$ satisfies $\mathbf{y}^\top M \mathbf{y} > \mathbf{y}^\top M' \mathbf{y}$. Let $\mathbf{y} = \mathbf{x}'$ be the positive Perron-Frobenius eigenvector of the irreducible matrix M', with $\|\mathbf{x}'\| = 1$. Then by the Rayleigh quotient we have

$$\lambda_{\max}(M) \geqslant \mathbf{x}'^\top M \mathbf{x}' > \mathbf{x}'^\top M' \mathbf{x}' = \lambda_{\max}(M'),$$

as required.

Case 2: $m > m'$. In this case, let L be the principal submatrix of M consisting of its first m' rows and columns. By Definition 3.2 we have $d_1 \geqslant d'_1$, $d_2 \geqslant d'_2$, $\ldots$, $d_{m'} \geqslant d'_{m'}$. Therefore $L \geqslant M'$, and hence $\lambda_{\max}(L) \geqslant \lambda_{\max}(M')$.

Since L is symmetric and non-negative, there exists a vector $\mathbf{y} \in \mathbb{R}^{m'}$ with $\mathbf{y} \geqslant \mathbf{0}$, $\|\mathbf{y}\| = 1$ satisfying $\lambda_{\max}(L) = \mathbf{y}^\top L \mathbf{y}$. Extend $\mathbf{y}$ with zeros to a vector $\mathbf{x} \in \mathbb{R}^m$. Then $\mathbf{x} \geqslant \mathbf{0}$ and $\|\mathbf{x}\| = 1$ and $\mathbf{y}^\top L \mathbf{y} = \mathbf{x}^\top M \mathbf{x} \leqslant \lambda_{\max}(M)$. Equality cannot occur here, for if it did, then $\mathbf{x}$ would be the unique Perron-Frobenius eigenvector of the irreducible matrix M and $\mathbf{x}$ would be positive, whereas $x_i = 0$ for $i > m'$. Thus $\lambda_{\max}(M) > \lambda_{\max}(L) \geqslant \lambda_{\max}(M')$, as required. $\square$

Lemma 3.4. *If $G \in \mathscr{B}_D$ is connected, then $\lambda_{max}(G) \leqslant \lambda_{max}(G_D)$.*

Proof. Let $D = \{d_1 \geqslant \cdots \geqslant d_m\}$ and $n \geqslant d_1$. Let $B = \left(\begin{smallmatrix} 0 & A \\ A^\top & 0 \end{smallmatrix}\right)$ be the adjacency matrix of G, where A is $m \times n$ with row sums given by D. Since G is connected, B is irreducible. Let $(\mathbf{x}, \mathbf{y})$ be the positive Perron-Frobenius eigenvector of B belonging to $\lambda_{\max}(G) = \sigma_1(A)$, with $\mathbf{x} = (x_1, \ldots, x_m)$, $\mathbf{y} = (y_1, \ldots, y_n)$:

$$\sigma_1(A)\left(\begin{smallmatrix} \mathbf{x} \\ \mathbf{y} \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 & A \\ A^\top & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} \mathbf{x} \\ \mathbf{y} \end{smallmatrix}\right), \tag{3.1}$$

and so $A\mathbf{y} = \sigma_1(A)\mathbf{x}$.

As we observed in Section 2, we have $\|\mathbf{x}\| = \|\mathbf{y}\|$, and so we may choose a normalization such that $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$.

We reorder the columns of A so that $y_1 \geqslant y_2 \geqslant \cdots \geqslant y_n > 0$. The rows are still in their original order, and so the row sums are $d_1 \geqslant \cdots \geqslant d_m$ in this order.

Let $\overleftarrow{A}$ be the matrix obtained from A by left-justifying each row, i.e., moving all the 1's of the row to the beginning of the row. Then $\left(\begin{smallmatrix} 0 & \overleftarrow{A} \\ \overleftarrow{A}^\top & 0 \end{smallmatrix}\right)$ is the adjacency matrix of G_D with $n - d_1$ zero rows and columns appended at the end, and therefore $\lambda_{\max}(G_D) = \sigma_1(\overleftarrow{A})$.

Since $y_1 \geqslant y_2 \geqslant \cdots \geqslant y_n \geqslant 0$ and since $\overleftarrow{A}$ is obtained from A by left-justifying each row, we have $\overleftarrow{A}\mathbf{y} \geqslant A\mathbf{y}$. Since $\mathbf{x} \geqslant \mathbf{0}$, we have $\mathbf{x}^\top \overleftarrow{A}\mathbf{y} \geqslant \mathbf{x}^\top A\mathbf{y}$. (2.2) yields

$$\begin{aligned}\lambda_{\max}(G_D) = \sigma_1(\overleftarrow{A}) = \max_{\substack{\mathbf{u} \in \mathbb{R}^m, \|\mathbf{u}\|=1 \\ \mathbf{v} \in \mathbb{R}^n, \|\mathbf{v}\|=1}} \mathbf{u}^\top \overleftarrow{A}\mathbf{v} \geqslant \mathbf{x}^\top \overleftarrow{A}\mathbf{y} \geqslant \mathbf{x}^\top A\mathbf{y} \\ = \mathbf{x}^\top \sigma_1(A)\mathbf{x} = \sigma_1(A) = \lambda_{\max}(G).\end{aligned} \tag{3.2}$$

□

Lemma 3.5. *An optimal graph must be connected.*

Proof. Let $G \in \mathscr{B}_D$ be an optimal graph. The graph G is bipartite, and one side of the bipartition (call it the first side) has degrees given by D. Let $G_1, \ldots, G_k$ be the connected components of G. Then $\lambda_{\max}(G) = \lambda_{\max}(G_i)$ for some i.

Like G, the component G_i is also bipartite with the bipartition inherited from that of G. Let D_i be the set of degrees of G_i on the first side of the bipartition.

If G is disconnected, then $D > D_i$, and therefore $\lambda_{\max}(G) \geqslant \lambda_{\max}(G_D) > \lambda_{\max}(G_{D_i}) \geqslant \lambda_{\max}(G_i)$, where the first inequality is by the optimality of G, the second by Theorem 3.3, and the third by Lemma 3.4 and the connectivity of G_i. This contradicts the equality above and proves that G must be connected. □

We are now ready to prove our main theorem.

Proof. (of Theorem 3.1). Let $G \in \mathscr{B}_D$ be optimal with adjacency matrix $B = \left(\begin{smallmatrix} 0 & A \\ A^\top & 0 \end{smallmatrix}\right)$. By Lemma 3.5 G is connected. We begin as in the proof of Lemma 3.4. We let $(\mathbf{x}, \mathbf{y})$ be the positive Perron-Frobenius eigenvector of B belonging to $\lambda_{\max}(G) = \sigma_1(A)$, with $\mathbf{x} = (x_1, \ldots, x_m)^\top$, $\mathbf{y} = (y_1, \ldots, y_n)^\top$, $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$. In other words, (3.1) holds, or equivalently

$$A\mathbf{y} = \sigma_1(A)\mathbf{x} \tag{3.3}$$

$$A^\top \mathbf{x} = \sigma_1(A)\mathbf{y} \tag{3.4}$$

However, this time we reorder both the rows and the columns of A so that $x_1 \geqslant x_2 \geqslant \cdots \geqslant x_m > 0$ and $y_1 \geqslant y_2 \geqslant \cdots \geqslant y_n > 0$, so now the row sums of A, which we still denote by $d_1, d_2, \ldots, d_m$, are not necessarily non-decreasing. As before, we let $\overleftarrow{A}$ be the matrix obtained from A by left-justifying each row. The graph with adjacency matrix $\left(\begin{smallmatrix} 0 & \overleftarrow{A} \\ \overleftarrow{A}^\top & 0 \end{smallmatrix}\right)$ is still isomorphic to G_D plus $n - d_1$ isolated vertices, and therefore $\lambda_{\max}(G_D) = \sigma_1(\overleftarrow{A})$. For the same reasons as before we have $\overleftarrow{A}\mathbf{y} \geqslant A\mathbf{y}$, and therefore (3.2) holds. Moreover, by the optimality of G we have equality throughout (3.2). In particular G_D is optimal and $\lambda_{\max}(G_D) = \sigma_1(A)$, so from now on we abbreviate $\sigma_1(A) = \sigma_1(\overleftarrow{A}) = \sigma_1$. Now $\overleftarrow{A}\mathbf{y} \geqslant A\mathbf{y}$ and $\mathbf{x}^\top \overleftarrow{A}\mathbf{y} = \mathbf{x}^\top A\mathbf{y}$ and $\mathbf{x} > \mathbf{0}$ give

$$\overleftarrow{A}\mathbf{y} = A\mathbf{y} = \sigma_1 \mathbf{x}. \tag{3.5}$$

The first two rows of (3.5) and $x_1 \geqslant x_2$ now give

$$y_1 + \cdots + y_{d_1} = \sigma_1 x_1 \geqslant \sigma_1 x_2 = y_1 + \cdots + y_{d_2},$$

and since $\mathbf{y} > \mathbf{0}$ we must have $d_1 \geqslant d_2$. The same argument with rows 2 and 3 shows $d_2 \geqslant d_3$, and so on. We have established that the row sums of A are non-decreasing, i.e.,

$$d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m. \tag{3.6}$$

Note that by (3.6), the columns of $\overleftarrow{A}$ are top-justified, i.e., the 1's are above the 0's. For this reason and $\mathbf{x} \geqslant \mathbf{0}$ we have $\overleftarrow{A}^\top \mathbf{x} \geqslant A^\top \mathbf{x}$, and hence $\mathbf{y}^\top \overleftarrow{A}^\top \mathbf{x} \geqslant \mathbf{y}^\top A^\top \mathbf{x}$ by $\mathbf{y} \geqslant \mathbf{0}$. The analog of (3.2) for $\overleftarrow{A}^\top$ now holds with equality throughout and we obtain

$$\overleftarrow{A}^\top \mathbf{x} = A^\top \mathbf{x} = \sigma_1 \mathbf{y}. \tag{3.7}$$

Our remaining task is to show that $d_1 = n$ and $A = \overleftarrow{A}$, and therefore G is isomorphic to G_D. For that purpose we need notation for rows of $\overleftarrow{A}$ with equal sums, and similarly for columns.

We introduce the following notation for the row sums of $\overleftarrow{A}$:

$$\begin{aligned} r_1 = d_1 = \cdots = d_{m_1} > r_2 = d_{m_1+1} = \cdots = d_{m_1+m_2} > \cdots > \\ > r_h = d_{m_1+\cdots+m_{h-1}+1} = \cdots = d_{m_1+\cdots+m_h}, \end{aligned} \tag{3.8}$$

where

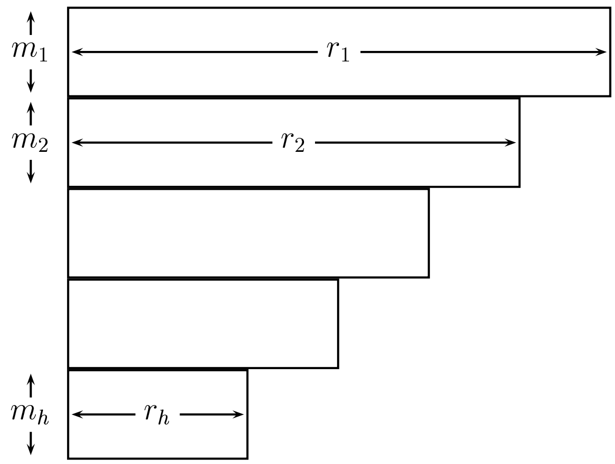
$$m_1 + \cdots + m_h = m.$$

This is illustrated in Figure 2.

From (3.5) we have $\sigma_1 x_i = (\overleftarrow{A}\mathbf{y})_i = y_1 + \cdots + y_{d_i}$. Therefore by (3.8) and $\mathbf{y} > \mathbf{0}$ we obtain

$$\begin{aligned} x_1 = \cdots = x_{m_1} > x_{m_1+1} = \cdots = x_{m_1+m_2} > \cdots > \\ x_{m_1+\cdots+m_{h-1}+1} = \cdots = x_{m_1+\cdots+m_h} > 0. \end{aligned} \tag{3.9}$$

Figure 2: The notation for the row sums of $\overleftarrow{A}$.



Analogously using (3.7) and (3.8) and $\mathbf{x} > \mathbf{0}$ we obtain

$$\begin{gathered} y_1 = \cdots = y_{r_h} > y_{r_h+1} = \cdots = y_{r_{h-1}} > \cdots > \\ y_{r_2+1} = \cdots = y_{r_1} > 0 = y_{r_1+1} = y_{r_1+2} = \cdots = y_n. \end{gathered} \tag{3.10}$$

From (3.10) and $\mathbf{y} > \mathbf{0}$, we conclude that

$$d_1 = r_1 = n.$$

We are now ready to show that $A = \overleftarrow{A}$. Since $d_1 = r_1 = n$, the first m_1 rows of A are all-1, and so are the first m_1 rows of $\overleftarrow{A}$. Now let $m_1 + 1 \leqslant i \leqslant m_1 + m_2$ be an index of one of the next m_2 rows. Both A and $\overleftarrow{A}$ have $d_i = r_2$ 1's in row i. Let the 1's in row i of A lie in columns $k_1, \ldots, k_{r_2}$. Then by (3.5) we have

$$\sum_{j=1}^{r_2} y_{k_j} = (A\mathbf{y})_i = (\overleftarrow{A}\mathbf{y})_i = \sum_{j=1}^{r_2} y_j. \tag{3.11}$$

However, by (3.10) the last $r_1 - r_2$ components of $\mathbf{y}$ are smaller than all other components. Therefore if any k_j lies in the range $\{r_2 + 1, \ldots, r_1\}$, it would follow that $\sum_{j=1}^{r_2} y_{k_j} < \sum_{j=1}^{r_2} y_j$, contradicting (3.11). Therefore $k_j = j$ for $j = 1 \ldots, r_2$, in other words rows i of A and $\overleftarrow{A}$ are the same.

An analogous argument can be applied to the next m_3 rows, and so on, and it follows that $\overleftarrow{A} = A$. □

The arguments of the proof of the above theorem yield.

Corollary 3.6. *Let the assumptions of Problem 1.1 holds. Then any* $H \in \mathcal{K}(p, q, e)$ *satisfying* $\max_{G \in \mathcal{K}(p,q,e)} \lambda_{max}(G) = \lambda_{max}(H)$ *is isomorphic to* G_D*, for some* $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$*, where* $m \leqslant p$ *and* $d_1 \leqslant q$.

4 Estimations of the Largest Eigenvalue

In this section we give lower and upper bounds for $\lambda_{\max}(G)$, where G is an optimal graph with a given adjacency matrix $\left(\begin{smallmatrix} 0 & A \\ A^\top & 0 \end{smallmatrix}\right)$. (Our upper bound improves the upper bound (2.4).)

Recall the concept of the second compound matrix $\Lambda_2 A$ of an $m \times n$ matrix $A = (A_{i,j})$ [6]: $\Lambda_2 A$ is an $\binom{m}{2} \times \binom{n}{2}$ matrix with rows indexed by (i_1, i_2), $1 \leqslant i_1 < i_2 \leqslant m$ and columns indexed by (j_1, j_2), $1 \leqslant j_1 < j_2 \leqslant n$. The entry in row (i_1, i_2) and column (j_1, j_2) of $\Lambda_2 A$ is given by

$$\Lambda_2 A_{(i_1,i_2)(j_1,j_2)} = \det \begin{pmatrix} A_{i_1,j_1} A_{i_1,j_2} \\ A_{i_2,j_1} A_{i_2,j_2} \end{pmatrix}. \tag{4.1}$$

Note that $(\Lambda_2 A)^\top = \Lambda_2 A^\top$. It follows from the Cauchy-Binet theorem that for matrices A, B of compatible dimensions one has $\Lambda_2(AB) = (\Lambda_2 A)(\Lambda_2 B)$. One also has $\Lambda_2 I = I$ and therefore $\Lambda_2 A^{-1} = (\Lambda_2 A)^{-1}$ for nonsingular A. In particular, the second compound matrix of an orthogonal matrix is orthogonal, and therefore the SVD carries over to the second compound: if the SVD of A is $A = U\Sigma V^\top$, then the SVD of $\Lambda_2 A$ is $(\Lambda_2 A) = (\Lambda_2 U)(\Lambda_2 \Sigma)(\Lambda_2 V)^\top$. It follows that if the singular values of A are $\sigma_1 \geqslant \sigma_2 \geqslant \cdots$, then the singular values of $\Lambda_2 A$ are $\sigma_i \sigma_j$, $i < j$. In particular, when the rank of A is larger than 1, equivalently $\Lambda_2 A \neq 0$, we have

$$\sigma_1 \sigma_2 = \sigma_1(\Lambda_2 A) = \max_{\mathbf{w} \neq \mathbf{0}} \frac{\|(\Lambda_2 A)\mathbf{w}\|}{\|\mathbf{w}\|}, \tag{4.2}$$

where the second equality follows by applying (2.2) to $\Lambda_2 A$.

We now specialize to A given by (2.1), which is the adjacency matrix of an optimal graph. Thus A is a matrix of 0's and 1's whose rows are left-justified and whose columns are top-justified. We use the notation (3.8) for the row sums of A. For such A the entries of $\Lambda_2 A$ can only be 0 or -1. Indeed, if in (4.1) $A_{i_2,j_2} = 1$, then $A_{i_1,j_2} = A_{i_2,j_1} = A_{i_1,j_1} = 1$ and the determinant vanishes. If $A_{i_2,j_2} = 0$ and the determinant does not vanish, then again $A_{i_1,j_2} = A_{i_2,j_1} = A_{i_1,j_1} = 1$ and the determinant equals -1. In the latter case we say that (i_1, i_2) and (j_1, j_2) are in a Γ-*configuration.*

To estimate $\sigma_1\sigma_2$ from below, we take a particular column vector $\mathbf{w}$ in (4.2): the (j_1, j_2), $j_1 < j_2$ entry of $\mathbf{w}$ is 1 if column (j_1, j_2) of $\Lambda_2 A$ is nonzero; otherwise this entry of $\mathbf{w}$ is zero. (The assumption $\Lambda_2 A \neq 0$ implies that $\mathbf{w} \neq \mathbf{0}$.) By (4.2) we have

$$\sigma_1 \sigma_2 \geqslant \frac{\|(\Lambda_2 A)\mathbf{w}\|}{\|\mathbf{w}\|}. \tag{4.3}$$

Since $\mathbf{w}$ is a vector of 0's and 1's, $\|\mathbf{w}\|^2$ is the number of nonzero entries of $\mathbf{w}$, that is to say, the number of nonzero columns of $\Lambda_2 A$. We count the nonzero columns (j_1, j_2), $j_1 < j_2$ of $\Lambda_2 A$ as follows. Fix j_2. There is a unique $k = 1, \ldots, h-1$ such that $r_{k+1} + 1 \leqslant j_2 \leqslant r_k$. If j_1 is chosen among $1, \ldots, r_{k+1}$, then there exist (i_1, i_2) such that (i_1, i_2) and (j_1, j_2) are in a Γ-configuration, and otherwise not. It follows that for our fixed j_2, there are r_{k+1} values of j_1 such that column (j_1, j_2) of $\Lambda_2 A$ is nonzero. We can vary j_2 without changing

k in $r_k - r_{k+1}$ ways, so $\Lambda_2 A$ has $r_{k+1}(r_k - r_{k+1})$ nonzero columns corresponding to the same k. Summing over k, we conclude that

$$\|\mathbf{w}\|^2 = \sum_{k=1}^{h-1} r_{k+1}(r_k - r_{k+1}). \tag{4.4}$$

By similar arguments we see that for $1 \leqslant k < l \leqslant h$, the vector $(\Lambda_2 A)\mathbf{w}$ has $m_k m_l$ entries equal to $-r_l(r_k - r_l)$, and that all other entries of $(\Lambda_2 A)\mathbf{w}$ vanish. Therefore

$$\|(\Lambda_2 A)\mathbf{w}\|^2 = \sum_{1 \leqslant k < l \leqslant h} m_k m_l [r_l(r_k - r_l)]^2. \tag{4.5}$$

From (4.3), (4.4) and (4.5), we obtain

$$\sigma_1^2 \sigma_2^2 \geqslant \omega \equiv \frac{\sum_{1 \leqslant k < l \leqslant h} m_k m_l [r_l(r_k - r_l)]^2}{\sum_{k=1}^{h-1} r_{k+1}(r_k - r_{k+1})}. \tag{4.6}$$

As we have noted above, we assume that $h > 1$, for otherwise A has rank 1. If $h = 1$ we define $\omega = 0$.

We can improve the lower bound (4.6) by the following consideration. The graph with adjacency matrix $\left(\begin{smallmatrix} 0 & A^\top \\ A & 0 \end{smallmatrix}\right)$ is isomorphic to the one with adjacency matrix $\left(\begin{smallmatrix} 0 & A \\ A^\top & 0 \end{smallmatrix}\right)$. Therefore we can repeat the work in this section with $A^\top$ replacing A. This amounts to transposing the Ferrers diagram illustrated in Figure 2. Instead of (4.6) we now have

$$\sigma_1^2 \sigma_2^2 \geqslant \omega' \equiv \frac{\sum_{1 \leqslant k < l \leqslant h} m'_k m'_l [r'_l(r'_k - r'_l)]^2}{\sum_{k=1}^{h-1} r'_{k+1}(r'_k - r'_{k+1})}, \tag{4.7}$$

where for $i = 1, \ldots, h$ we have $r'_i = m_1 + \cdots + m_{h-i+1}$ and $m'_i = r_{h-i+1} - r_{h-i+2}$ ($r_{h+1} = 0$).

Combining (4.6) and (4.7) we obtain

$$\sigma_1^2 \sigma_2^2 \geqslant \omega^* \equiv \max\{\omega, \omega'\}. \tag{4.8}$$

We are now ready to estimate σ_1^2 from above.

Theorem 4.1. *Let $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$ be a set of positive integers, where $d_1 > d_m$. Then*

$$\lambda_{max}(G_D)^2 \leqslant \frac{e(G_D) + \sqrt{e(G_D)^2 - 4\omega^*(G_D)}}{2}, \tag{4.9}$$

where $\omega^*(G_D)$ is defined in (4.8). Assume that in the Ferrers diagram given in Figure 2 $h = 2$. I.e. the degree of the vertices in each group of G_D have exactly two distinct values. Then equalities hold in (4.6), (4.7), (4.8) and (4.9). In particular

$$\omega^*(D) = \omega = \omega' = m_1 m_2 r_2 (r_1 - r_2). \tag{4.10}$$

Proof. Since the eigenvalues of $A^\top A$ are $\lambda_{\max}(G_D)^2 = \sigma_1^2, \sigma_2^2, \ldots, \sigma_r^2, 0, 0, \ldots$, we have $\sum_{i=1}^r \sigma_i^2 = \operatorname{trace} A^\top A = \sum_{i,j} A_{i,j}^2 = e$. Let us denote $a = \sigma_1^2 + \sigma_2^2$, so that $a \leqslant e = e(G_D)$, and $b = \sigma_1^2\sigma_2^2$, so that $b \geqslant \omega^*$ by (4.8). Solving for σ_1^2 we obtain $\sigma_1^2 = \frac{a+\sqrt{a^2-4b}}{2} \leqslant \frac{e+\sqrt{e^2-4\omega^*}}{2}$.

Assume that $h = 2$. Then A has rank 2, $\Lambda_2 A$ has rank 1, and $a = e$. Furthermore the definitions of ω, ω' yield the equalities (4.10). To complete the proof, we show that equality holds in (4.3) and therefore also in (4.6), i.e., $b = \omega$.

Since $\Lambda_2 A$ has rank 1 and its elements are only 0 and -1, all its nonzero rows are equal. Say it has c nonzero rows, each with d elements of -1. The trace of $(\Lambda_2 A)^\top(\Lambda_2 A)$ is the sum of squares of the singular values of $\Lambda_2 A$, which equals $(\sigma_1(\Lambda_2 A))^2 = \sigma_1^2\sigma_2^2$ in our case. This trace also equals the sum of squares of the elements of $\Lambda_2 A$, namely cd.

On the other hand, our chosen vector $\mathbf{w}$ satisfies $\|\mathbf{w}\|^2 = d$ and $\|(\Lambda_2 A)\mathbf{w}\|^2 = cd^2$ (because each of the c nonzero rows of $\Lambda_2 A$ multiplied by $\mathbf{w}$ gives $-d$). Hence $\frac{\|(\Lambda_2 A)\mathbf{w}\|^2}{\|\mathbf{w}\|^2} = cd$. Thus both sides of (4.3) are equal to $\sqrt{cd}$. □

We suspect that under the conditions of Theorem 4.1 for $h \geqslant 3$ one has strict inequality in (4.9).

5 A Minimization Problem

The first step in proving Conjecture 1.2 is to show its validity in the case $h = 2$ in Figure 2. We note that for $h = 2$, (4.9) is tight by Theorem 4.1. Theorem 4.1 also implies that equality holds in (4.6), (4.7) and (4.8). This motivates us to consider the problem of minimizing $\omega^*(G)$.

Let $n_1 := r_2$, $n_2 := r_1 - r_2$. Then the condition that the chain graph G has e edges is equivalent to

$$m_1 n_1 + m_1 n_2 + m_2 n_1 = e. \tag{5.1}$$

Formula (4.6) for the case $h = 2$ gives

$$\omega = m_1 m_2 n_1 n_2. \tag{5.2}$$

Let $\mathcal{K}_2(p, q, e) \subseteq \mathcal{K}(p, q, e)$ be set of all subgraphs of $K_{p,q}$ isomorphic to some G_D whose Ferrers diagram, given in Figure 2, satisfies the condition $h = 2$. By the above discussion for $h = 2$, the problem of finding $\max_{G \in \mathcal{K}_2(p,q,e)} \lambda_{\max}(G)$ is equivalent to the following minimization problem over the integers.

Problem 5.1. *Let p, q and e be integers satisfying $2 \leqslant p \leqslant q$ and $3 \leqslant e < pq$. Find the minimum of $m_1 m_2 n_1 n_2$ in positive integers m_1, m_2, n_1 and n_2 satisfying $m_1 + m_2 \leqslant p$, $n_1 + n_2 \leqslant q$ and the constraint (5.1).*

Note if $p = q$, then Problem 5.1 remains invariant under the duality of exchanging (m_1, m_2) with (n_1, n_2). Conjecture 1.2 implies that any minimal solution of Problem 5.1 satisfies the condition $\min(m_2, n_2) = 1$.

In order to prove Conjecture 1.2 in the cases discussed in Theorem 8.1 we need to consider a problem of minimizing $m_1m_2n_1n_2$ under certain constraints, where m_1, m_2, n_1 and n_2 are real numbers. We start with the following simple lemma.

Lemma 5.2. *Let a, b and e be positive real numbers satisfying $e > a + b$. Assume that*

$$ax + by = e, \quad 1 \leqslant x,\ 1 \leqslant y. \tag{5.3}$$

Then

$$xy \geqslant \min\left(\frac{e-a}{b}, \frac{e-b}{a}\right). \tag{5.4}$$

Equality holds if and only if

1. *$x = 1$ when $a < b$;*

2. *$y = 1$ when $b < a$;*

3. *$x = 1$ or $y = 1$ when $a = b$.*

Proof. Set $by = e - ax$ and observe that $f(x) := byx = (e - ax)x$. Note that f is a parabola, with its maximum at $x_0 := \frac{e}{2a}$. So f is decreasing for $x > x_0$ and increasing for $x < x_0$. The minimum of $xy = \frac{f}{b}$, given the constraints $x \geqslant 1$, $y \geqslant 1$ is achieved only when $x = 1$ and $y = \frac{e-a}{b} > 1$ (the minimum possible value of x), or when $y = 1$ and $x = \frac{e-b}{a} > 1$ (where x is the maximum possible value). For $a < b$ and $x = 1$ we have $xy = \frac{e-a}{b}$, which is the LHS of (5.4). For $b < a$ and $y = 1$ we have $xy = \frac{e-b}{a}$, which is the RHS of (5.4). $\square$

Proposition 5.3. *Let $2 \leqslant r, e \in \mathbb{N}$ and assume that*

$$e = lr + r - 1, \;\; r \leqslant p, q \leqslant l + 1 + \frac{l}{r-1}. \tag{5.5}$$

Let $G = (V, W, E) \in \mathcal{K}(p, q, e)$. Then $\#V \geqslant r$ and $\#W \geqslant r$.

Proof. Assume to the contrary that $\#V \leqslant r - 1$. Since G is not a complete bipartite graph,

$$e < (r-1)q \leqslant (r-1)\left(l + 1 + \frac{l}{r-1}\right) = lr + r - 1 = e,$$

which is impossible. Replacing q by p we deduce that $\#W \geqslant r$. $\square$

Hence if p, q and e satisfy (5.5), then for $D \in \mathcal{K}_2(p, q, e)$ we must have $m_1 + m_2 \geqslant r$ and $n_1 + n_2 \geqslant r$. Since m_1, m_2, n_1, n_2 are positive integers, they satisfy the following constraints

$$m_{\geqslant}1,\ m_2 \geqslant 1,\ n_1 \geqslant 1,\ n_2 \geqslant 1,\ m_1 + m_2 \geqslant r,\ n_1 + n_2 \geqslant r. \tag{5.6}$$

Theorem 5.4. *Let $2 \leqslant r \in \mathbb{N}$, $e \in [r^2+1, \infty)$ and consider the minimum of $\omega = m_1 m_2 n_1 n_2$ subject to m_1, m_2, n_1, $n_2 \in \mathbb{R}$, (5.1) and (5.6). Then the minimum is $\frac{(r-1)(e-r+1)}{r}$, and it is achieved only in one of the two cases*

$$(m_1, m_2) = (r-1, 1),\ (n_1, n_2) = \left(\frac{e-r+1}{r}, 1\right) \tag{5.7}$$

$$(m_1, m_2) = \left(\frac{e-r+1}{r}, 1\right),\ (n_1, n_2) = (r-1, 1). \tag{5.8}$$

Proof. Let ϖ be the minimum value of ω subject (5.1) and (5.6). Note that since for the values of m_1, m_2, n_1, n_2 given in (5.7) we have $\omega = \frac{(r-1)(e-r+1)}{r}$, we deduce that $\varpi \leqslant \frac{(r-1)(e-r+1)}{r}$. Since all the functions are symmetric in (m_1, m_2) and (n_1, n_2), we will always assume that $m_1 + m_2 \leqslant n_1 + n_2$. As $m_1 \geqslant 1$ and $m_2 \geqslant 1$, we have $(m_1 - 1)(m_2 - 1) \geqslant 0$, which implies $m_1 m_2 \geqslant m_1 + m_2 - 1$. Similarly $n_1 n_2 \geqslant n_1 + n_2 - 1$. Thus

$$\omega = m_1 m_2 n_1 n_2 \geqslant (m_1 + m_2 - 1)(n_1 + n_2 - 1) \geqslant (m_1 + m_2 - 1)^2.$$

Suppose that $m_1 + m_2 \geqslant \frac{e}{r}$. Then

$$\omega \geqslant (m_1 + m_2 - 1)^2 \geqslant \left(\frac{e}{r} - 1\right)^2 = \frac{(e-r)^2}{r^2}.$$

Since $e \geqslant r^2 + 1$ and $r \geqslant 2$, we obtain

$$(e-r)^2 - r(r-1)(e-r+1) = (e - r^2 - 1)(r^2 - r + 2) + 1 \geqslant 0 \cdot 0 + 1.$$

Hence $\omega > \frac{(r-1)(e-r+1)}{r}$ if $m_1 + m_2 \geqslant \frac{e}{r}$. Thus to find the value of ϖ, we may assume that $m_1 + m_2 < \frac{e}{r}$.

Fix m_1, m_2 that satisfy the conditions

$$m_1 \geqslant 1,\ m_2 \geqslant 1,\ \frac{e}{r} > m_1 + m_2 \geqslant r. \tag{5.9}$$

Now let us find the minimum of $n_1 n_2$ subject to $n_1 \geqslant 1$, $n_2 \geqslant 1$ and (5.1). The constraint (5.1) is equivalent to (5.3) with $a = m_1 + m_2$, $b = m_1$, $x = n_1$ and $y = n_2$. Also $a + b = 2m_1 + m_2 < r(m_1 + m_2) \leqslant e$. Since $a > b$, Lemma 5.2 implies that $n_1 n_2$ is at a minimum when

$$n_2 = 1,\ n_1 := n_1(e, m_1, m_2) = \frac{e-b}{a} = \frac{e - m_1}{m_1 + m_2}. \tag{5.10}$$

Clearly

$$n_1(e, m_1, m_2) > \frac{e - (m_1 + m_2)}{m_1 + m_2} > \frac{e - \frac{e}{r}}{\frac{e}{r}} = r - 1 \geqslant 1,$$

and hence $n_1(e, m_1, m_2) + 1 \geqslant r$. Thus the problem of minimizing $m_1 m_2 n_1 n_2$ subject to (5.1) and (5.6) is equivalent to the problem

$$\text{minimize } \tau := m_1 m_2 n_1(e, m_1, m_2) = \frac{(e - m_1) m_1 m_2}{m_1 + m_2} \text{ subject to (5.9).} \tag{5.11}$$

Fix m_1. Since the function $\frac{t}{m_1 + t}$ increases for $t > 0$, the minimum of τ in (5.11) is achieved only in the following two cases:

1. Case 1: $m_2 = r - m_1$ if $1 \leqslant m_1 \leqslant r-1$;

2. Case 2: $m_2 = 1$ if $m_1 \geqslant r-1$.

Consider first Case 1. Assume first that $r=2$. Then $m_1 = m_2 = 1$, and the minimum of τ subject to Case 1 is $\frac{(e-1)}{2}$.

Now assume that $r \geqslant 3$. Then $\tau = f(m_1)$, where $f(t) := \frac{t(r-t)(e-t)}{r}$. Note that $f(t)$ is a cubic with zeros at 0, r and e. Also $f(t) < 0$ for $t < 0$ and $f(t) > 0$ for $t > e$. Hence $f'(t) = 0$ for some $t = t_1 \in (0,r)$ and some $t = t_2 \in (r,e)$. Note that $f(t)$ increases on $(-\infty, t_1)$ and decreases on (t_1, t_2).

We need to find $\min_{t\in[1,r-1]} f(t)$. Clearly

$$rf'(t) = (r-t)(e-t) - t(e-t) - t(r-t) = (r-2t)(e-2t) - t^2.$$

As $(r-2)(e-2) \geqslant e-2 \geqslant r^2-1 \geqslant 8$, we deduce that $f'(1) > 0$. As $r - 2(r-1) = 2-r < 0$ and $(e-2r+2) \geqslant (r^2-2r+3) = (r-1)^2+2 > 0$, it follows that $f'(r-1) < 0$. So $1 < t_1 < r-1$. Hence

$$\min_{t\in[1,r-1]} f(t) = \min(f(1), f(r-1)) = f(r-1) = \frac{(e-r+1)(r-1)}{r},$$

which is achieved only for $m_1 = r-1$ and $m_2 = 1$.

We now consider Case 2. In this case $\tau = g(m_1)$, where

$$g(t) = \frac{(e-t)t}{t+1} = e+1-t-\frac{e+1}{t+1}.$$

Thus on $[0,\infty)$, the function $g'(t)$ vanishes at the point

$$t_0 = \sqrt{e+1} - 1 > \sqrt{r^2} - 1 = r-1.$$

Note that t_0 is the unique solution of (5.1), where $m_1 = n_1 = t$ and $m_2 = n_2 = 1$. So $f(t)$ increases on $[0, t_0]$ and decreases on the interval $[t_0, \infty)$. Our assumption that $m_1 + m_2 = m_1 + 1 \leqslant n_1 + n_2 = n_1 + 1$ is equivalent to $m_1 \leqslant n_1$. So $m_1 \leqslant t_0 \leqslant n_1$. The assumption that $m_1 + m_2 = m_1 + 1 \geqslant r$ means that $m_1 \geqslant r-1$. Hence $g(m_1)$ has a unique minimum at $m_1 = r-1$. This corresponds to $n_1 = \frac{e-r+1}{r}$. Interchanging (m_1, m_2) with (n_1, n_2) we obtain the second solution $(m_1, m_2) = (\frac{e-r+1}{r}, 1)$, $(n_1, n_2) = (r, 1)$. $\square$

Theorem 5.5. *Suppose one of the following conditions holds.*

1. $r = 2$, $e \geqslant 3$ *is odd and* $2 \leqslant p \leqslant q$, $l = \frac{e-1}{2} < q$.

2. $3 \leqslant r \in \mathbb{N}$ *and (5.5) holds.*

Then $\min_{G\in\mathcal{K}_2(p,q,e)} \lambda_{max}(G)$ *is achieved only for* G_D *isomorphic to the graph obtained from* $K_{r-1,l+1}$ *by adding one vertex to the group of* $r-1$ *vertices and connecting it to* l *vertices in the group of* $l+1$ *vertices.*

Proof. Assume that G_D has the Ferrers diagram given in Figure 2 with $h=2$. Let $n_1 = r_2$ and $n_2 = r_1 - r_2$. Assume first that $r = 2$ and $3 \leqslant e$ is odd. Then $m_1 \geqslant 1$, $m_2 \geqslant 1$, $n_1 \geqslant 1$ and $n_2 \geqslant 1$, so $m_1 + m_2 \geqslant 2$ and $n_1 + n_2 \geqslant 2$. Then for $e \geqslant 5$ the theorem follows from Theorem 5.4 for $r=2$ and Theorem 4.1. For $e = 3$ the theorem is trivial. For $r \geqslant 3$ the theorem follows from Proposition 5.3, Theorem 5.4 and Theorem 4.1. $\square$

6 A special case of Problem 5.1

We now discuss a special case of Problem 5.1 that is not covered by Theorem 5.4.

Theorem 6.1. *Let $e = 3k+1$, where $k \geqslant 7$ is an integer. Consider the minimum of $\omega = m_1m_2n_1n_2$, where m_1, m_2, n_1 and n_2 are positive integers satisfying the constraints $m_1(n_1+n_2)+m_2n_1 = e$, $m_1+m_2 \geqslant 3$, $n_1+n_2 \geqslant 3$; in other words, (5.1) and (5.6) with $r = 3$ hold. Then the minimum of ω is $2k$, and it is achieved if and only if one of the following cases holds:*

$$(m_1, m_2) = (1, 2),\ (n_1, n_2) = (k, 1) \tag{6.1}$$

$$(m_1, m_2) = (k, 1),\ (n_1, n_2) = (1, 2). \tag{6.2}$$

Proof. Clearly, if (6.1) or (6.2) holds, then $\omega = 2k$. Thus it is enough to show that for all integer values of m_1, m_2, n_1 and n_2 satisfying the constraints that are different from the values given in (6.1) and (6.2), we have $\omega > 2k$.

Since we can interchange m_1 with n_1 and m_2 with n_2, we assume without loss of generality that $n_1+n_2 \geqslant m_1+m_2$. We denote the product m_1m_2 by X. Since $m_1+m_2 \geqslant 3$, it follows that $X \geqslant 2$.

Case 1: $m_1 + m_2 \geqslant k$. Since $n_1 + n_2 \geqslant m_1 + m_2 \geqslant k$, we have $m_1m_2 \geqslant k-1$ and $n_1n_2 \geqslant k-1$. This implies $\omega = m_1m_2n_1n_2 \geqslant (k-1)^2 > 2k$ since $k \geqslant 7$.

Case 2: $3 < m_1 + m_2 < k$. Hence $X \geqslant 3$. Suppose $X \geqslant k-1$. Since $n_1+n_2 \geqslant 4$, we have $n_1n_2 \geqslant 3$. Thus $\omega = m_1m_2n_1n_2 \geqslant 3(k-1) > 2k$ since $k \geqslant 7$.

So for the remaining part of Case 2 we assume that $X < k-1$, and hence $\lfloor \frac{2k}{X} \rfloor \geqslant 2$. We will now show that $n_1n_2 \geqslant \lfloor \frac{2k}{X} \rfloor + 1$, from which it will follow that $\omega = Xn_1n_2 > X\frac{2k}{X} = 2k$, as required.

Assume to the contrary that $n_1n_2 < \lfloor \frac{2k}{X} \rfloor + 1$. Since $n_1n_2 \leqslant \lfloor \frac{2k}{X} \rfloor$ we have $n_1 + n_2 \leqslant \lfloor \frac{2k}{X} \rfloor + 1$, and hence $n_1 \leqslant \lfloor \frac{2k}{X} \rfloor$. We now obtain an upper bound for e.

Clearly

$$e = m_1(n_1+n_2) + m_2n_1 \leqslant m_1\left(\left\lfloor \frac{2k}{X} \right\rfloor + 1\right) + m_2n_1 \leqslant m_1\left(\left\lfloor \frac{2k}{X} \right\rfloor + 1\right) + m_2\left\lfloor \frac{2k}{X} \right\rfloor.$$

Observe that that for any $0 < a \in \mathbb{R}$ we have the inequality

$$m_1(a+1) + m_2a \leqslant m_1m_2(a+1) + a = X(a+1) + a$$

and hence

$$e \leqslant X\left(\left\lfloor \frac{2k}{X} \right\rfloor + 1\right) + \left\lfloor \frac{2k}{X} \right\rfloor = X\left\lfloor \frac{2k}{X} \right\rfloor + X + \left\lfloor \frac{2k}{X} \right\rfloor. \tag{6.3}$$

Let $f(x) = x + \frac{2k}{x}$. Since f is strictly convex on $(0,\infty)$, it follows that $f(X) \leqslant \max(f(3), f(k-2)) = \max(3 + \frac{2k}{3}, k - 2 + \frac{2k}{k-2})$. Hence $f(X) < k+1$ for $k > 6$. We also note that in the range $[3, k-2]$, $f(x)$ has a unique minimum at $x = \sqrt{2k}$. Furthermore, $f(x)$ is strictly increasing after that point.

Consider the function $g(x) = x + \lfloor \frac{2k}{x} \rfloor$ on the interval $x \in (0,\infty)$. Note that $g(x)$ is piecewise linear, where each linear piece has slope 1, and is continuous from the left, with jumps at $x_i = \frac{2k}{i}$ for $i \in \mathbb{N}$. So $g(x_i) = f(x_i)$ for $i \in N$, and $g(x) < f(x)$ if $0 < x \neq x_i$ for $i \in N$. This implies $g(X) = X + \lfloor \frac{2k}{X} \rfloor \leqslant f(X) < k+1$ for $k > 6$. Since $g(X)$ is an integer, we deduce that $g(X) \leqslant k$ when $k > 6$ and $X \in [3, k-2]$. Use (6.3) to deduce that

$$e \leqslant X \left\lfloor \frac{2k}{X} \right\rfloor + g(X) \leqslant X \frac{2k}{X} + g(X) \leqslant 2k + k = 3k.$$

This contradicts the assumption that $e = 3k + 1$, and completes Case 2.

Case 3: $m_1 + m_2 = 3$. Then $m_1 m_2 = 2$ and $e = 3n_1 + m_1 n_2$. Assume first that $m_1 = 2$ and $m_2 = 1$. Since $e = 3k+1$ it follows that $n_2 \geqslant 2$. So $3n_1 n_2 = n_2(e - 2n_2)$. Since $e \geqslant 22$, the minimum of $n_1 n_2$ is achieved either for $n_2 = 2$ or for the maximum possible value of n_2 obtained when $n_1 = 1$. For $n_2 = 2$ we have $n_1 = k - 1$ and $\omega = 4(k-1) > 2k$ if $k > 2$. For $n_1 = 1$ we have $n_2 = \frac{e-3}{2}$, which may not be an integer, and $\omega = (e-3) = 3k - 2 > 2k$ for $k > 2$.

Assume finally that $m_1 =$ and $m_2 = 2$. Then $e = 3n_1 + n_2$. Lemma 5.2 yields that $n_1 n_2 \geqslant \frac{e-1}{3} = k$, and equality holds if and only if $n_2 = 1$ and $n_1 = k$. This completes Case 3 and the proof of the theorem. ☐

We used software to show that Theorem 6.1 holds for $k = 2, 3, 4, 5, 6$.

7 C-matrices

Let $\mathbb{R}^p_{+\searrow} := \{\mathbf{c} = (c_1, \ldots, c_p) \in \mathbb{R}^p,\ c_1 \geqslant \cdots \geqslant c_p \geqslant 0\}$. With each $\mathbf{c} \in \mathbb{R}^p_{+\searrow}$ we associate the following symmetric matrix.

$$M(\mathbf{c}) = [c_{\min(i,j)}]_{i,j=1}^p. \tag{7.1}$$

The following result is well-known [4, §3.3, pp.110–111].

Proposition 7.1. *Let $\mathbf{c} = (c_1, \ldots, c_p) \in \mathbb{R}^p_{+\searrow}$. Then all the minors of $M(\mathbf{c})$ are nonnegative. In particular $M(\mathbf{c})$ is a nonnegative definite matrix. If $c_1 > \cdots > c_p > 0$, then all the principal minors of $M(\mathbf{c})$ are positive, i.e., $M(\mathbf{c})$ is positive definite.*

Corollary 7.2. *Let $\mathbf{c} = (c_1, \ldots, c_p) \in \mathbb{R}^p_{+\searrow}$. Then the rank of $M(\mathbf{c})$ is equal to the number of distinct positive elements in $\{c_1, \ldots, c_p\}$.*

Proof. Let $\{c_{i_1}, \ldots, c_{i_k}\}$ be the set of all distinct positive elements in $\{c_1, \ldots, c_p\}$. Hence the rank of $M(\mathbf{c})$ is at most k. Let F be the principal submatrix of $M(\mathbf{c})$ based on the rows and columns $\{i_1, \ldots, i_k\}$. Proposition 7.1 yields that rank $F = k$. ☐

In what follows we assume that $\mathbf{c} = (c_1, \ldots, c_p) \in \mathbb{R}^p_{+\searrow}$ unless stated otherwise. Assume that $c_1 \geqslant \cdots \geqslant c_m > 0 = c_{m+1} = \cdots = c_p$. Denote by $\mathbf{c}_+ := (c_1, \ldots, c_m)$. Then $M(\mathbf{c}_+)$ is the principal submatrix of $M(\mathbf{c})$ obtained from $M(\mathbf{c})$ by deleting the last $p - m$ zero rows and columns. Let

$$\lambda_1(\mathbf{c}) \geqslant \lambda_2(\mathbf{c}) \geqslant \cdots \geqslant \lambda_p(\mathbf{c}) \geqslant 0$$

be the p eigenvalues of $M(\mathbf{c})$. Let m' be the number of distinct elements in $\{c_1, \ldots, c_m\}$. Corollary 7.2 yields that $M(\mathbf{c})$ has exactly m' positive eigenvalues and $\lambda_i(\mathbf{c}) = \lambda_i(\mathbf{c}_+)$ for $i = 1, \ldots, m$.

Let $\mathrm{S}_m(\mathbb{R})$ be the space of $m \times m$ real symmetric matrices. Since $\lambda_1(M)$ is a convex function on $\mathrm{S}_m(\mathbb{R})$ by

$$\max_{\|\mathbf{z}\|=1} \mathbf{z}^\top \frac{A+B}{2} \mathbf{z} \leqslant \frac{\max_{\|\mathbf{x}\|=1} \mathbf{x}^\top A \mathbf{x} + \max_{\|\mathbf{y}\|=1} \mathbf{y}^\top B \mathbf{y}}{2},$$

we obtain the following result.

Proposition 7.3. *Let* $\mathrm{C} \subset \mathbb{R}^p_{+\searrow}$ *be a compact convex set. Let* $\mathcal{E}(\mathrm{C})$ *be the set of the extreme points of* C. *Then* $\max_{\mathbf{c}\in\mathrm{C}} \lambda_1(\mathbf{c}) = \max_{\mathbf{c}\in\mathcal{E}(C)} \lambda_1(\mathbf{c})$.

We show that $\lambda_1(G_D) = \lambda_1(\mathbf{d})$ for a corresponding vector $\mathbf{d} \in \mathbb{R}^p_{+\searrow}$. Let $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$ be a set of positive integers. Assume that $m \leqslant p$ and let $\mathbf{d} = (d_1, \ldots, d_m, 0, \ldots, 0) \in \mathbb{R}^p_{+\searrow}$. Let $G(\mathbf{d})$ denote the chain graph with degrees $\mathbf{d}$, that is to say the chain graph G_D with $p-m$ additional isolated vertices, where $D = \{d_1, \ldots, d_m\}$. Let $A(\mathbf{d})$ be the representation matrix of $G(\mathbf{d})$. Note that $A(\mathbf{d}_+)$ is the representation matrix of G_D. Clearly $A(\mathbf{d})A(\mathbf{d})^\top = M(\mathbf{d})$. Hence

$$\lambda_{\max}(G_D)^2 = \lambda_1(\mathbf{d}) = \lambda_1(\mathbf{d}_+). \tag{7.2}$$

Thus $M(\mathbf{d})$ can be viewed as a continuous version of $G(\mathbf{d})$. The main idea of the proof of Conjecture 1.2, under the conditions discussed in the Introduction, is to replace the maximum discussed in Problem 1.1 with the maximization problem discussed in Proposition 7.3 with a carefully chosen C.

We now bring a few inequalities for $\lambda_1(\mathbf{d})$ needed later, which can be viewed as a generalizations of Proposition 2.1 and Theorem 4.1.

Proposition 7.4. *Let* $\mathbf{c} = (c_1 \ldots, c_p) \in \mathbb{R}^p_{+\searrow}$. *Then*

$$e(\mathbf{c}) := \operatorname{trace} M(\mathbf{c}) = \sum_{i=1}^p c_i = \sum_{i=1}^p \lambda_i(\mathbf{c}), \tag{7.3}$$

$$\sum_{i=1}^p \lambda_i(\mathbf{c})^2 = \operatorname{trace} M(\mathbf{c})^2 = \sum_{i=1}^p (2i-1)c_i^2, \tag{7.4}$$

$$\sum_{1\leqslant i<j\leqslant p} \lambda_i(\mathbf{c})\lambda_j(\mathbf{c}) = \sum_{1\leqslant i<j\leqslant p} c_j(c_i - c_j). \tag{7.5}$$

Hence $\lambda_1(\mathbf{c}) \leqslant e(\mathbf{c})$. *Equality holds if and only if* $M(\mathbf{c})$ *has rank one. Moreover,*

$$\lambda_1(\mathbf{c}) \leqslant \sqrt{\sum_{i=1}^p (2i-1)c_i^2}. \tag{7.6}$$

A sharper upper estimate of $\lambda_1(\mathbf{c})$ for $p \geqslant 2$ is given as follows. Assume that the set $\{c_1, \ldots, c_p\}$ consists of $h \geqslant 2$ distinct positive numbers. Then

$$\lambda_1(\mathbf{c}) \leqslant \frac{(2\alpha_h - 1)e(\mathbf{c}) + \sqrt{e(\mathbf{c})^2 - 4\alpha_h\beta}}{2\alpha_h}, \tag{7.7}$$

where

$$\alpha_h = \frac{h}{2(h-1)}, \qquad \beta = \sum_{1 \leqslant i < j \leqslant p} c_j(c_i - c_j).$$

For a fixed β, the right-hand side of (7.7) is an increasing sequence for $h = 2, 3, \ldots$, and its limit as $h \to \infty$ is the right-hand side of (7.6).

Proof. The equalities (7.3), (7.4) are straightforward. The equality (7.5) follows from them and the identity

$$2 \sum_{1 \leqslant i < j \leqslant p} \lambda_i \lambda_j = \left(\sum_{i=1}^{p} \lambda_i \right)^2 - \sum_{i=1}^{p} \lambda_i^2. \tag{7.8}$$

Since all $\lambda_i(\mathbf{c})$ are real, the inequality (7.6) follows from (7.4).

We now show how the estimate (7.7) follows from (7.5). By Corollary 7.2 the rank of $M(\mathbf{c})$ is exactly h, and therefore exactly h eigenvalues of $M(\mathbf{d})$ are positive. Thus in the left-hand side of the equalities (7.3)–(7.5), i and j can run from 1 to h only. For $h = 2$, (7.7) follows with equality from (7.3) and (7.5).

Assume that $h \geqslant 3$. We let $\lambda_1(\mathbf{c}) = x$ and $e(\mathbf{c}) = e$ and rewrite (7.5) as follows:

$$x(e - x) = \beta - \sum_{2 \leqslant i < j \leqslant h} \lambda_i(\mathbf{c}) \lambda_j(\mathbf{c}). \tag{7.9}$$

In (7.9) we are free to choose $\lambda_2(\mathbf{c}), \ldots, \lambda_h(\mathbf{c})$ subject to $x + \sum_{2 \leqslant i \leqslant h} \lambda_i(\mathbf{c}) = e$, and wish to maximize x.

Observe that the right-hand side of (7.9) is always nonnegative by (7.5) and the definition of β. Thus (7.9) has two solutions x between 0 and e, and we are interested in the larger one and want to maximize it. This is equivalent to choosing $\lambda_2(\mathbf{c}), \ldots, \lambda_h(\mathbf{c})$ so as to minimize the right-hand side of (7.9), or equivalently to maximize $\sum_{2 \leqslant i < j \leqslant h} \lambda_i(\mathbf{c}) \lambda_j(\mathbf{c})$. It is well-known that a sum of the form $\sum_{1 \leqslant i < j \leqslant k} a_i a_j$ can only increase if the a_i are each replaced by their arithmetic mean $\frac{\sum a_i}{k}$. Indeed, $(\sum 1 \cdot a_i)^2 \leqslant (\sum 1^2)(\sum a_i^2) = k \sum a_i^2$. Therefore $2 \sum_{\mathbf{i}<j} a_i a_j = (\sum a_i)^2 - \sum a_i^2 \leqslant (\sum a_i)^2 - \frac{1}{k}(\sum a_i)^2 = (\sum a_i)^2 \frac{k-1}{k} = 2\binom{k}{2} \left(\frac{\sum a_i}{k} \right)^2$.

Thus the upper estimate on x is achieved if we set each of $\lambda_2(\mathbf{c}), \ldots, \lambda_h(\mathbf{c})$ equal to y. Then x and y are subject to $x + (h-1)y = e$ and $x(e-x) + \binom{h-1}{2} y^2 = \beta$. Eliminating y, we see that x should satisfy

$$x(e - x) + \frac{h-2}{2(h-1)}(e - x)^2 = \beta, \tag{7.10}$$

and the larger solution of (7.10) yields (7.7) for $h \geqslant 3$.

The left-hand side of (7.10) is a quadratic in x, which is positive for $0 < x < e$ and increases with h. Therefore the larger solution of (7.10) increases with h. When we take (7.10) to the limit $h \to \infty$, we obtain $x(e-x) + \frac{1}{2}(e-x)^2 = \beta$, or equivalently

$$x^2 = e^2 - 2\beta = \sum_{i=1}^{p} (2i-1)c_i^2, \tag{7.11}$$

and the positive solution of (7.11) is equal to the right-hand side of (7.6). □

8 A proof of Conjecture 1.2 in certain cases

Theorem 8.1. *Let $2 \leqslant r \leqslant l$ be two positive integers. Assume that $e = rl + r - 1$. Suppose one of the following conditions holds:*

1. *$r = 2$ and $2 \leqslant p \leqslant q$, $l = \frac{e-1}{2} < q$;*

2. *$3 \leqslant r \leqslant l$ and $r \leqslant p \leqslant l+1 \leqslant q \leqslant l+1+\frac{l}{r-1}$.*

Let $G_{r,l+1}$ be the graph obtained from $K_{r-1,l+1}$ by adding one vertex to the group of $r-1$ vertices and connecting it to l vertices in the group of $l+1$ vertices. Then $\lambda_{max}(G) \leqslant \lambda_{max}(G_{r,l+1})$, for all $G \in \mathcal{K}(p,q,e)$. Equality holds if and only if G is isomorphic to $G_{r,l+1}$.

Proof. Corollary 3.6 implies that in order to find $\max_{G \in \mathcal{K}(p,q,e)}$, it is enough to consider graphs $G_D = (U, V, E)$, for some $D = \{d_1 \geqslant d_2 \geqslant \cdots \geqslant d_m\}$, where $m \leqslant p$ and $d_1 \leqslant q$. We are going to assume that $\#U = m \leqslant \#V = d_1$ (if this is not satisfied consider the isomorphic graph $G'_D = (V, U, E)$). Let $\mathbf{d} = (d_1, \ldots, d_m)$ be the degree sequence of D.

Since $\mathcal{K}(e,p,q)$ does not contain a complete bipartite graph, we know that $m \geqslant 2$. Proposition 5.3 yields that $m \geqslant r$ for $r \geqslant 3$. Let $\delta_i := d_i - d_m$ for $i = 1, \ldots, m$. We define s by $\delta_s > 0 = \delta_{s+1} = \cdots = \delta_m$, and put $\boldsymbol{\delta} := (\delta_1, \ldots, \delta_s)^\top$. Thus switching from $\mathbf{d}$ to $\boldsymbol{\delta}$ amounts to deleting the first d_m columns of the Ferrers diagram of $\mathbf{d}$, and then deleting empty rows. The resulting Ferrers diagram has a total of $e' := e - md_m = \sum_{i=1}^{s} \delta_i$ components equal to 1 and the rest are zero. Note that $\delta_1 \leqslant q - d_m$. As $h \geqslant 2$, we have that $\delta_s \geqslant 1$. Hence $e' \leqslant e-1$ and $\frac{e'}{s} \geqslant 1$.

We now consider the following polyhedron in $\mathbb{R}^s$:

$$P := \{(x_1, \ldots, x_s)^\top \in \mathbb{R}^s, \quad x_1 \geqslant x_2 \geqslant \cdots \geqslant x_s \geqslant 0, \ \sum_{i=1}^{s} x_i = e'\}. \tag{8.1}$$

Using the notation

$$\mathbf{1}_{n,i} := (\underbrace{1, \ldots, 1}_{i}, 0, \ldots, 0)^\top \in \mathbb{R}^n, \quad i = 1, \ldots, n, \tag{8.2}$$

it is clear that the extreme points of P are $\frac{e'}{i}\mathbf{1}_{s,i}$, $i = 1, \ldots, s$.

Let us define

$$\mathbf{a}_i(\mathbf{d}) = (a_{1,i}, \ldots, a_{m,i})^\top := \frac{e'}{i}\mathbf{1}_{m,i} + d_m \mathbf{1}_{m,m}, \quad i = 1, \ldots, s. \tag{8.3}$$

We note that $\mathbf{d} \in \mathrm{C}(\mathbf{d}) := \operatorname{conv}\{\mathbf{a}_1(\mathbf{d}), \ldots, \mathbf{a}_s(\mathbf{d})\}$. Indeed, $\boldsymbol{\delta} \in P$, and therefore there exist $\alpha_1, \ldots, \alpha_s \geqslant 0$ satisfying $\sum_{i=1}^s \alpha_i = 1$ and $\sum_{i=1}^s \alpha_i \frac{e'}{i}\mathbf{1}_{s,i} = \boldsymbol{\delta}$. Then

$$\begin{aligned}\sum_{i=1}^s \alpha_i \mathbf{a}_i(\mathbf{d}) = \sum_{i=1}^s \alpha_i \left(\frac{e'}{i}\mathbf{1}_{m,i} + d_m \mathbf{1}_{m,m}\right) = \left(\sum_{i=1}^s \alpha_i \frac{e'}{i}\mathbf{1}_{m,i}\right) + d_m \mathbf{1}_{m,m} \\ (d_1, \ldots, d_s, d_m, \ldots, d_m)^\top = (d_1, \ldots, d_s, d_{s+1}, \ldots, d_m)^\top = \mathbf{d}.\end{aligned}$$

Since $\mathbf{d}$ is a convex combination of $\mathbf{a}_1(\mathbf{d}), \ldots, \mathbf{a}_s(\mathbf{d})$, it follows that $M(\mathbf{d})$ is the same convex combination of $M(\mathbf{a}_1(\mathbf{d})), \ldots, M(\mathbf{a}_s(\mathbf{d}))$. Combine (7.2) with Proposition 7.3 to obtain

$$\lambda_{\max}(G_D)^2 = \lambda_1(M(\mathbf{d})) \leqslant \max_{1 \leqslant k \leqslant l} \lambda_1(M(\mathbf{a}_k(\mathbf{d}))). \tag{8.4}$$

The vector $\mathbf{a}_k(\mathbf{d})$ has the form $\mathbf{a}_k(\mathbf{d}) = (\underbrace{x, \ldots, x}_{k}, \underbrace{y, \ldots, y}_{m-k})^\top$ with $x = \frac{e'}{k} + d_m$ and $y = d_m$.

Therefore the first k rows of $M(\mathbf{a}_k(\mathbf{d}))$ are equal to $\mathbf{a}_k(\mathbf{d})$ and the last $m-k$ rows are equal to $y\mathbf{1}_{m,m}$. Proposition 7.1 and Corollary 7.2 yield that $M(\mathbf{a}_k(\mathbf{d}))$ is a nonnegative definite matrix of rank 2. It satisfies

$$\lambda_1(M(\mathbf{a}_k(\mathbf{d}))) + \lambda_2(M(\mathbf{a}_k(\mathbf{d}))) = \operatorname{trace} M(\mathbf{a}_k(\mathbf{d})) = k\left(\frac{e'}{k} + d_m\right) + (m-k)d_m = e. \tag{8.5}$$

The product $\lambda_1(M(\mathbf{a}_k(\mathbf{d})))\lambda_2(M(\mathbf{a}_k(\mathbf{d})))$ is equal to the sum

$$\sum_{i<j} \lambda_i(M(\mathbf{a}_k(\mathbf{d})))\lambda_j(M(\mathbf{a}_k(\mathbf{d}))),$$

which in turn equals the coefficient of λ^{m-2} in the characteristic polynomial

$$\prod_i (\lambda - \lambda_i(M(\mathbf{a}_k(\mathbf{d})))).$$

This coefficient equals in turn the sum of all 2×2 principal minors of $M(\mathbf{a}_k(\mathbf{d}))$. There are $k(m-k)$ contributing minors, each of the form $\det\left(\begin{smallmatrix} x & y \\ y & y \end{smallmatrix}\right) = y(x-y)$. Therefore

$$\lambda_1(M(\mathbf{a}_k(\mathbf{d})))\lambda_2(M(\mathbf{a}_k(\mathbf{d}))) = \omega(\mathbf{a}_k(\mathbf{d})) := k(m-k)\frac{e'}{k}d_m. \tag{8.6}$$

Hence

$$\lambda_1(M(\mathbf{a}_k(\mathbf{d}))) = \frac{e + \sqrt{e^2 - 4\omega(a_k(\mathbf{d}))}}{2}. \tag{8.7}$$

Thus the maximum possible value of $\lambda_1(M(\mathbf{a}_k(\mathbf{d})))$ is achieved for the minimum value of $\omega(\mathbf{a}_k(\mathbf{d}))$. This situation corresponds to the minimization problem we studied in Theorem 5.4. We put

$$m_1 = k, \quad m_2 = m - k, \quad n_1 = d_m, \quad n_2 = \frac{e'}{k}.$$

Clearly $m_1 \geqslant 1$ and $n_1 \geqslant 1$. Also $m_2 = m-k \geqslant s+1-k \geqslant 1$ and $n_2 = \frac{e'}{k} \geqslant \frac{e'}{s} \geqslant 1$. Recall that $m = m_1 + m_2 \geqslant r$. We claim that for each $2 \leqslant r \in \mathbb{N}$, the inequality $n_1 + n_2 \geqslant r$ holds. For $r = 2$ this inequality follows from the inequalities $n_1 \geqslant 1, n_2 \geqslant 1$. Assume now that $r \geqslant 3$. Observe that

$$n_1 + n_2 = d_m + \frac{e'}{k} \geqslant d_m + \frac{e'}{s} \geqslant d_m + \frac{e'}{m-1} = d_m + \frac{e - md_m}{m-1} = \frac{e - d_m}{m-1}.$$

Recall that G_D is not complete bipartite. Since $d_1 \geqslant \cdots \geqslant d_m$, we deduce that $d_m \leqslant \frac{e-1}{m}$. Hence

$$\frac{e - d_m}{m-1} \geqslant f(m) := \frac{e}{m-1} + \frac{1}{m(m-1)}.$$

So $f(m)$ is a decreasing function for $m > 1$. For $m = p = l + 1$, obtain $f(l+1) > \frac{e}{l} = \frac{rl+r-1}{l} > r$ if $r \geqslant 3$. Hence $n_1 + n_2 \geqslant r$ for any $r \geqslant 2$. Theorem 5.4 implies the inequality

$$\omega(\mathbf{a}_k(\mathbf{d})) \leqslant \frac{(r-1)(e-r+1)}{r}. \tag{8.8}$$

Hence

$$\lambda_1(M(\mathbf{a}_k(\mathbf{d}))) \leqslant \frac{e + \sqrt{e^2 - (\frac{(r-1)(e-r+1)}{r})^2}}{2} = \lambda_{\max}(G_{r,l+1})^2,$$

where the last equality follows from Theorem 4.1. We use (8.4) to deduce

$$\lambda_{\max}(G_D) \leqslant \lambda_{\max}(G_{r,l+1}) \text{ for any } G_D \in \mathcal{K}(p,q,e). \tag{8.9}$$

It is left to show that equality holds in (8.9) if and only if $D = D_* := \{d_1 = \cdots = d_{r-1} = l+1 > d_r = l\}$. Let $\mathbf{d}_* = (l+1, \ldots, l+1, 1)$ be the corresponding degree sequence of D_*. We now consider the equality case in (8.8). Theorem 5.4 asserts that equality holds only if one of the two conditions in (5.7) holds.

Assume first that the first condition of (5.7) holds. So $n_1 = \frac{e-r+1}{r} = l$. On the other hand $n_1 = d_m$. So $d_m = l$. Also $m = m_1 + m_2 = r - 1 + 1 = r$. Furthermore, $n_2 = \frac{e'}{k} = 1$. This can happen if and only if $\delta_1 = \cdots = \delta_k = 1$. Hence $d_1 = \cdots = d_s = l + 1$ and $d_{s+1} = d_r = l$. Since $e = lr + r - 1$, we deduce that $s = r - 1$.

Assume now that the second condition holds in (8.8). So $d_m = n_1 = r - 1$ and $\frac{e'}{k} = 1$. Hence $d_1 = \cdots = d_s = r > d_{s+1} = \cdots = d_m = r - 1$. We have $m_1 = \frac{e-r+1}{r} = l = k$ and $m_2 = 1$. So $m = m_1 + m_2 = l + 1$. Since $e = rl + r - 1$, we deduce that $s = r - 1$. Hence $D = D^* = \{d_1 = \cdots = d_l = r > d_{l+1} = r - 1\}$. Note that G_{D^*} is isomorphic to $G_{D_*} = G_{r,l+1} = (U_*, V_*, E)$. More precisely, $G_{D_*} = (V_*, U_*, E)$. Assume first that $r \geqslant 3$. Then $\#V_* = l + 1 > r = \#U_*$. This case is ruled out since we agreed to consider only

$G_D = (U, V, E)$ where $\#U \leqslant \#V$. If $r = 2$, then $\#V_* = \frac{e+1}{2} = l + 1$ and $\#U = 2$. If $e \geqslant 5$, then this case is ruled out as above. If $e = 3$, then any $G \in \mathcal{K}(2, 2, 3)$ is isomorphic to $G_{2,2}$, and the theorem trivially holds in this case. In particular any $G_D \in \mathcal{K}(2, 2, 3)$ is equal to G_{D_*}.

Let $G_D = (U, V, E) \in \mathcal{K}(p, q, e)$, and assume that $\#U \leqslant \#V$ and $D \neq D_*$. The above arguments show that $\omega(\mathbf{a}_k(\mathbf{d})) > \omega(\mathbf{a}_{r-1}(\mathbf{d}_*))$ for $k = 1, \ldots, s$. Hence $\lambda_1(M(\mathbf{a}_k(\mathbf{d})) < \lambda_{\max}(G_{r,l+1})^2$ for $k = 1, \ldots, s$, and (8.4) yields that $\lambda_{\max}(G_D) < \lambda_{\max}(G_{r,l+1})$. □

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