國立交通大學

應用數學系

博士論文

圖的譜半徑與度數列之研究

Spectral Radius and Degree Sequence of a Graph

博 士 生：劉家安

指導教授：翁志文 教授

中華民國一百零四年六月

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摘要

令 G 為一 n 點的簡單圖，G 的**譜半徑** $\rho(G)$ 為 G 之鄰接矩陣的最大特徵值。對於每個不大於 n 的自然數 ℓ，本論文給出一個用 G 圖中前 ℓ 大的點度數所表示之譜半徑可達上界；此上界的應用非常廣泛，如圖的團數、無號拉普拉斯譜半徑、以及廣義 r 分圖。我們將此證明概念應用於二分圖譜半徑上的研究，而解決以下前人所提的猜想：給定正整數 $k < p < q + 1$，在所有從完全二分圖 $K_{p,q}$(兩個分部分別為 p 點和 q 點) 扣掉 k 邊後所可能產生的子圖中，擁有最大譜半徑的，為此扣掉的 k 邊皆和 q 點分部中的同一點相連。

關鍵字：圖，二分圖，鄰接矩陣，譜半徑，度數列。

Spectral Radius and Degree Sequence of a Graph

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Abstract

Let G be a simple graph of order n. The *spectral radius* $\rho(G)$ of G is the largest eigenvalue of its adjacency matrix. For each positive integer ℓ at most n, this dissertation gives a sharp upper bound for $\rho(G)$ by a function of the first ℓ vertex degrees in G, which generalizes a series of previous results. Applications of these bounds on the clique number, signless Laplace spectral radius, and generalized r-partite graphs are provided. The idea of the above result also applies to bipartite graphs. Let k, p, q be positive integers with $k < p < q+1$. We prove a conjecture stating that the maximum spectral radius of a simple bipartite graph obtained from the complete bipartite graph $K_{p,q}$ of bipartition orders p and q by deleting k edges is attained when the deleted edges are all incident on a common vertex which is located in the partite set of order q.

Keywords: graph, bipartite graph, adjacency matrix, spectral radius, degree sequence.

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Table of Contents

List of Figures

Chapter 1

Introduction

Algebraic graph theory is a branch of mathematics that studies graphs by using algebraic properties of associated matrices. It has proven to be effective in treating graphs. More in particular, spectral graph theory studies the relation between graph properties and the eigenvalues of the adjacency matrix, Laplace matrix, or the signless Laplace matrix of a graph. There is a large amount of literature on spectral graph theory, well documented in several surveys and books, such as Biggs [5], Cvetković, Doob and Sachs [16] (also see [15]), and Seidel [39].

Spectral graph theory is a useful subject. The founders of Google computed the Perron-Frobenius eigenvector of the web graph and became billionaires. The largest eigenvalue, also known as the spectral radius, of a graph is the largest eigenvalue of its adjacency matrix. The basic information about the spectral radius of a (possibly directed) graph is provided by Perron-Frobenius theory [8, Section 2.2]. The second largest eigenvalue of a graph gives information about expansion and randomness properties [8, Chapter 4]. The smallest eigenvalue gives information about independence number [26] and chromatic number [27, 44]. The second least eigenvalue of Laplace matrix has been referred to as the algebraic connectivity of a graph [23]. Interlacing inequalities between the eigenvalues of two graphs give information about their substructure relations [25, Chapter 5]. Even the trivial fact that eigenvalue multiplicities must be integral provides strong restrictions. For example, Moore graphs are classified from this method [7, Theorem 6.7.1].

This dissertation is aiming at the relation between the spectral radius and degree sequence of a graph. Let G be a simple graph of n vertices and e edges with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. The spectral radius $\rho(G)$ of G is the largest eigenvalue of its adjacency matrix and has been studied by many authors. It is well-known that $\rho(G) \leq d_1$ [35, Chapter 2]. In 1985 [9, Corollary 2.3], Brualdi and Hoffman proved that if $e \leq k(k-1)/2$ then

$$\rho(G) \leq k-1. \tag{1.0.1}$$

In 1987 [41], Stanley improved (1.0.1) and showed hat

$$\rho(G) \leq \frac{-1+\sqrt{1+8e}}{2}. \tag{1.0.2}$$

If G is connected, in 1998 [29, Theorem 2] Yuan Hong improved (1.0.2) and showed that

$$\rho(G) \leq \sqrt{2e-n+1}. \tag{1.0.3}$$

In 2001 [30, Theorem 2.3], Hong *et al.* improved (1.0.3) and showed that

$$\rho(G) \leq \frac{d_n - 1 + \sqrt{(d_n+1)^2 + 4(2e - nd_n)}}{2}. \tag{1.0.4}$$

In 2004 [40, Theorem 2.2], Jinlong Shu and Yarong Wu showed that

$$\rho(G) \leq \frac{d_\ell - 1 + \sqrt{(d_\ell+1)^2 + 4(\ell-1)(d_1 - d_\ell)}}{2} \tag{1.0.5}$$

for $1 \leq \ell \leq n$. Moreover, they showed in [40, Theorem 2.5] that if $a + b \geq d_1 + 1$ then (1.0.5) improves (1.0.4) where a is the number of vertices with the largest degree d_1 and b is the number of vertices with the second largest degree. In Section 3.2 we present the following upper bounds for $\rho(G)$ in terms of the degree sequence of G which improves (1.0.5).

Let H, H' be two simple graphs with vertices sets $V(H) \cap V(H)' = \phi$. The *sum* $H + H'$ of H and H' is the graph obtained from H and H' by adding an edge between x and y for each pair $(x, y) \in V(H) \times V(H')$.

Theorem A. Let ℓ be a positive integer with $1 \leq \ell \leq n$. Then

$$\rho(G) \leq \phi_\ell := \frac{d_\ell - 1 + \sqrt{(d_\ell+1)^2 + 4\sum_{i=1}^{\ell-1}(d_i - d_\ell)}}{2}.$$

Furthermore, if G is connected then the above equality holds if and only if G is regular or there exists $2 \leq t \leq \ell$ and a regular graph H of order $n-t+1$ such that $G = K_{t-1} + H$.

This result also improves (1.0.4) since ϕ_n is exactly the upper bound in (1.0.4).

There are several applications of Theorem A. The spectral radius of the signless Laplace matrix of G is denoted by $q(G)$. Let $\Delta_{ij} = d_i + d_j - 2$ for each pair of adjacent vertices $i \sim j$ in G be the vertex degrees of the line graph G^ℓ of G, and $\Delta_1 \geq \Delta_2 \geq \ldots \geq \Delta_e$ be a renumbering of them in non-increasing order. Then for $1 \leq \ell \leq e$, we have

$$q(G) \leq \psi_\ell := 2 + \frac{\Delta_\ell - 1 + \sqrt{(\Delta_\ell + 1)^2 + 4\sum_{i=1}^{\ell-1}(\Delta_i - \Delta_\ell)}}{2}$$

with equality if and only if $\Delta_1 = \Delta_e$ or there exists $2 \leq t \leq \ell$ such that $e - 1 = \Delta_1 = \Delta_{t-1} > \Delta_t = \Delta_e$.

Let $3 \leq j \leq n$ be the smallest integer such that $\sum_{i=1}^{j} d_i < \ell(\ell - 1)$. We prove in Section 3.3 that

$$\phi_j = \min\{\phi_k \mid 1 \leq k \leq n\}.$$

Turán's Theorem [42], proved in 1941, is a seminal result in extremal graph theory. In its concise form it states that

$$\frac{n}{n-d} \leq \omega(G)$$

where d is the average vertex degree and $\omega(G)$ is the clique number of G. In 1986, Wilf [45] proved that

$$\frac{n}{n-\rho(G)} \leq \omega(G).$$

There is also a lower bound for $\omega(G)$ presented by ϕ_j :

$$\frac{n}{n-\phi_j} < \omega(G) + \frac{1}{3}.$$

In a series of papers, Bojilov and others have generalized the concept of an r-partite graph. Let $d(v)$ denote the degree of vertex v in G. They define a parameter, say $\theta(G)$, to be the smallest integer r for which $V(G)$ has an r-partition:

$$V(G) = V_1 \cup V_2 \cup \ldots \cup V_r, \text{ such that } d(v) \leq n - n_i, \text{ where } n_i = |V_i|,$$

for all $v \in V_i$ and for $i = 1, 2, \ldots, r$. Bojilov *et al.* [6] proved that

$$\theta(G) \leq \omega(G)$$

and Khadzhiivanov and Nenov [32] proved that

$$\frac{n}{n-d} \leq \theta(G).$$

Despite this bound, Elphick and Wocjan [21] demonstrated that

$$\frac{n}{n-\rho(G)} \not\leq \theta(G),$$

i.e., $n/(n-\rho(G)) > \theta(G)$ in some graphs. We prove in Section 4.5 that

$$\frac{n}{n-\rho(G)} \leq \frac{n}{n-\phi_j} < \theta(G) + \frac{1}{3}.$$

Brualdi and Hoffman proposed the problem of finding the maximum spectral radius of a graph with precisely e edges in 1976 [3, p.438], and ten years later they gave a conjecture in [9] that the maximum spectral radius of a graph with e edges is attained by taking a complete graph and adding a new vertex which is adjacent to a corresponding number of vertices in the complete graph. This conjecture was proved by Peter Rowlinson in [38]. See [41, 24] also for the proof of partial cases of this conjecture.

The bipartite graphs analogue of the Brualdi-Hoffman conjecture was settled by A. Bhattacharya, S. Friedland, and U.N. Peled [4] with the following statement: For a connected bipartite graph G, $\rho(G) \leq \sqrt{e}$ with equality iff G is a complete bipartite graph. Moreover, they proposed the problem to determine graphs with maximum spectral radius in the class of bipartite graphs with bipartition orders p and q, and e edges. They then gave Conjecture B below.

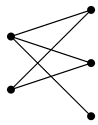
Conjecture B. Let $\mathcal{K}(p,q,e)$ denote the family of e-edge subgraphs of the complete bipartite graph $K_{p,q}$ with bipartition orders p and q, and $1 < e < pq$ be integers. An extremal graph that solves

$$\max_{G\in\mathcal{K}(p,q,e)} \rho(G)$$

is obtained from a complete bipartite graph by adding one vertex and a corresponding number of edges.

Conjecture B does not indicate that the adding vertex goes into which partite set of a complete bipartite graph. For $e \geq pq - \min(p,q)$, let $K_{p,q}^e$ denote the graph which is obtained from $K_{p,q}$ by deleting $pq-e$ edges incident on a common vertex in the partite set of order no less than that of the other partite set. Figure 1.1 gives a such graph.

In 2010 [12], Yi-Fan Chen, Hung-Lin Fu, In-Jae Kim, Eryn Stehr and Brendon Watts determined $\rho(K_{p,q}^e)$ and gave an affirmative answer to Conjecture B when $e = pq-2$. Furthermore, they refined Conjecture B for the case when the number of edges



$K_{2,3}^5$

Figure 1.1: The graph $K_{2,3}^5$.

is at least $pq - \min(p,q) + 1$ to the following conjecture.

Conjecture C. Suppose $0 < pq - e < \min(p,q)$. Then for $G \in \mathcal{K}(p,q,e)$,

$$\rho(G) \le \rho(K_{p,q}^e).$$

Let H, H' be two bipartite graphs with given ordered bipartitions $V(H) = X \cup Y$ and $V(H') = X' \cup Y'$, where $V(H) \cap V(H') = \phi$. The bipartite sum $H \oplus H'$ of H and H' (with respect to the given ordered bipartitions) is the graph obtained from H and H' by adding an edge between x and y for each pair $(x,y) \in X \times Y' \cup X' \times Y$. For example, $K_{p,q}^e = K_{p-pq+e,q-1} \oplus N_{pq-e,1}$ where $N_{s,t}$ denotes the bipartite graph with bipartition orders s,t and without any edges. We apply the idea of Theorem A to the bipartite graphs and give Theorem D in Section 5.3.

Theorem D. Let G be a simple bipartite graph with bipartition orders p and q, and corresponding degree sequences $d_1 \ge d_2 \ge \cdots \ge d_p$ and $d'_1 \ge d'_2 \ge \cdots \ge d'_q$. For $1 \le s \le p$ and $1 \le t \le q$, let $X_{s,t} = d_s d'_t + \sum_{i=1}^{s-1}(d_i - d_s) + \sum_{j=1}^{t-1}(d'_j - d'_t)$ and $Y_{s,t} = \sum_{i=1}^{s-1}(d_i - d_s) \cdot \sum_{j=1}^{t-1}(d'_j - d'_t)$. Then the spectral radius

$$\rho(G) \le \phi_{s,t} := \sqrt{\frac{X_{s,t} + \sqrt{X_{s,t}^2 - 4Y_{s,t}}}{2}}.$$

Furthermore, if G is connected then the above equality holds if and only if there exists nonnegative integers $s' < s$ and $t' < t$, and a biregular graph H of bipartition orders $p - s'$ and $q - t'$ respectively such that $G = K_{s',t'} \oplus H$.

Based on Theorem D, in Section 5.5 we solve Conjecture C, and Conjecture B under the assumption that $0 < pq - e < \min(p,q)$.

The following preprints and papers are included in this dissertation:

1. Chia-an Liu and Chih-wen Weng, Spectral radius and degree sequence of a graph, *Linear Algebra Appl.* 438 (2013) 3511-3515.

2. Chia-an Liu and Chih-wen Weng, Spectral radius of bipartite graphs, *Linear Algebra Appl.* 474 (2015) 30-43.

3. Clive Elphick and Chia-an Liu, A (forgotten) bound for the spectral radius of a graph, to appear in *Taiwanese Journal of Mathematics* DOI: 10.11650/tjm.19.2015.5393.

This dissertation is organized as follows.

In Chapter 2 we introduce definitions, terminologies and some results concerning the graphs, matrices of graphs, and spectra of graphs.

In Chapter 3 we prove Theorem A.

In Chapter 4 several applications of Theorem A are introduced. Moreover, partial result of Theorem A is written in a different statement.

In Chapter 5 we focus on the bipartite graphs. We prove Theorem D, and then give affirmative answers to Conjecture C (and then Conjecture B under additional assumptions).

Chapter 2

Preliminaries

In this chapter we review some definitions and basic concepts concerning the graphs, spectra of graphs, and matrices.

2.1 Graphs

The following basic knowledge of graphs is referred to [43].

Definition 2.1.1. A *graph* G is a triple consisting of a *vertex set* $V(G)$, an *edge set* $E(G)$, and a relation that associates with each edge two vertices (not necessarily distinct) called its endpoints. The *order* of G is the number of vertices in G, i.e. $|V(G)|$.

Definition 2.1.2. A *loop* is an edge whose endpoints are equal. *Multiple edges* are edges having the same pair of endpoints. A *simple graph* is a graph having no loops or multiple edges. We specify a simple graph by its vertex set and edge set, treating the edge set as a set of unordered pairs of vertices and writing $e = uv$ (or $e = vu$) for an edge e with endpoints u and v.

Definition 2.1.3. Let G be a loopless graph with vertex set $V(G)$ and edge set $E(G)$. If vertex $v \in V(G)$ is an endpoint of $e \in E(G)$, then v and e are *incident*. The *degree* of vertex v is the number of incident edges. The *degree sequence* of a graph is the list of vertex degrees, usually written in nonincreasing order, as $d_1 \geq d_2 \geq \cdots \geq d_n$ where $n = |V(G)|$. G is *regular* if $d_1 = d_n$, and G is *k-regular* if $d_1 = d_n = k$.

Definition 2.1.4. The *complement* $\overline{G}$ of a simple graph G is the simple graph with vertex set $V(G)$ defined by $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$. A *clique* in a graph is a set of pairwise adjacent vertices.

Definition 2.1.5. An *independent set* (or *stable set*) in a graph is a set of pairwise nonadjacent vertices. A graph G is *bipartite* if $V(G)$ is the union of two disjoint (possibly empty) independent sets called *partite sets* of G.

Definition 2.1.6. Let G be a bipartite graph with p and q vertices in its partite sets and corresponding degree sequences $d_1 \geq d_2 \geq \cdots \geq d_p$ and $d'_1 \geq d'_2 \geq \cdots \geq d'_q$. We say that G is *biregular* if $d_1 = d_p$ and $d'_1 = d'_q$.

Definition 2.1.7. The *chromatic number* of a graph G, written $\chi(G)$, is the minimum number of colors needed to label the vertices so that adjacent vertices receive different colors. A graph G is *k-partite* if $V(G)$ can be expressed as the union of k (possibly empty) independent sets.

This generalizes the idea of bipartite graphs, which are 2-partite.

Definition 2.1.8. The *line graph* of a simple graph G, written G^ℓ, is the graph whose vertices are the edges of G, with $ef \in E(G^\ell)$ when $e = uv$ and $f = vw$ in G for some $u, v, w \in V(G)$.

Figure 2.1: An example of a simple graph and its line graph.

Definition 2.1.9. The *clique number* of a graph G, written $\omega(G)$, is the maximum size of a set of pairwise adjacent vertices in G.

Definition 2.1.10. An *isomorphism* from a simple graph G to a simple graph H is a bijection $f : V(G) \to V(H)$ such that $uv \in E(G)$ if and only if $f(u)f(v) \in E(H)$. We say "G is *isomorphic* to H", written $G \cong H$, if there is an isomorphism from G to H.

Proposition 2.1.11. *[43, Proposition 1.1.24] On any set of (simple) graphs, the isomorphism relation is an equivalence relation.*

Definition 2.1.12. An *isomorphism class* of graphs is an equivalence class of graphs under isomorphism relation.

When discussing a graph G, we have a fixed vertex set, but our structural comments apply also to every graph isomorphic to G. Our conclusions are independent of the names (labels) of the vertices. Thus, we use the informal expression "unlabeled graph" to mean an isomorphism class of graphs.

Definition 2.1.13. A *path* is a simple graph whose vertices can be ordered so that two vertices are adjacent if and only if they are consecutive in the list. A *cycle* is a graph with an equal number of vertices and edges whose vertices can be placed around a circle so that two vertices are adjacent if and only if they appear consecutively along the circle. The (unlabeled) path and cycle with n vertices are denoted by P_n and C_n, respectively; an *n-cycle* is a cycle with n vertices.

P_5 C_5

Figure 2.2: The graphs P_5 and C_5.

Definition 2.1.14. A *complete graph* is a simple graph whose vertices are pairwise adjacent; the (unlabeled) complete graph with n vertices is denoted by K_n. A *complete bipartite graph* is a simple bipartite graph such that two vertices are adjacent if and only if they are in different partite sets. When the sets have sizes s and t, the (unlabeled) complete bipartite graph is denoted by $K_{s,t}$.

K_5 $\qquad$ $K_{2,3} = K_{3,2}$

Figure 2.3: The graphs K_5, $K_{2,3}$, and $K_{3,2}$.

Definition 2.1.15. The n-vertex star, denoted by S_n, is the complete bipartite graph $K_{1,n-1}$ for $n \geq 2$. The n-vertex wheel W_n is formed by connecting an isolated vertex to all vertices of an $(n-1)$-cycle, for $n \geq 4$.

$S_7 = K_{1,6}$ $\qquad$ W_7

Figure 2.4: The graphs S_7 and W_7.

Definition 2.1.16. A *walk* is a list $v_0, e_1, v_1, \ldots, e_k, v_k$ of vertices and edges such that, for $1 \leq i \leq k$, the edge e_i has endpoints v_{i-1} and v_i. A u, v-*walk* has first vertex u and last vertex v; these are its endpoints.

Definition 2.1.17. A graph G is *connected* if it has a u, v-walk whenever $u, v \in V(G)$ (otherwise, G is *disconnected*).

2.2 Graph spectrum

The background of graph spectrum mentioned in this section is referred to [8].

Definition 2.2.1. Let G be a simple graph. The *adjacency matrix* of G is the 0-1 matrix $A = A(G)$ indexed by the vertex set $V(G)$ of G, where $A_{xy} = 1$ if and only if $xy \in E(G)$.

Note that the degree of vertex v is the sum of the entries of A in the row indexed by v.

Definition 2.2.2. Let G be a simple graph and D be the diagonal matrix indexed by the vertex set $V(G)$ such that D_{xx} is the degree of x. The *Laplace matrix* of G is $L(G) = L = D - A$, and the *signless Laplace matrix* of G is $Q(G) = Q = D + A$.

Definition 2.2.3. The *spectrum* of a simple graph G is by definition the spectrum of its adjacency matrix A, that is, its set of eigenvalues together with their multiplicities. The spectral radius $\rho(G)$ of G is the largest eigenvalue of its adjacency matrix A. Let $q(G)$ be the largest eigenvalue of the signless Laplace matrix $Q(G)$ of G.

2.3 Nonnegative matrices

Let $M = (m_{ij})$ be an $n \times n$ matrix. We say that M is *positive* (resp. *nonnegative*) if $m_{ij} > 0$ (resp. $m_{ij} \geq 0$) for all i, j. We say that M is *reducible* if the indices $1, 2, \cdots, n$ can be divided into two disjoint nonempty sets $i_1, i_2, \cdots, i_\mu$ and $j_1, j_2, \cdots, j_\nu$ where $\mu + \nu = n$ such that $m_{i_\alpha j_\beta} = 0$ for $\alpha = 1, 2, \cdots, \mu$ and $\beta = 1, 2, \cdots \nu$. A square matrix is called *irreducible* if it is not reducible. Simply considering the adjacent relation of a graph and the definition of irreducible matrices, we have the following proposition.

Proposition 2.3.1. *The adjacency matrix of a simple graph G is irreducible if and only if G is connected.* □

The following lemma is a part of the Perron-Frobenius Theorem [35, Chapter 2]. Note that according to the Perron-Frobenius Theorem, the spectral radius of a symmetric nonnegative matrix is equal to its largest eigenvalue.

Theorem 2.3.2. *If M is a nonnegative $n \times n$ matrix with spectral radius $\rho(M)$ and row-sums $r_1, r_2, \ldots, r_n$, then*

$$\rho(M) \leq \max_{1 \leq i \leq n} r_i.$$

Moreover, if M is irreducible then the above equality holds if and only if the row-sums of M are all equal.

2.4 Quotient matrices

Let M be a real matrix described in the following block form

$$M = \begin{pmatrix} M_{1,1} & \cdots & M_{1,m} \\ \vdots & & \vdots \\ M_{m,1} & \cdots & M_{m,m} \end{pmatrix},$$

where the diagonal blocks $M_{i,i}$ are square. Let b_{ij} denote the average row-sum of $M_{i,j}$, i.e. b_{ij} is the sum of entries in $M_{i,j}$ divided by the number of rows. Then $B = (b_{ij})$ is called a *quotient matrix* of M. If in addition for each pair i, j, $M_{i,j}$ has constant row-sum, then B is called an *equitable quotient matrix* of M. The following lemma is direct from the definition of matrix multiplication [8, Chapter 2].

Lemma 2.4.1. *Let B be an equitable quotient matrix of M with an eigenvalue θ. Then M also has the eigenvalue θ.*

Chapter 3

Spectral Radius and Degree Sequence of a Graph

In Chapter 3 we give a series of upper bounds in terms of the degree sequence of a simple graph, which generalizes some previous results. Throughout this chapter let G be a simple graph of n vertices and e edges with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Note that $\sum_{i=1}^{n} d_i = 2e$.

3.1 Known upper bounds for the spectral radius $\rho(G)$

We shall review previous known results of upper bounds of spectral radius of graph G in expression of part or all of the degree sequence.

In 1985 [9, Corollary 2.3], Brualdi and Hoffman showed the following result.

Theorem 3.1.1. *Let k be the smallest positive integer such that $e \leq k(k-1)/2$. Then*

$$\rho(G) \leq k - 1.$$

Furthermore, if G is connected then the above equality holds if and only if G is isomorphic to the complete graph K_n of order n.

In 1987 [41], Stanley improved Theorem 3.1.1 and showed the following result.

Theorem 3.1.2. *Let G be a simple graph. Then*

$$\rho(G) \le \frac{-1+\sqrt{1+8e}}{2}.$$

If G is connected then the above equality holds if and only if G is isomorphic to K_n.

If G is connected, in 1998 [29, Theorem 2] Yuan Hong improved Theorem 3.1.2 and showed the following result.

Theorem 3.1.3. *If G is connected then*

$$\rho(G) \le \sqrt{2e-n+1}$$

with equality holds if and only if G is isomorphic to the star $K_{1,n-1}$ or K_n.

Definition 3.1.4. Let H, H' be two simple graphs with vertices sets $V(H) \cap V(H)' = \phi$. The *sum* $H+H'$ of H and H' is the graph obtained from H and H' by adding an edge between x and y for each pair $(x,y) \in V(H) \times V(H')$.

In 2001 [30, Theorem 2.3], Hong *et al.* improved Theorem 3.1.3 and showed the following result.

Theorem 3.1.5. *Let G be a simple graph. Then*

$$\rho(G) \le \frac{d_n - 1 + \sqrt{(d_n+1)^2 + 4(2e - nd_n)}}{2}.$$

Furthermore, if G is connected then the above equality holds if and only if G is regular or there exists $2 \le t \le n$ and a regular graph H of order $n-t+1$ such that $G = K_{t-1} + H$.

In 2004 [40, Theorem 2.2], Jinlong Shu and Yarong Wu improved Theorem 2.3.2 in the case that A is the adjacency matrix of G by showing the following result.

Theorem 3.1.6. *Let ℓ be a positive integer with $1 \le \ell \le n$. Then*

$$\rho(G) \le \frac{d_\ell - 1 + \sqrt{(d_\ell+1)^2 + 4(\ell-1)(d_1 - d_\ell)}}{2}.$$

Furthermore, if G is connected then the above equality holds if and only if G is regular or there exists $2 \le t \le \ell$ and a regular graph H of order $n-t+1$ such that $G = K_{t-1} + H$.

Moreover, they also showed in [40, Theorem 2.5] that if $p + q \geq d_1 + 1$ then Theorem 3.1.6 improves Theorem 3.1.5 where p is the number of vertices with the largest degree d_1 and q is the number of vertices with the second largest degree. The special case $\ell = 2$ of Theorem 3.1.6 is reproved [18].

3.2 New upper bounds ϕ_ℓ for $\rho(G)$

We give a series of sharp upper bounds of $\rho(G)$ in Theorem 3.2.1 in terms of the degree sequence of G which improves Theorem 3.1.1 to Theorem 3.1.6.

Theorem 3.2.1. *Let ℓ be a positive integer with $1 \leq \ell \leq n$. Then*

$$\rho(G) \leq \phi_\ell := \frac{d_\ell - 1 + \sqrt{(d_\ell + 1)^2 + 4\sum_{i=1}^{\ell-1}(d_i - d_\ell)}}{2}.$$

Furthermore, if G is connected then the above equality holds if and only if G is regular or there exists $2 \leq t \leq \ell$ and a regular graph H of order $n - t + 1$ such that $G = K_{t-1} + H$.

Remark 3.2.2. This result improves Theorem 3.1.3 and Theorem 3.1.6 since ϕ_n is exactly the upper bounds in Theorem 3.1.3 and is at most the upper bound appearing in Theorem 3.1.6. Additionally, generalized from this research, a similar upper bound of the spectral radius in terms of the average 2-degree sequence of a graph is presented in [31].

Proof of Theorem 3.2.1. Let the vertices be labeled by $1, 2, \ldots, n$ with degrees $d_1 \geq d_2 \geq \cdots \geq d_n$, respectively. For each $1 \leq i \leq \ell - 1$, let $x_i \geq 1$ be a variable to be determined later. Let $U = diag(x_1, x_2, \ldots, x_{\ell-1}, 1, 1, \ldots, 1)$ be a diagonal matrix of size $n \times n$. Then $U^{-1} = diag(x_1^{-1}, x_2^{-1}, \ldots, x_{\ell-1}^{-1}, 1, 1, \ldots, 1)$.

Let $B = U^{-1}AU$. Notice that A and B have the same eigenvalues.

Let $r_1, r_2, \ldots, r_n$ be the row-sums of B. Then for $1 \leq i \leq \ell - 1$ we have

$$\begin{aligned} r_i &= \sum_{k=1}^{\ell-1} \frac{x_k}{x_i} a_{ik} + \sum_{k=\ell}^{n} \frac{1}{x_i} a_{ik} = \frac{1}{x_i} \sum_{k=1}^{n} a_{ik} + \frac{1}{x_i} \sum_{k=1}^{\ell-1} (x_k - 1) a_{ik} \\ &\leq \frac{1}{x_i} d_i + \frac{1}{x_i} \left(\sum_{k=1, k\neq i}^{\ell-1} x_k - (\ell - 2) \right), \end{aligned} \tag{3.2.1}$$

and for $\ell \le j \le n$ we have

$$\begin{aligned} r_j &= \sum_{k=1}^{\ell-1} x_k a_{jk} + \sum_{k=\ell}^{n} a_{jk} = \sum_{k=1}^{n} a_{jk} + \sum_{k=1}^{\ell-1} (x_k - 1) a_{jk} \\ &\le d_\ell + \left(\sum_{k=1}^{\ell-1} x_k - (\ell - 1) \right). \end{aligned} \tag{3.2.2}$$

For $1 \le i \le \ell - 1$ let

$$x_i = 1 + \frac{d_i - d_\ell}{\phi_\ell + 1} \ge 1, \tag{3.2.3}$$

where ϕ_ℓ is defined in Theorem 3.2.1. Clearly that ϕ_ℓ has the following quadratic equation

$$(\phi_\ell + 1)^2 - (d_\ell + 1)(\phi_\ell + 1) - \sum_{i=1}^{\ell-1} (d_i - d_\ell) = 0.$$

Therefore

$$\sum_{k=1}^{\ell-1} x_k - (\ell - 1) = (\phi_\ell + 1) - (d_\ell + 1) = \phi_\ell - d_\ell, \tag{3.2.4}$$

and hence for $1 \le i \le \ell - 1$

$$x_i(\phi_\ell + 1) = d_i + 1 + \sum_{k=1}^{\ell-1} x_k - (\ell - 1) = d_i + x_i + \sum_{k=1, k \ne i}^{\ell-1} x_k - (\ell - 2). \tag{3.2.5}$$

By (3.2.5) for $1 \le i \le \ell - 1$ we have

$$r_i \le \frac{1}{x_i} d_i + \frac{1}{x_i} \left(\sum_{k=1, k \ne i}^{\ell-1} x_k - (\ell - 2) \right) = \phi_\ell,$$

and by (3.2.4) for $\ell \le j \le n$ we have

$$r_j \le d_\ell + \left(\sum_{k=1}^{\ell-1} x_k - (\ell - 1) \right) = \phi_\ell.$$

Hence by Theorem 2.3.2,

$$\rho(G) = \rho(B) \le \max_{1 \le i \le n} \{r_i\} \le \phi_\ell. \tag{3.2.6}$$

The first part of Theorem 3.2.1 follows.

To prove the second part of Theorem 3.2.1, suppose that G is connected. The sufficient condition of $\phi_\ell = \rho(G)$ follows from the fact that

$$\phi_\ell \le \frac{d_\ell - 1 + \sqrt{(d_\ell + 1)^2 + 4(\ell - 1)(d_1 - d_\ell)}}{2}$$

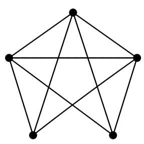
and applying the second part in Theorem 3.1.6.

To prove the necessary condition of $\phi_\ell = \rho(G)$, suppose $\phi_\ell = \rho(G)$. The connectivity of G implies that A is irreducible, and so as B because U is a diagonal matrix with positive entries on the diagonal. From (3.2.6) we have $\phi_\ell = \max_{1\le i\le n}\{r_i\}$ and then by the second part of Theorem 2.3.2 and the irreducibility of B the r_i's are all equal. It follows that the equalities in (3.2.1) and (3.2.2) all hold. If $d_1 = d_\ell$, then $d_1 = \phi_1 = \phi_\ell = \rho(G)$, and G is regular by the second part of Theorem 2.3.2. Suppose $2 \le t \le \ell$ such that $d_{t-1} > d_t = d_\ell$. Then $x_i > 1$ for $1 \le i \le t-1$ by (3.2.3). For each $1 \le i \le \ell - 1$, the equality in (3.2.1) implies that $a_{ik} = 1$ for $1 \le k \le t-1$, $k \ne i$. For each $\ell \le j \le n$, the equality in (3.2.2) implies that $a_{jk} = 1$ for $1 \le k \le t-1$ and $d_j = d_\ell$. Hence $n - 1 = d_1 = d_{t-1} > d_t = d_\ell = d_n$. It follows that $G = K_{t-1} + H$ for some regular graph H of order $n - t + 1$.

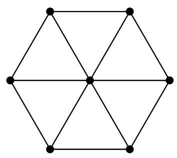
We complete the proof. $\square$

We give two examples which meet the equalities in Theorem 3.2.1.

Example 3.2.3. Consider the graph K_5^- obtained by deleting one edge from the complete graph K_5 on 5 vertices. Its degree sequence is $d_1 = d_3 = 5 - 1$ and $d_4 = d_5 = 3$, so $\rho(K_5^-) = \phi_4(K_5^-) = 1 + \sqrt{7}$. Consider the wheel graph W_7 on 7 vertices. Its degree sequence is $d_1 = 7 - 1$ and $d_2 = d_7 = 3$, so $\rho(W_7) = \phi_2(W_7) = 1 + \sqrt{7}$.



K_5^-



W_7

Figure 3.1: Two examples meet the equalities in Theorem 3.2.1.

3.3 The sequence $\phi_1, \phi_2, \ldots, \phi_n$

The sequence $\phi_1, \phi_2, \ldots, \phi_n$ is not necessarily non-increasing. i.e. the upper bound ϕ_ℓ of $\rho(G)$ is not always getting better. For example, the path P_n of n vertices has $2 = d_1 = d_{n-2} > d_{n-1} = d_n = 1$, and it is immediate to check that if $n \geq 6$ then $\phi_1 = \phi_2 = 2 < \sqrt{n-1} = \phi_{n-1} = \phi_n$.

Clearly that for all $1 \leq s < t \leq n$, $d_s = d_t$ implies that $\phi_s = \phi_t$. However, $\phi_s = \phi_t$ dose not imply $d_s = d_t$. For example, in the graph with degree sequence $(4, 3, 3, 2, 1, 1)$, one can check that $\phi_4 = \phi_5 = 3$ but $d_4 > d_5$.

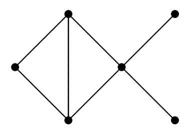


Figure 3.2: A graph with $\phi_4 = \phi_5 = 3$, but $d_4 > d_5$.

Recall that $d_s = d_{s+1}$ implies $\phi_s = \phi_{s+1}$ for $1 \leq s \leq n-1$. The following proposition describes the shape of the sequence $\phi_1, \phi_2, \ldots, \phi_n$.

Proposition 3.3.1. *Let $1 \leq s \leq n-1$ and suppose $d_s > d_{s+1}$. Then*

$$\phi_s \succeq \phi_{s+1} \quad \textit{iff} \quad \sum_{i=1}^{s} d_i \succeq s(s-1),$$

where $\succeq \ \in \{>, =\}$.

Proof. Recall that

$$\phi_s = \frac{d_s - 1 + \sqrt{(d_s+1)^2 + 4\sum_{i=1}^{s-1}(d_i - d_s)}}{2}.$$

The proposition follows from the following equivalent relations step by step:

$$
\begin{aligned}
& \phi_s \succeq \phi_{s+1} \\
\Leftrightarrow \quad & d_s - d_{s+1} + \sqrt{(d_s+1)^2 + 4\sum_{i=1}^{s-1}(d_i - d_s)} \\
& \qquad \succeq \sqrt{(d_{s+1}+1)^2 + 4\sum_{i=1}^{s}(d_i - d_{s+1})} \\
\Leftrightarrow \quad & \sqrt{(d_s+1)^2 + 4\sum_{i=1}^{s-1}(d_i - d_s)} \succeq 2s - (d_s+1) \qquad (3.3.1) \\
\Leftrightarrow \quad & (d_s+1)^2 + 4\sum_{i=1}^{s}(d_i - d_s) \succeq 4s^2 - 4s(d_s+1) + (d_s+1)^2 \\
\Leftrightarrow \quad & \sum_{i=1}^{s} d_i \succeq s(s-1),
\end{aligned}
$$

where the relation in (3.3.1) is obtained from the second by taking square on both sides, simplifying it, and deleting the common term $d_s - d_{s+1}$. Notice that if $2s - (d_s + 1) < 0$ in (3.3.1) then in the case that $\succeq$ is $=$, all statements fails, and in the case that $\succeq$ is $>$ the left hand side of (3.3.1) is at least $d_s + 1$, which is greater than $|2s - (d_s + 1)|$, so the equivalent relation in the next step holds. □

We have known that $d_s = d_{s+1}$ implies $\phi_s = \phi_{s+1}$. Combining with Proposition 3.3.1 we have the following results.

Lemma 3.3.2. *(i) If $\sum_{i=1}^{s} d_i \geq s(s-1)$ then $\phi_s \geq \phi_{s+1}$.*

(ii) If $\sum_{i=1}^{s} d_i < s(s-1)$ then $\phi_s \leq \phi_{s+1}$.

(iii) $\phi_s = \phi_{s+1}$ iff $d_s = d_{s+1}$ or $\sum_{i=1}^{s} d_i = s(s-1)$.

□

Corollary 3.3.3. *Let $n \geq 3$ and ℓ be the smallest integer such that $\sum_{i=1}^{\ell} d_i < \ell(\ell-1)$. Then for $1 \leq j \leq n$*

$$\phi_j = \min\{\phi_k \mid 1 \leq k \leq n\}$$

if and only if $d_j = d_\ell$, or $d_j = d_{\ell-1}$ with $\sum_{i=1}^{\ell-1} d_i = (\ell-1)(\ell-2)$.

Proof. For $1 \leq s \leq \ell - 1$, from Lemma 3.3.2(i) we have $\phi_s \geq \phi_{s+1}$ since $\sum_{i=1}^{s} d_i \geq s(s-1)$. For $\ell \leq t \leq n-1$, notice that $\sum_{i=1}^{t} d_i < t(t-1)$ implies $d_t < t-1$, and hence $\sum_{i=1}^{t+1} d_i < t(t-1) + (t-1) < t(t+1)$. From Lemma 3.3.2(ii) we have $\phi_\ell \leq \phi_{\ell+1} \leq \cdots \leq \phi_n$ since $\sum_{i=1}^{\ell} d_i < \ell(\ell-1)$. Hence $\phi_\ell = \min\{\phi_k \mid 1 \leq k \leq n\}$.

If $\sum_{i=1}^{s} d_i = s(s-1)$ then $s-1 \geq d_s \geq d_{s+1}$, and $\sum_{i=1}^{s+1} d_i \leq s(s-1) + (s-1) < s(s+1)$. Hence $\sum_{i=1}^{s} d_i > s(s-1)$ for $1 \leq s \leq \ell - 2$. The second part immediately follows from Lemma 3.3.2(iii), and the result follows. □

Chapter 4

Applications of the New Upper Bounds ϕ_ℓ

The best degree-based bounds ϕ_ℓ for the spectral radius $\rho(G)$ of graphs are obtained in Chapter 3. We give applications of them in this chapter.

4.1 A different approach of ϕ_ℓ

This chapter begins by demonstrating that a bound for the spectral radius dating from 1983 is equivalent to $\min\{\phi_\ell \mid 1 \le \ell \le n\}$. In 1983, Edwards and Elphick proved the following result in [19, Theorem 8] (and its corollary).

Theorem 4.1.1. *The spectral radius*

$$\rho(G) \le y - 1$$

where $y = y(G) > 0$ is defined by the equality

$$y(y-1) = \sum_{k=1}^{\lfloor y \rfloor} d_k + (y - \lfloor y \rfloor) d_{\lceil y \rceil}. \tag{4.1.1}$$

They also showed that $1 \le y \le n$ and that y is a single-valued function of G in [19, Lemma 3].

This bound is exact for regular graphs because, we then have that

$$d = \rho(G) \le y - 1 = \frac{1}{y}\left(\sum_{k=1}^{\lfloor y \rfloor} d + (y - \lfloor y \rfloor) d\right) = d$$

where d is the common vertex degree.

The bound is also exact for various bidegree graphs. For example, let G be the star graph $K_{1,n-1}$ on n vertices which has $\rho(G) = \sqrt{n-1}$. It is easy to show that $y > 1$. Then the equation 4.1.1 becomes

$$y(y-1) = (n-1) + \lfloor y \rfloor - 1 + (y - \lfloor y \rfloor) = n - 2 + y,$$

so $y = 1 + \sqrt{n-1}$.

Similarly let G be the wheel graph on n vertices ($n \geq 4$), which has $\rho(G) = 1 + \sqrt{n}$. It is straightforward to show that $y = 2 + \sqrt{n}$, so again the bound is exact.

The following theorem combines Theorem 3.2.1 and Theorem 4.1.1 which are over 30 years!

Theorem 4.1.2. *Let a be the smallest integer such that $\sum_{i=1}^{a} d_i \leq a(a-1)$. Then*

$$y - 1 = \phi_{a+1} = \frac{d_{a+1} - 1 + \sqrt{(d_{a+1}+1)^2 + 4\sum_{i=1}^{a}(d_i - d_{a+1})}}{2},$$

where y is defined in (4.1.1).

Proof. Observing the definition of y, we have $\lfloor y \rfloor = a$. Hence the equation (4.1.1) can be written as

$$y(y-1) = \sum_{i=1}^{a} d_i + (y-a)d_{a+1}. \tag{4.1.2}$$

Note that if y is an integer then $y = a$. Hence in (4.1.2) the term $(y-a)d_a = (y-a)d_{a+1} = 0$. Therefore

$$y^2 - y(1 + d_{a+1}) - \sum_{i=1}^{a}(d_i - d_{a+1}) = 0.$$

The result follows by directly solving the above quadratic equation. □

4.2 Upper bounds for the spectral radius $q(G)$ of signless Laplace matrix of G

Let $q(G)$ denote the spectral radius of the signless Laplace matrix of G. In this section we investigate graph and line graph degree-based bounds for $q(G)$ and then compare them experimentally.

The following well-known Lemma (see, for example, Lemma 2.1 in [11]) provides an equality between the spectral radii of the signless Laplace matrix and the adjacency matrix of the line graph of a graph.

Lemma 4.2.1. *If G^ℓ denotes the line graph of G then*

$$q(G) = 2 + \rho(G^\ell).$$

Let $\Delta_{ij} = d_i + d_j - 2$ for each pair of adjacent vertices $i \sim j$ in G be the vertex degrees of G^ℓ, and $\Delta_1 \geq \Delta_2 \geq \ldots \geq \Delta_e$ be a renumbering of them in non-increasing order. Cvetković *et al.* proved the following theorem using Lemma 4.2.1 and Theorem 2.3.2.

Theorem 4.2.2. *(Theorem 4.7 in [17]) Let G be a simple connected graph. Then*

$$q(G) \leq 2 + \Delta_1$$

with equality if and only if G is regular or biregular.

The following lemma is proved in various ways in [40, 18, 34].

Lemma 4.2.3. *Let G be a simple connected graph. Then*

$$\rho(G) \leq \frac{d_2 - 1 + \sqrt{(d_2-1)^2 + 4d_1}}{2}$$

with equality if and only if G is regular or $n - 1 = d_1 > d_2 = d_n$.

Chen *et al.* combined Lemma 4.2.1 and Lemma 4.2.3 to prove the following result.

Theorem 4.2.4. *(Theorem 3.4 in [14]) Let G be a simple connected graph. Then*

$$q(G) \leq 2 + \frac{\Delta_2 - 1 + \sqrt{(\Delta_2-1)^2 + 4\Delta_1}}{2}$$

with equality if and only if G is regular, or biregular, or the tree obtained by joining an edge to the centers of two stars $K_{1,\frac{n}{2}-1}$ with even n, or $n-1 = d_1 = d_2 > d_3 = d_n = 2$.

Recall Theorem 3.2.1 as a lemma.

Lemma 4.2.5. *Let ℓ be a positive integer with $1 \leq \ell \leq n$. Then*

$$\rho(G) \leq \phi_\ell := \frac{d_\ell - 1 + \sqrt{(d_\ell+1)^2 + 4\sum_{i=1}^{\ell-1}(d_i - d_\ell)}}{2}.$$

Furthermore, if G is connected then the above equality holds if and only if G is regular or there exists $2 \leq t \leq \ell$ such that $n-1 = d_1 = d_{t-1} > d_t = d_n$.

Combining Lemma 4.2.1 and Lemma 4.2.5 provides the following series of upper bounds for the signless Laplacian spectral radius.

Theorem 4.2.6. *Let ℓ be a positive integer with $1 \leq \ell \leq e$. Then*

$$q(G) \leq \psi_\ell := 2 + \frac{\Delta_\ell - 1 + \sqrt{(\Delta_\ell+1)^2 + 4\sum_{i=1}^{\ell-1}(\Delta_i - \Delta_\ell)}}{2}. \tag{4.2.1}$$

Furthermore, if G is connected then the above equality holds if and only if $\Delta_1 = \Delta_e$ or there exists $2 \leq t \leq \ell$ such that $e - 1 = \Delta_1 = \Delta_{t-1} > \Delta_t = \Delta_e$.

Proof. Since G is simple, G^ℓ is simple. Hence it is a direct result of Lemma 4.2.1 and Lemma 4.2.5. □

Remark 4.2.7. Note that Theorem 4.2.6 generalizes both Theorem 4.2.2 and Theorem 4.2.4 since those bounds are precisely ψ_1 and ψ_2 in (4.2.1) respectively.

We list all the extremal graphs with equalities in (4.2.1) in the following. From Theorem 4.2.2 the graphs with $q(G) = \psi_1$, i.e. $\Delta_1 = \Delta_e$, are regular or biregular.

From Theorem 4.2.4 the graphs with $q(G) < \psi_1$ and $q(G) = \psi_2$, i.e. $e - 1 = \Delta_1 > \Delta_2 = \Delta_e$, are the tree obtained by joining an edge to the centers of two stars $K_{1,\frac{n}{2}-1}$ with even n (where Figure 4.1 is an example of such graph with $n = 6$), or $n - 1 = d_1 = d_2 > d_3 = d_n = 2$.

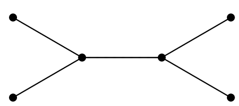


Figure 4.1: The tree obtained by joining an edge to the centers of two stars $K_{1,2}$.

The only graph with $q(G) < \min\{\psi_i | i = 1, 2\}$ and $q(G) = \psi_3$, i.e. $m - 1 = \Delta_1 = \Delta_2 > \Delta_3 = \Delta_e$, is the 4-vertex graph $K_{1,3}^+$ obtained by adding one edge to $K_{1,3}$.

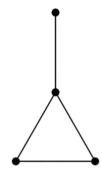


Figure 4.2: The graph $K_{1,3}^+$.

We now prove that no graph satisfies $q(G) < \min\{\psi_i | 1 \leq i < k-1\}$ and $q(G) = \psi_k$ where $e \geq k \geq 4$. Let G be a counter-example such that $e-1 = \Delta_1 = \Delta_{k-1} > \Delta_k = \Delta_e$. Since $\Delta_3 = e - 1$ there are at least 3 edges incident to all other edges in G. If these 3 edges form a 3-cycle then there is nowhere to place the fourth edge, which is a contradiction. Hence they are incident to a common vertex, and G has to be a star graph. However a star graph is biregular so $q(G) = \psi_1$, which completes the proof.

Nikiforov [37] has recently strengthened various upper bounds for $q(G)$ with the following theorem.

Theorem 4.2.8. *If G is a graph with n vertices, e edges, maximum degree d_1 and minimum degree d_n, then*

$$q(G) \leq \min\left(2d_1, \frac{1}{2}\left(d_1 + 2d_n - 1 + \sqrt{(d_1 + 2d_n - 1)^2 + 16e - 8(n - 1 + d_1)d_n}\right)\right).$$

Equality holds if and only if G is regular or G has a component of order $d_1 + 1$ in which every vertex is of degree d_1 or d_n, and all other components are d_n-regular.

It is straightforward to compare the above bounds experimentally using the named graphs and LineGraph function in Wolfram Mathematica. Theorem 4.2.8 is exact for some graphs (eg. Wheels W_n for $n \geq 5$) for which Theorems 4.2.4 and 4.2.6 are inexact, and Theorems 4.2.4 and 4.2.6 are exact for some graphs (eg. complete bipartite graphs $K_{p,q}$ with $2 \leq \min(p, q)$) for which Theorem 4.2.8 is inexact. Tabulated below are the numbers of named irregular graphs on 10, 16, 25 and 28 vertices in Mathematica and the average values of q and the bounds in Theorems 4.2.8, 4.2.4 and 4.2.6.

n	irrregular graphs	$q(G)$	Theorem 4.2.8	Theorem 4.2.4	Theorem 4.2.6
10	59	9.3	10.0	10.3	9.8
16	48	10.3	11.2	11.5	11.0
25	25	11.5	13.4	13.1	12.6
28	21	11.2	12.6	12.7	12.2

Theorem 4.2.4 gives results that are broadly equal on average to Theorem 4.2.8, and Theorem 4.2.6 gives results which are on average modestly better. This is unsurprising since more data is involved in Theorem 4.2.6 than in the other two theorems.

4.3 A lower bound for $q(G)$

Elphick and Wocjan [21] defined a measure of graph irregularity, $\nu = \nu(G)$, as follows:

$$\nu = \frac{n \sum d_i^2}{4e^2},$$

where $\nu \geq 1$ with equality only for regular graphs.

It is well known that $q(G) \geq 2\rho(G)$ and Hofmeister [28] has proved that $\rho(G)^2 \geq (\sum d_i^2)/n$, so it is immediate that

$$q(G) \geq 2\rho(G) \geq \frac{4e\sqrt{\nu}}{n}.$$

Liu and Liu [33] improved this bound in the following theorem, for which we provide a simpler proof using Lemma 4.2.1.

Theorem 4.3.1. *Let G be a graph with irregularity ν and signless Laplace spectral radius $q(G)$. Then*

$$q(G) \geq \frac{4e\nu}{n}.$$

This is exact for complete bipartite graphs.

Proof. Let G^ℓ denote the line graph of G. From Lemma 4.2.1 we know that $q(G) = 2 + \rho(G^\ell)$ and it is well known that $|V(G^\ell)| = e$ and $|E(G^\ell)| = (\sum d_i^2/2) - e$. Therefore

$$q(G) = 2 + \rho(G^\ell) \geq 2 + \frac{2|E(G^\ell)|}{|V(G^\ell)|} = 2 + \frac{2}{e}\left(\frac{\sum d_i^2}{2} - e\right) = \frac{\sum d_i^2}{e} = \frac{4e\nu}{n}.$$

For the complete bipartite graph $K_{s,t}$,

$$q(G) = s + t = \frac{st(s+t)}{st} = \frac{\sum d_i^2}{e} = \frac{4e\nu}{n}.$$

□

4.4 Lower bounds for the clique number

Turán's Theorem [42], proved in 1941, is a seminal result in extremal graph theory. In its concise form it states that

$$\frac{n}{n-d} \leq \omega(G)$$

where d is the average vertex degree.

Edwards and Elphick [19] proved the following lower bound for the clique number.

Theorem 4.4.1. *Let G be a simple graph of n vertices. Then*

$$\frac{n}{n - y(G) + 1} < \omega(G) + \frac{1}{3},$$

where $y(G)$ is defined in (4.1.1).

In 1986, Wilf [45] proved that

$$\frac{n}{n - \rho(G)} \leq \omega(G).$$

Note, however, that

$$\frac{n}{n - y(G) + 1} \nleq \omega(G),$$

since for example $\frac{n}{n-y+1} = 2.13$ for $K_{7,9}$, and $\frac{n}{n-y+1} = 3.1$ for $K_{3,3,4}$.

Nikiforov [36] proved a conjecture due to Edwards and Elphick [19] that:

Theorem 4.4.2. *Let G be a simple graph with e edges. Then*

$$\frac{2e}{2e - \rho(G)^2} \leq \omega(G).$$

Experimentally, bound in Theorem 4.4.2 performs better than bound in Theorem 4.4.1 for most graphs.

4.5 Generalized r-partite graphs

In a series of papers, Bojilov and others have generalized the concept of an r-partite graph. They define a parameter, say $\theta(G)$, to be the smallest integer r for which $V(G)$ has an r-partition:

$$V(G) = V_1 \cup V_2 \cup ... \cup V_r, \text{ such that } d(v) \leq n - n_i, \text{ where } n_i = |V_i|,$$

for all $v \in V_i$ and for $i = 1, 2, ..., r$.

Note that $\theta(G) \leq \omega(G)$ in [6], and Khadzhiivanov and Nenov [32] proved that

$$\frac{n}{n-d} \leq \theta(G).$$

Despite this bound, Elphick and Wocjan [21] demonstrated that

$$\frac{n}{n-\rho(G)} \nleq \theta(G),$$

i.e., $n/(n-\rho(G)) > \theta(G)$ in some graphs.

However, it is proved below in Corollary 4.5.5 that:

$$\frac{n}{n-\rho(G)} \leq \frac{n}{n-y(G)+1} < \theta(G) + \frac{1}{3}.$$

Definition 4.5.1. If H is any graph of order n with degree sequence $d_H(1) \geq d_H(2) \geq ... \geq d_H(n)$, and if H^* is any graph of order n with degree sequence $d_{H^*}(1) \geq d_{H^*}(2) \geq ... \geq d_{H^*}(n)$, such that $d_H(i) \leq d_{H^*}(i)$ for all i, then H^* is said to *dominate* H.

Erdös [22] proved that if G is any graph of order n, then there exists a graph G^* of order n, where $\chi(G^*) = \omega(G) = r$, such that G^* dominates G and G^* is complete r-partite.

Theorem 4.5.2. *If G is any graph of order n, then there exists a graph G^* of order n, where $\omega(G^*) = \theta(G) = r$, such that G^* dominates G, and G^* is complete r-partite.*

Proof. Let G be a generalized r-partite graph with $\theta(G) = r$ and $n_i = |V_i|$ for $1 \leq i \leq r$, and let G^* be the complete r-partite graph $K_{n_1,...,n_r}$. Let $d(v)$ denote the degree of vertex v in G and $d^*(v)$ denote the degree of vertex v in G^*. Clearly $\chi(G^*) = \omega(G^*) = r$, and by the definition of a generalized r-partite graph,

$$d^*(v) = n - n_i \geq d(v)$$

for all $v \in V_i$ and for $1 \leq i \leq r$. Therefore G^* dominates G. $\square$

Recall that $y(G)$ is defined in Theorem 4.1.1.

Lemma 4.5.3. *(Lemma 4 in [19]) Assume G^* dominates G. Then $y(G^*) \geq y(G)$.*

Theorem 4.5.4. *Let G be a simple graph of n vertices. Then*

$$\frac{n}{n - y(G) + 1} < \theta(G) + \frac{1}{3}.$$

Proof. Let G^* be any graph of order n, where $\omega(G^*) = \theta(G)$ such that G^* dominates G. (By Theorem 4.5.2 at least one such graph G^* exists.) Then, using Lemma 4.5.3 and Theorem 4.4.1,

$$\frac{n}{n - y(G) + 1} \leq \frac{n}{n - y(G^*) + 1} < \omega(G^*) + \frac{1}{3} = \theta(G) + \frac{1}{3} \leq \omega(G) + \frac{1}{3}.$$

$\square$

Corollary 4.5.5. *Let G be a simple graph of n vertices. Then*

$$\frac{n}{n - \rho(G)} < \theta(G) + \frac{1}{3}.$$

Proof. Immediate since $\rho(G) \leq y(G) - 1$. $\square$

Chapter 5

Spectral Radius of Bipartite Graphs

Brualdi and Hoffman proposed the problem of finding the maximum spectral radius of a graph with precisely e edges in 1976 [3, p.438], and ten years later they gave a conjecture in [9] that the maximum spectral radius of a graph with e edges is attained by taking a complete graph and adding a new vertex which is adjacent to a corresponding number of vertices in the complete graph. This conjecture was proved by Peter Rowlinson in [38]. See [41, 24] also for the proof of partial cases of this conjecture.

The next problem is then to determine graphs with maximum spectral radius in the class of connected graphs with n vertices and e edges. The cases $e \leq n+5$ when n is sufficiently large are settled by Brualdi and Solheid [10], and the cases $e-n = \binom{r}{2}-1$ by F. K. Bell [1].

The bipartite graphs analogue of the Brualdi-Hoffman conjecture was settled by A. Bhattacharya, S. Friedland, and U.N. Peled [4] with the following statement: For a connected bipartite graph G, $\rho(G) \leq \sqrt{e}$ with equality iff G is a complete bipartite graph. Moreover, they proposed the problem to determine graphs with maximum spectral radius in the class of bipartite graphs with bipartition orders p and q, and e edges. They then gave Conjecture 5.1.1 below.

5.1 Conjectures B and C

From now on the graphs considered are simple bipartite. Let $\mathcal{K}(p,q,e)$ denote the family of e-edge bipartite graphs with bipartition orders p and q.

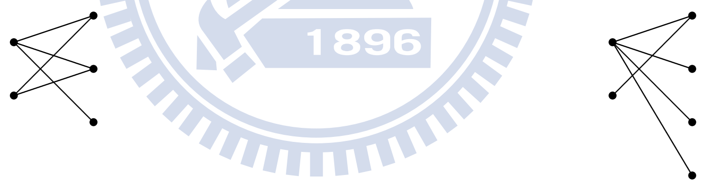
Conjecture 5.1.1. *Let p, q, e be positive integers with $1 < e < pq$. An extremal graph that solves*

$$\max_{G \in \mathcal{K}(p,q,e)} \rho(G)$$

is obtained from a complete bipartite graph by adding one vertex and a corresponding number of edges.

Moreover, in [4, Theorem 8.1] Conjecture 5.1.1 was proved in the case that $e = st - 1$ for some positive integers s, t satisfying $2 \leq s \leq p < t \leq q \leq t + (t-1)/(s-1)$. They also indicated that the only extremal graph is obtained from $K_{s,t}$ by deleting an edge.

Conjecture 5.1.1 does not indicate into which partite set of a complete bipartite graph the adding vertex goes. For $e \geq pq - \max(p, q)$ (resp. $e \geq pq - \min(p, q)$), let ${}^{e}K_{p,q}$ (resp. $K^{e}_{p,q}$) denote the graph which is obtained from $K_{p,q}$ by deleting $pq - e$ edges incident on a common vertex which belongs to the partite set of order no larger than (resp. no less than) that of the other partite set. Then the extremal graph in Conjecture 5.1.1 is either ${}^{e}K_{s,t}$ or $K^{e}_{s,t}$ for some positive integers $s \leq p$ and $t \leq q$ which meet the constraints of the number of edges. Figure 5.1 gives two such graphs.



$K^{5}_{2,3} = {}^{5}K_{2,3}$ ${}^{5}K_{2,4}$

Figure 5.1: The graphs $K^{5}_{2,3}$, ${}^{5}K_{2,3}$ and ${}^{5}K_{2,4}$.

In 2010 [12], Yi-Fan Chen, Hung-Lin Fu, In-Jae Kim, Eryn Stehr and Brendon Watts determined $\rho(K^{e}_{p,q})$ and gave an affirmative answer to Conjecture 5.1.1 when $e = pq - 2$ and $\min(p, q) \geq 2$. Furthermore, they refined Conjecture 5.1.1 for the case when the number of edges is at least $pq - \min(p, q) + 1$ to the following conjecture.

Conjecture 5.1.2. *Let p, q, e be positive integers with $0 < pq - e < \min(p, q)$. Then for $G \in \mathcal{K}(p, q, e)$,*

$$\rho(G) \leq \rho(K^{e}_{p,q}).$$

This chapter is organized as follows. Known results that we need are provided in Section 5.2. Theorem 5.3.3 in Section 5.3 presents a series of sharp upper bounds of $\rho(G)$ in terms of the degree sequence of G. Some special cases of Theorem 5.3.3 are further investigated in Section 5.4 with which Corollary 5.4.2 is the most useful in this paper. We prove Conjecture 5.1.2 as an application of Corollary 5.4.2 in Section 5.5. Finally we propose another conjecture which is a general refinement of Conjecture 5.1.1 in Section 5.6.

5.2 Known results

Basic results are provided in this section for later use.

Lemma 5.2.1. *([4, Proposition 2.1]) Let G be a simple bipartite graph with e edges. Then*

$$\rho(G) \leq \sqrt{e}$$

with equality iff G is a disjoint union of a complete bipartite graph and isolated vertices.

Let G be a simple bipartite graph with bipartition orders p and q, and degree sequences $d_1 \geq d_2 \geq \cdots \geq d_p$ and $d'_1 \geq d'_2 \geq \cdots \geq d'_q$ respectively. We say that G is *biregular* if $d_1 = d_p$ and $d'_1 = d'_q$.

Lemma 5.2.2. *([2, Lemma 2.1]) Let G be a simple connected bipartite graph. Then*

$$\rho(G) \leq \sqrt{d_1 d'_1}$$

with equality iff G is biregular.

5.3 A series of sharp upper bounds $\phi_{s,t}$ of $\rho(G)$

We give a series of sharp upper bounds of $\rho(G)$ in terms of the degree sequence of a bipartite graph G in this section. The following set-up is for the description of extremal graphs of our upper bounds.

Definition 5.3.1. Let H, H' be two bipartite graphs with given ordered bipartitions $V(H) = X \cup Y$ and $V(H') = X' \cup Y'$, where $V(H) \cap V(H') = \phi$. The *bipartite sum* $H \oplus H'$ of H and H' (with respect to the given ordered bipartitions) is the graph obtained from H and H' by adding an edge between x and y for each pair $(x, y) \in X \times Y' \cup X' \times Y$.

Example 5.3.2. Let $N_{s,t}$ denote the bipartite graph with bipartition orders s, t and without any edges. Then for $p \leq q$ and e meeting the required constraints, ${}^eK_{p,q} = K_{p-1,q-pq+e} \oplus N_{1,pq-e}$ and $K^e_{p,q} = K_{p-pq+e,q-1} \oplus N_{pq-e,1}$.

Theorem 5.3.3. *Let G be a simple bipartite graph with bipartition orders p and q, and corresponding degree sequences $d_1 \geq d_2 \geq \cdots \geq d_p$ and $d'_1 \geq d'_2 \geq \cdots \geq d'_q$. For $1 \leq s \leq p$ and $1 \leq t \leq q$, let $X_{s,t} = d_s d'_t + \sum_{i=1}^{s-1}(d_i - d_s) + \sum_{j=1}^{t-1}(d'_j - d'_t)$ and $Y_{s,t} = \sum_{i=1}^{s-1}(d_i - d_s) \cdot \sum_{j=1}^{t-1}(d'_j - d'_t)$. Then*

$$\rho(G) \leq \phi_{s,t} := \sqrt{\frac{X_{s,t} + \sqrt{X^2_{s,t} - 4Y_{s,t}}}{2}}.$$

Furthermore, if G is connected then the above equality holds if and only if there exists nonnegative integers $s' < s$ and $t' < t$, and a biregular graph H of bipartition orders $p - s'$ and $q - t'$ respectively such that $G = K_{s',t'} \oplus H$.

Before proving Theorem 5.3.3, we mention some simple properties of $\phi_{s,t}$.

Lemma 5.3.4. *(i)* $\phi_{1,1} = \sqrt{d_1 d'_1}$.

(ii) If $d_k = d_s$ then $\phi_{k,t} = \phi_{s,t}$. If $d'_\ell = d'_t$ then $\phi_{s,\ell} = \phi_{s,t}$.

(iii)

$$\phi^2_{s,t} \geq \max\left(\sum_{i=1}^{s-1}(d_i - d_s), \sum_{j=1}^{t-1}(d'_j - d'_t)\right) \tag{5.3.1}$$

with equality iff $d_s d'_t = 0$. Moreover, if the equality in (5.3.1) holds then $\phi^2_{s,t} = e$.

(iv) $\phi^4_{s,t} - X_{s,t}\phi^2_{s,t} + Y_{s,t} = 0$.

Proof. (i), (ii), (iv) are immediate from the definition of $\phi_{s,t}$. Clearly $d_s d'_t = 0$ if and only if

$$\max\left(\sum_{i=1}^{s-1}(d_i - d_s), \sum_{j=1}^{t-1}(d'_j - d'_t)\right) = e.$$

Hence (iii) follows by using that $X_{s,t} \geq \sum_{i=1}^{s-1}(d_i - d_s) + \sum_{j=1}^{t-1}(d'_j - d'_t)$ with equality iff $d_s d'_t = 0$ to simplify $\phi_{s,t}$.

□

We set up notations for the use in the proof of Theorem 5.3.3. For $1 \leq k \leq s-1$, let

$$x_k = \begin{cases} 1 + \dfrac{d'_t(d_k - d_s)}{\phi^2_{s,t} - \sum_{i=1}^{s-1}(d_i - d_s)}, & \text{if } \phi^2_{s,t} > \sum_{i=1}^{s-1}(d_i - d_s); \\ 1, & \text{if } \phi^2_{s,t} = \sum_{i=1}^{s-1}(d_i - d_s), \end{cases} \tag{5.3.2}$$

and for $1 \leq \ell \leq t-1$ let

$$x'_\ell = \begin{cases} 1 + \dfrac{d_s(d'_\ell - d'_t)}{\phi^2_{s,t} - \sum_{j=1}^{t-1}(d'_j - d'_t)}, & \text{if } \phi^2_{s,t} > \sum_{j=1}^{t-1}(d'_j - d'_t); \\ 1, & \text{if } \phi^2_{s,t} = \sum_{j=1}^{t-1}(d'_j - d'_t). \end{cases} \tag{5.3.3}$$

Note that $x_k, x'_\ell \geq 1$ because of Lemma 5.3.4(iii). The relations between the above parameters are given in the following.

Lemma 5.3.5. *(i) Suppose $\phi^2_{s,t} > \sum_{a=1}^{s-1}(d_a - d_s)$. Then*

$$\frac{1}{x_i}\left(d_i d'_t + \sum_{h=1}^{t-1}(d'_h - d'_t) + \sum_{k=1}^{s-1}(x_k - 1)d_i\right) = \phi^2_{s,t}$$

for $1 \leq i \leq s-1$, and

$$d_s d'_t + \sum_{h=1}^{t-1}(d'_h - d'_t) + \sum_{k=1}^{s-1}(x_k - 1)d_s = \phi^2_{s,t}.$$

(ii) Suppose $\phi^2_{s,t} > \sum_{b=1}^{t-1}(d'_b - d'_t)$. Then

$$\frac{1}{x'_j}\left(d_s d'_j + \sum_{h=1}^{s-1}(d_h - d_s) + \sum_{\ell=1}^{t-1}(x'_\ell - 1)d'_j\right) = \phi^2_{s,t}$$

for $1 \leq j \leq t-1$, and

$$d_s d'_t + \sum_{h=1}^{s-1}(d_h - d_s) + \sum_{\ell=1}^{t-1}(x'_\ell - 1)d'_t = \phi^2_{s,t}.$$

Proof. Referring to (5.3.2) and Lemma 5.3.4(iv),

$$\begin{aligned}
&\frac{1}{x_i}\left(d_i d'_t + \sum_{h=1}^{t-1}(d'_h - d'_t) + \sum_{k=1}^{s-1}(x_k - 1)d_i\right)\\
= \;&\frac{1}{\phi_{s,t}^2 - \sum_{k=1}^{s-1}(d_k - d_s) + d'_t(d_i - d_s)}\\
&\times\left(\phi_{s,t}^2\left(d_i d'_t + \sum_{h=1}^{t-1}(d'_h - d'_t)\right) - \sum_{h=1}^{t-1}(d'_h - d'_t)\sum_{k=1}^{s-1}(d_k - d_s)\right)\\
= \;&\phi_{s,t}^2
\end{aligned}$$

for $1 \le i \le s-1$, and

$$\begin{aligned}
&d_s d'_t + \sum_{h=1}^{t-1}(d'_h - d'_t) + \sum_{k=1}^{s-1}(x_k - 1)d_s\\
= \;&\frac{1}{\phi_{s,t}^2 - \sum_{k=1}^{s-1}(d_k - d_s)}\left(\phi_{s,t}^2\left(d_s d'_t + \sum_{h=1}^{t-1}(d'_h - d'_t)\right) - \sum_{h=1}^{t-1}(d'_h - d'_t)\sum_{k=1}^{s-1}(d_k - d_s)\right)\\
= \;&\phi_{s,t}^2.
\end{aligned}$$

Hence (i) follows. Similarly, referring to (5.3.3) and Lemma 5.3.4(iv) we have (ii). □

Let $U = \{u_i \mid 1 \le i \le p\}$ and $V = \{v_j \mid 1 \le j \le q\}$ be the bipartition of G such that d_i is the degree of u_i for $1 \le i \le p$, d'_j is the degree of v_j for $1 \le j \le q$, $d_1 \ge d_2 \cdots \ge d_p$ and $d'_1 \ge d'_2 \cdots \ge d'_q$. For $1 \le i, j \le p$, let n_{ij} denote the numbers of common neighbors of u_i and u_j, i.e., $n_{ij} = |G(u_i) \cap G(u_j)|$ where $G(u)$ is the set of neighbors of the vertex u in G. Similarly, for $1 \le i, j \le q$ let $n'_{ij} = |G(v_i) \cap G(v_j)|$. Since G is bipartite, the adjacency matrix A and its square A^2 look like the following in block form:

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}, \quad A^2 = \begin{pmatrix} BB^T & 0 \\ 0 & B^T B \end{pmatrix} = \begin{pmatrix} (n_{ij})_{1\le i,j\le p} & 0 \\ 0 & (n'_{ij})_{1\le i,j\le q} \end{pmatrix}. \tag{5.3.4}$$

We have the following properties of n_{ij} and n'_{ij}.

Lemma 5.3.6. *(i) For $1 \le i \le p$ and $1 \le j \le q$, $n_{ii} = d_i$ and $n'_{jj} = d'_j$.*

(ii) For $1 \le i, j \le p$, $n_{ij} \le d_i$ with equality if and only if $G(u_j) \supseteq G(u_i)$.

(iii) For $1 \le i, j \le q$, $n'_{ij} \le d'_i$ with equality if and only if $G(v_j) \supseteq G(v_i)$.

(iv) For $1 \le i \le p$,

$$\sum_{k=1}^{p} n_{ik} = \sum_{j:\ u_i v_j \in E(G)} d'_j \le (d_i - t + 1)d'_t + \sum_{h=1}^{t-1} d'_h.$$

(v) For $1 \le j \le q$,

$$\sum_{k=1}^{q} n'_{jk} = \sum_{i:\ u_i v_j \in E(G)} d_i \le (d'_j - s + 1)d_s + \sum_{h=1}^{s-1} d_h.$$

Proof. (i)-(iii) are immediate from the definition of n_{ij}. Counting the pairs (u_k, v_j) such that $v_j \in G(u_i) \cap G(u_k)$ in two orders (j,k) and (k,j), we have the first equality in (iv). The second inequality of (iv) is clear since d'_j is non-increasing. (v) is similar to (iv). □

The proof of Theorem 5.3.3

Proof. Clearly $\rho(A)^2 = \rho(A^2)$. In the following we will show that $\rho(A^2) \le \phi^2_{s,t}$. Let

$$U = diag(\underbrace{x_1, x_2, \cdots, x_{s-1}, 1, \cdots, 1}_{p}, \underbrace{x'_1, x'_2, \cdots, x'_{t-1}, 1, \cdots, 1}_{q})$$

be a diagonal matrix of order $p+q$. Let $C = U^{-1}A^2U$. Then A^2 and C are similar and with the same spectrum. Let $r_1, \cdots, r_p, r'_1, \cdots, r'_q$ be the row-sums of C. Referring to (5.3.4), we have

$$\begin{aligned}
r_i &= \sum_{k=1}^{s-1} \frac{x_k}{x_i} n_{ik} + \sum_{k=s}^{p} \frac{1}{x_i} n_{ik} \\
&= \frac{1}{x_i}\sum_{k=1}^{p} n_{ik} + \frac{1}{x_i}\sum_{k=1}^{s-1}(x_k - 1)n_{ik} \quad \text{for} \quad 1 \le i \le s-1; && (5.3.5)\\
r_i &= \sum_{k=1}^{s-1} x_k n_{ik} + \sum_{k=s}^{p} n_{ik} = \sum_{k=1}^{p} n_{ik} + \sum_{k=1}^{s-1}(x_k - 1)n_{ik} \quad \text{for} \quad s \le i \le p; && (5.3.6)\\
r'_j &= \sum_{\ell=1}^{t-1} \frac{x'_\ell}{x'_j} n'_{j\ell} + \sum_{\ell=t}^{q} \frac{1}{x'_j} n'_{j\ell} \\
&= \frac{1}{x'_j}\sum_{\ell=1}^{q} n'_{j\ell} + \frac{1}{x'_j}\sum_{\ell=1}^{t-1}(x'_\ell - 1)n'_{j\ell} \quad \text{for} \quad 1 \le j \le t-1; && (5.3.7)\\
r'_j &= \sum_{\ell=1}^{t-1} x'_\ell n'_{j\ell} + \sum_{\ell=t}^{q} n'_{j\ell} = \sum_{\ell=1}^{q} n'_{j\ell} + \sum_{\ell=1}^{t-1}(x'_\ell - 1)n'_{j\ell} \quad \text{for} \quad t \le j \le q. && (5.3.8)
\end{aligned}$$

If $\phi^2_{s,t} = \sum_{a=1}^{s-1}(d_a - d_s)$ then $x_k = 1$ for $1 \le k \le s-1$ by (5.3.2) and $\phi^2_{s,t} = e$ by Lemma 5.3.4(iii). Hence (5.3.5) and (5.3.6) become

$$r_i = \sum_{k=1}^{p} n_{ik} = \sum_{j:\ u_i v_j \in E(G)} d'_j \le e = \phi^2_{s,t} \tag{5.3.9}$$

for $1 \le i \le p$. Suppose $\phi_{s,t}^2 > \sum_{a=1}^{s-1}(d_a - d_s)$. Referring to (5.3.5) and (5.3.6), for $1 \le i \le s-1$

$$r_i \le \frac{1}{x_i}\left((d_i - t + 1)d'_t + \sum_{h=1}^{t-1} d'_h\right) + \frac{1}{x_i}\sum_{k=1}^{s-1}(x_k - 1)d_i = \phi_{s,t}^2 \tag{5.3.10}$$

and for $s \le i \le p$

$$\begin{aligned} r_i &\le (d_i - t + 1)d'_t + \sum_{h=1}^{t-1} d'_h + \sum_{k=1}^{s-1}(x_k - 1)d_i && (5.3.11)\\ &\le (d_s - t + 1)d'_t + \sum_{h=1}^{t-1} d'_h + \sum_{k=1}^{s-1}(x_k - 1)d_s = \phi_{s,t}^2, && (5.3.12)\end{aligned}$$

where the inequalities are from Lemma 5.3.6(ii)(iv) and the non-increasing of degree sequence, and the equalities are from Lemma 5.3.5(i). Thus, $r_i \le \phi_{s,t}^2$ for $1 \le i \le p$. Similarly, referring to (5.3.7), (5.3.8), Lemma 5.3.6(iii)(v), the non-increasing of degree sequence, and Lemma 5.3.5(ii) we have $r'_j \le \phi_{s,t}^2$ for $1 \le j \le q$. Hence $\rho(A^2) = \rho(C) \le \phi_{s,t}^2$ by Theorem 2.3.2.

To verify the second part of Theorem 5.3.3, assume that G is connected. We prove the sufficient conditions of $\rho(G) = \phi_{s,t}$. If $s' = 0$ and $t' = 0$ then G is biregular. By Lemma 5.2.2 and Lemma 5.3.4(i)(ii), $\rho(G) = \sqrt{d_1 d'_1} = \phi_{s,t}$. Suppose $s' = 0$ and $t' \ge 1$. Then $d_1 = d_p$ and $p = d'_1 = d'_{t'} \ge d'_{t'+1} = d'_q$. We take the equatable quotient matrix E of A with respect to the partition $\{\{1, \dots, p\}, \{p+1, \dots, p+t'\}, \{p+t'+1, \dots, p+q\}\}$. Hence

$$E = \begin{pmatrix} 0 & t' & d_s - t' \\ p & 0 & 0 \\ d'_t & 0 & 0 \end{pmatrix}.$$

The eigenvalues of E are 0 and $\pm\sqrt{d_s d'_t + t'(p - d'_t)} = \pm\phi_{s,t}$. By Lemma 2.4.1, $\phi_{s,t}$ is also an eigenvalue of A. Since $\rho(G) \le \phi_{s,t}$ has been shown in the first part, we have $\rho(G) = \phi_{s,t}$. Similarly for the case $s' \ge 1$ and $t' = 0$. Suppose $s' \ge 1$ and $t' \ge 1$. Then $q = d_1 = d_{s'} \ge d_{s'+1} = d_p$ and $p = d'_1 = d'_{t'} \ge d'_{t'+1} = d'_q$. We take the equatable quotient matrix F of A with respect to the partition $\{\{1, \dots, s'\}, \{s'+1, \dots, p\}, \{p+$

$1, \ldots, p+t'\}, \{p+t'+1, \ldots, p+q\}\}$. Hence

$$F = \begin{pmatrix} 0 & 0 & t' & q-t' \\ 0 & 0 & t' & d_s - t' \\ s' & p-s' & 0 & 0 \\ s' & d'_t - s' & 0 & 0 \end{pmatrix}.$$

Then the eigenvalues of F are

$$\pm\sqrt{\frac{X_{s,t} \pm \sqrt{X_{s,t}^2 - 4Y_{s,t}}}{2}}.$$

We see $\phi_{s,t}$ is an eigenvalue of F, and by Lemma 2.4.1 $\phi_{s,t}$ is also an eigenvalue of A. Hence $\rho(G) = \phi_{s,t}$. Here we complete the proof of the sufficient conditions of $\phi_{s,t} = \rho(G)$.

To prove the necessary conditions of $\rho(G) = \phi_{s,t}$, suppose $\rho(G) = \phi_{s,t}$. Then by Theorem 2.3.2 $r_i = r'_j = \phi_{s,t}^2$ for $1 \le i \le p$ and $1 \le j \le q$. Let $s' < s$ and $t' < t$ be the smallest nonnegative integers such that $d_{s'+1} = d_s$ and $d'_{t'+1} = d'_t$, respectively. We prove either $d_1 = d_p$ or $q = d_1 = d_{s'} > d_{s'+1} = d_p$ in the following. The connectedness of G implies $d_s d'_t > 0$ so that

$$\phi_{s,t}^2 > \max\left(\sum_{i=1}^{s-1}(d_i - d_s), \sum_{j=1}^{t-1}(d'_j - d'_t)\right)$$

by Lemma 5.3.4(iii). Hence the equalities in (5.3.10) to (5.3.12) all hold. The choose of s' and the equalities in (5.3.12) imply that $d_{s'+1} = d_s = d_p$. If $s' = 0$ then $d_1 = d_p$. Suppose $s' \ge 1$. For $1 \le i \le s'$, since $d_i > d_s$ and $\phi_{s,t}^2 > \sum_{a=1}^{s-1}(d_a - d_s)$, we have $x_i > 1$ by (5.3.2). The equalities in (5.3.10) imply $n_{ik} = d_i$ and then $G(u_k) \supseteq G(u_i)$ by Lemma 5.3.6(ii) for $1 \le k \le s'$ and $1 \le i \le s-1$. Similarly the equalities in (5.3.11) imply $G(u_k) \supseteq G(u_i)$ for $1 \le k \le s'$ and $s \le i \le p$ by Lemma 5.3.6(ii). That is,

$$G(u_1) = G(u_2) = \cdots = G(u_{s'}) \supseteq G(u_i) \quad \text{for} \quad s'+1 \le i \le p.$$

Due to the connectedness of G, $d_1 = d_{s'} = q$. The result follows. Similarly, either $d'_1 = d'_q$ or $p = d'_1 = d'_{t'} > d'_{t'+1} = d'_q$. Clearly that the graphs with those degree sequences are $K_{s',t'} + H$ for some biregular graph H of bipartition orders $p-s'$ and $q-t'$

respectively. Here we complete the proof for the necessary conditions of $\phi_{s,t} = \rho(G)$, and also for Theorem 5.3.3. $\square$

Remark 5.3.7. Other previous results shown by the style of the above proof can be found in [40, 34, 13, 31]. Similar earlier results are referred to [9, 10, 41, 29, 30].

5.4 A few special cases of Theorem D

In this section we study some special cases of $\phi_{s,t}$ in Theorem 5.3.3. We follow the notations in Theorem 3.3. As $\phi_{1,1} = \sqrt{d_1 d'_1}$ in Lemma 5.3.4(i), Theorem 5.3.3 provides another proof of $\rho(G) \leq \sqrt{d_1 d'_1}$ in Lemma 5.2.2. Applying Theorem 5.3.3 and simplifying the formula $\phi_{s,t}$ in cases $(s,t) = (1,q)$ and $(s,t) = (p,1)$, we have the following corollary.

Corollary 5.4.1. *(i)* $\rho(G) \leq \phi_{1,q} = \sqrt{e - (q - d_1)d'_q}$.

(ii) $\rho(G) \leq \phi_{p,1} = \sqrt{e - (p - d'_1)d_p}$.

$\square$

We quickly observe that

$$X_{p,q} = d_p d'_q + (e - pd_p) + (e - qd'_q) = 2e - (pd_p + qd'_q - d_p d'_q) \tag{5.4.1}$$

and

$$Y_{p,q} = (e - pd_p)(e - qd'_q). \tag{5.4.2}$$

Hence we have the following corollary.

Corollary 5.4.2.

$$\rho(G) \leq \sqrt{\frac{2e - (pd_p + qd'_q - d_p d'_q) + \sqrt{(pd_p + qd'_q - d_p d'_q)^2 - 4d_p d'_q(pq - e)}}{2}}.$$

$\square$

By adding an isolated vertex if necessary, we might assume $d_p = 0$ and find $\phi_{p,q} = \sqrt{e}$ from Corollary 5.4.2. Hence Theorem 5.3.3 provides another proof of $\rho(G) \leq \sqrt{e}$ in Lemma 5.2.1.

5.5 Proof of Conjecture C

When e, p, q are fixed, the formula

$$\phi_{p,q}(d_p, d'_q) = \sqrt{\frac{2e - (pd_p + qd'_q - d_pd'_q) + \sqrt{(pd_p + qd'_q - d_pd'_q)^2 - 4d_pd'_q(pq-e)}}{2}} \tag{5.5.1}$$

obtained in Corollary 5.4.2 is a 2-variable function. The following lemma will provide shape of the function $\phi_{p,q}(d_p, d'_q)$.

Lemma 5.5.1. *If* $1 \le d'_q \le p-1$ *and* $qd'_q \le e$ *then*

$$\frac{\partial \phi_{p,q}(d_p, d'_q)}{\partial d_p} < 0.$$

Proof. Referring to (5.5.1), it suffices to show that

$$\begin{aligned}
&\frac{\partial}{\partial d_p}\left(2e - (pd_p + qd'_q - d_pd'_q) + \sqrt{(pd_p + qd'_q - d_pd'_q)^2 - 4d_pd'_q(pq-e)}\right) \\
&= -p + d'_q + \frac{(pd_p + qd'_q - d_pd'_q)(p - d'_q) - 2d'_q(pq-e)}{\sqrt{(pd_p + qd'_q - d_pd'_q)^2 - 4d_pd'_q(pq-e)}}
\end{aligned} \tag{5.5.2}$$

is negative. If $qd'_q = e$ then (5.5.2) has negative value $2(d'_q - p)$. Indeed if the numerator of the fraction in (5.5.2) is not positive then (5.5.2) has negative value. Thus assume that it is positive and $qd'_q < e$. From simple computation to have the fact that

$$\begin{aligned}
&\left((pd_p + qd'_q - d_pd'_q) - 2d'_q \cdot \frac{pq-e}{p-d'_q}\right)^2 - \left((pd_p + qd'_q - d_pd'_q)^2 - 4d_pd'_q(pq-e)\right) \\
= \ &\frac{4d'^2_q(pq-e)}{(p-d'_q)^2} \cdot (qd'_q - e) < 0,
\end{aligned}$$

we find that the fraction in (5.5.2) is strictly less than $p - d'_q$, so the value in (5.5.2) is negative. □

Remark 5.5.2. From Example 5.3.2, if $p \le q$ then the graphs ${}^eK_{p,q} = K_{p-1,q-pq+e} + N_{1,pq-e}$ and $K^e_{p,q} = K_{p-pq+e,q-1} + N_{pq-e,1}$ satisfy the equalities in Theorem 5.3.3. Hence $\rho({}^eK_{p,q}) = \phi_{p,q}(q-pq+e, p-1)$ and $\rho(K^e_{p,q}) = \phi_{p,q}(q-1, p-pq+e)$; the latter is expanded as

$$\rho(K^e_{p,q}) = \sqrt{\frac{e + \sqrt{e^2 - 4(q-1)(p-pq+e)(pq-e)}}{2}} \tag{5.5.3}$$

by (5.5.1).

Lemma 5.5.3. *Suppose* $0 < pq - e < \min(p, q)$, $1 \le d_p \le q-1$, $1 \le d'_q \le p-1$ *and*

$$d_p + d'_q = e - (p-1)(q-1). \tag{5.5.4}$$

Then

$$\phi_{p,q}(d_p, d'_q) \le \rho(K^e_{p,q}).$$

Proof. From symmetry, we assume $p \le q$. Referring to (5.5.1) and (5.5.3), we only need to show that

$$e - (pd_p + qd'_q - d_pd'_q) + \sqrt{(pd_p + qd'_q - d_pd'_q)^2 - 4d_pd'_q(pq-e)} \tag{5.5.5}$$

$$\le \sqrt{e^2 - 4(q-1)(p-pq+e)(pq-e)}. \tag{5.5.6}$$

From (5.5.4), we have

$$e - (pd_p + qd'_q - d_pd'_q) = (p - d'_q - 1)(q - d_p - 1) \ge 0 \tag{5.5.7}$$

and

$$\begin{aligned} d_pd'_q =& \frac{(d_p + d'_q)^2 - [2d_p - (d_p + d'_q)]^2}{4} \\ \ge& \frac{(e-(p-1)(q-1))^2 - [2(q-1) - (e-(p-1)(q-1))]^2}{4} \\ =&(q-1)(p-pq+e). \end{aligned} \tag{5.5.8}$$

Hence the equation (5.5.5) is at most

$$e - (pd_p + qd'_q - d_pd'_q) + \sqrt{(pd_p + qd'_q - d_pd'_q)^2 - 4(q-1)(p-pq+e)(pq-e)}. \tag{5.5.9}$$

Set $a = e - (pd_p + qd'_q - d_pd'_q)$ and $b = 4(q-1)(p-pq+e)(pq-e)$. Note that $a \ge 0$ by (5.5.7) and $b \ge 0$ by the relations between p, q, e. Using the fact that

$$\sqrt{e^2 - b} - \sqrt{(e-a)^2 - b} \ge \sqrt{e^2} - \sqrt{(e-a)^2} = a \tag{5.5.10}$$

from the concave property of the function $y = \sqrt{x}$, we find the value in (5.5.9) is at most that in (5.5.6) and the result follows. □

The proof of Conjecture 5.1.2

Proof. By Theorem 5.3.3, $\rho(G) \le \phi_{p,q}(d_p, d'_q)$. Note that the assumption $0 < pq - e < \min(p, q)$ implies $1 \le d_p \le q - 1$ and $1 \le d'_q \le p - 1$. Let $e_p = e - (p-1)(q-1) - d'_q$. Clearly that $1 \le e_p \le d_p$ and $qd'_q \le e$. By Lemma 5.5.1, $\phi_{p,q}(d_p, d'_q) \le \phi_{p,q}(e_p, d'_q)$. With e_p in the role of d_p in Lemma 5.5.3, we have $\phi_{p,q}(e_p, d'_q) \le \rho(K^e_{p,q})$. This completes the proof. $\square$

5.6 Concluding remark

We give a series of sharp upper bounds for the spectral radius of bipartite graphs in Theorem 5.3.3. One of these upper bounds can be presented only by five variables: the number e of edges, bipartition orders p and q, and the minimal degrees d_p and d'_q in the corresponding partite sets as shown in Corollary 5.4.2. We apply this bound when three variables e, p, q are fixed to prove Conjecture 5.1.2, a refinement of Conjecture 5.1.1 in the assumption that $0 < pq - e < \min(p, q)$. To conclude this paper we propose the following general refinement of Conjecture 5.1.1.

Conjecture 5.6.1. *Let $G \in \mathcal{K}(p, q, e)$. Then*

$$\rho(G) \le \rho(K^e_{s,t})$$

for some positive integers $s \le p$ and $t \le q$ such that $0 \le st - e \le \min(s, t)$.

We believe that the function $\phi_{p,q}(d_p, d'_q)$ in (5.5.1) will still play an important role in solving Conjecture 5.6.1. Two of the key points might be to investigate the shape of the 4-variable function $\phi_{p,q}(d_p, d'_q)$ with variables p, q, d_p, d'_q, and to check that for which sequence s, t, d_s, d'_t such that $s \le p$ and $t \le q$ and $0 \le st - e \le \min(s, t)$, there exists a bipartite graph H with e edges whose spectral radius satisfying $\rho(H) = \phi_{s,t}(d_s, d'_t)$, where s, t are the bipartition orders of H and d_s and d'_t are corresponding minimum degrees.

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