

An Introduction to the Theory of Graph Spectra

DRAGOŠ CVETKOVIĆ, PETER ROWLINSON
and SLOBODAN SIMIĆ

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Preface

This book has been written primarily as an introductory text for graduate students interested in algebraic graph theory and related areas. It is also intended to be of use to mathematicians working in graph theory and combinatorics, to chemists who are interested in quantum chemistry, and in part to physicists, computer scientists and electrical engineers using the theory of graph spectra in their work. The book is almost entirely self-contained; only a little familiarity with graph theory and linear algebra is assumed.

In addition to more recent developments, the book includes an up-to-date treatment of most of the topics covered in *Spectra of Graphs* by D. Cvetković, M. Doob and H. Sachs [CvDSa], where spectral graph theory was characterized as follows:

The theory of graph spectra can, in a way, be considered as an attempt to utilize linear algebra including, in particular, the well-developed theory of matrices, for the purposes of graph theory and its applications. However, that does not mean that the theory of graph spectra can be reduced to the theory of matrices; on the contrary, it has its own characteristic features and specific ways of reasoning fully justifying it to be treated as a theory in its own right.

Spectra of Graphs has been out of print for some years; it first appeared in 1980, with a second edition in 1982 and a Russian edition in 1984. The third English edition appeared in 1995, with new material presented in two Appendices and an additional Bibliography of over 300 items. The original edition summarized almost all results related to the theory of graph spectra published before 1978, with a bibliography of 564 items. A review of results in spectral graph theory which appeared mostly between 1978 and 1984 can be found in *Recent Results in the Theory of Graph Spectra* by D. Cvetković, M. Doob, I. Gutman and A. Torgašev [CvDGT]. This second monograph, published in 1988, contains over 700 further references, reflecting the rapid

growth of interest in graph spectra. Today we are witnessing an explosion of the literature on the topic: there exist several thousand papers in mathematics, chemistry, physics, computer science and other scientific areas that develop or use some parts of the theory of graph spectra. Consequently a truly comprehensive text with a complete bibliography is no longer practicable, and we have concentrated on what we see as the central concepts and the most useful techniques.

The monograph [CvDSa] has been used for many years both as an introductory text book and as a reference book. Since it is no longer available, we decided to write a new book which would nowadays be more suitable for both purposes. In this sense, the book is a replacement for [CvDSa]; but it is not a substitute because *Spectra of Graphs* will continue to serve as a reference for more advanced topics not covered here. The content has been influenced by our previous books from the same publisher, namely *Eigenspaces of Graphs* [CvRS2] and *Spectral Generalizations of Line Graphs: on Graphs with Least Eigenvalue -2* [CvRS7]. Nevertheless, very few sections of the present text are taken from these more specialized sources. For further reading we recommend not only the books mentioned above but also [BroCN], [Big2], [Chu2] and [GoRo].

The spectra considered here are those of the adjacency matrix, the Laplacian, the normalized Laplacian, the signless Laplacian and the Seidel matrix of a finite simple graph. In Chapters 2–6, the emphasis is on the adjacency matrix. In Chapter 1, we introduce the various matrices associated with a graph, together with the notation and terminology used throughout the book. We include proofs of the necessary results in matrix theory usually omitted from a first course on linear algebra, but we assume familiarity with the fundamental concepts of graph theory, and with basic results such as the orthogonal diagonalizability of symmetric matrices with real entries. Chapter 2 is concerned with the effects of constructing new graphs from old, and graph angles are used in place of walk generating functions to provide streamlined proofs of some classical results. Chapter 3 deals with the relations between the spectrum and structure of a graph, while Chapter 4 discusses the extent to which the spectrum can characterize a graph. Chapter 5 explores the relation between structure and just one eigenvalue, a relation made precise by the relatively recent notion of a star complement. Chapter 6 is concerned with spectral techniques used to prove graph-theoretical results which themselves make no reference to eigenvalues. Chapter 7 is devoted to the Laplacian, the normalized Laplacian and the signless Laplacian; here the emphasis is on the Laplacian because the normalized Laplacian is the subject of the monograph *Spectral Graph Theory* by F. R. K. Chung [Chu2], while the theory of the signless

Laplacian is still in its infancy. In Chapter 8 we discuss sundry topics that did not fit readily into earlier sections of the book, and in Chapter 9 we provide a small selection of applications, mostly outwith mathematics.

The tables in the Appendix provide lists of the various spectra, characteristic polynomials and angles of all connected graphs with up to 5 vertices, together with relevant data for connected graphs with 6 vertices, trees with up to 9 vertices, and cubic graphs with up to 12 vertices. We are indebted to M. Lepović for creating the graph catalogues for Tables A1, A3, A4 and A5, and for computing the data. We are grateful to D. Stevanović for the graph diagrams that appear with these tables: they were produced using *Graphviz* (open source graph visualization software developed by AT&T, www.graphviz.org/), in particular, the programs ‘circo’ (Tables A1, A3, A5) and ‘neato’ (Table A4). Table A2 is taken from *Eigenspaces of Graphs*.

Chapters 2, 4 and 9 were drafted by D. Cvetković, Chapters 1, 5 and 6 by P. Rowlinson, and Chapters 3, 7 and 8 by S. Simić. However, each of the authors added contributions to all of the chapters, which were then re-written in an effort to refine the text and unify the material. Hence all three authors are collectively responsible for the book. We have endeavoured to find a style that is concise enough to enable the extensive material to be treated in a book of limited size, yet intuitive enough to make the book readily accessible to the intended readership. The choice of consistent notation was a challenge because of conflicts in the ‘standard’ notation for several of the topics covered; accordingly we hope that readers will understand if their preferred notation has not been used. The proofs of some straightforward results in the text are relegated to the exercises. These appear at the end of the relevant chapter, along with notes which serve as a guide to a bibliography of over 500 selected items.

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1

Introduction

In Section 1.1 we define various types of graph spectra, and in Section 1.2 we introduce graph-theoretic notation and terminology which will be used throughout the book. In Section 1.3 we establish the results from matrix theory that will be required.

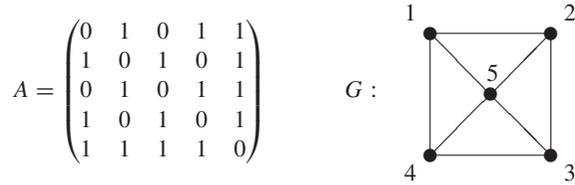
1.1 Graph spectra

Let G be a finite undirected graph without loops or multiple edges, and suppose that its vertices are labelled $1, 2, \dots, n$. If vertices i and j are joined by an edge, we say that i and j are *adjacent* and write $i \sim j$. We consider first the spectrum of the $(0, 1)$ -adjacency matrix A of G defined as follows: $A = A(G) = (a_{ij})$ where

$$a_{ij} = \begin{cases} 1 & \text{if } i \sim j \\ 0 & \text{otherwise.} \end{cases}$$

Thus A is a symmetric matrix with zero diagonal; its entries may be taken as 0 and 1 in any field, but throughout this book the entries are treated as real numbers. An example of a graph and its adjacency matrix is given in Fig. 1.1.

The eigenvalues of A are the n roots of the characteristic polynomial $\det(xI - A)$, and so they are algebraic integers. They are independent of the labelling of the vertices of G because similar matrices have the same characteristic polynomial: if the labels are permuted we obtain a $(0, 1)$ -adjacency matrix $A' = P^{-1}AP$ where P is a permutation matrix. Accordingly we speak of the *characteristic polynomial of G* , denoted by $P_G(x)$, and the *spectrum of G* , which consists of the n *eigenvalues of G* . Since A is a symmetric matrix with real entries, these eigenvalues are real. We usually denote them by $\lambda_1, \lambda_2, \dots, \lambda_n$, and unless we indicate otherwise, we shall assume that

Figure 1.1 A labelled graph G and its adjacency matrix A .

$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Where necessary, we use the notation $\lambda_i = \lambda_i(G)$ ($i = 1, 2, \dots, n$). The largest eigenvalue $\lambda_1(G)$ is called the *index* of G . For an integer $k \geq 0$, the k -th *spectral moment* of G is $\sum_{i=1}^n \lambda_i^k$, denoted by s_k . Note that s_k is the trace of A^k , and that the first n spectral moments determine the spectrum of G .

The eigenvalues of A are the real numbers λ satisfying $A\mathbf{x} = \lambda\mathbf{x}$ for some non-zero vector $\mathbf{x} \in \mathbb{R}^n$. Each such vector \mathbf{x} is called an *eigenvector* of the matrix A (or of the labelled graph G) corresponding to the eigenvalue λ . The relation $A\mathbf{x} = \lambda\mathbf{x}$ can be interpreted in the following way: if $\mathbf{x} = (x_1, x_2, \dots, x_n)^\top$ then

$$\lambda x_u = \sum_{v \sim u} x_v \quad (u = 1, 2, \dots, n), \quad (1.1)$$

where the summation is over all neighbours v of the vertex u . We note two straightforward consequences of these equations, which are called the *eigenvalue equations* for G .

Proposition 1.1.1. *If the graph G has maximum degree $\Delta(G)$ then $|\lambda| \leq \Delta(G)$ for every eigenvalue λ of G .*

Proof. With the notation above, let u be a vertex for which $|x_u|$ is maximal. Using Equation (1.1), we have:

$$|\lambda||x_u| \leq \sum_{v \sim u} |x_v| \leq |\Delta(G)||x_u|.$$

Since $x_u \neq 0$, the result follows. \square

The second observation is left as an exercise for the reader.

Proposition 1.1.2. *The graph G is regular (of degree r) if and only if the all-1 vector is an eigenvector of G (with corresponding eigenvalue r).*

If λ is an eigenvalue of A then the set $\{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} = \lambda\mathbf{x}\}$ is a subspace of \mathbb{R}^n , called the *eigenspace* of λ and denoted by $\mathcal{E}(\lambda)$ or $\mathcal{E}_A(\lambda)$. Such eigenspaces are called *eigenspaces of G* . Of course, relabelling the vertices of

G will result in a permutation of coordinates in eigenvectors (and eigenspaces). Since A is symmetric with real entries, it can be diagonalized by an orthogonal matrix. Hence the eigenspaces are pairwise orthogonal; and by stringing together orthonormal bases of the eigenspaces we obtain an orthonormal basis of \mathbb{R}^n consisting of eigenvectors (cf. Section 1.3). Moreover, the dimension of $\mathcal{E}_A(\lambda)$ is equal to the multiplicity of λ as a root of $P_G(x)$. In other words, the geometric multiplicity of λ is the same as the algebraic multiplicity of λ ; accordingly we refer only to the *multiplicity* of λ . A *simple* eigenvalue is an eigenvalue of multiplicity 1. If G has distinct eigenvalues $\mu_1, \mu_2, \dots, \mu_m$ with multiplicities k_1, k_2, \dots, k_m respectively, we shall write $\mu_1^{k_1}, \mu_2^{k_2}, \dots, \mu_m^{k_m}$ for the spectrum of G . (We often omit those K_i equal to 1.)

Example 1.1.3. For the graph G in Fig. 1.1 we have

$$\begin{aligned} P_G(x) &= \begin{vmatrix} x & -1 & 0 & -1 & -1 \\ -1 & x & -1 & 0 & -1 \\ 0 & -1 & x & -1 & -1 \\ -1 & 0 & -1 & x & -1 \\ -1 & -1 & -1 & -1 & x \end{vmatrix} \\ &= x^5 - 8x^3 - 8x^2 = x^2(x+2)(x^2 - 2x - 4). \end{aligned}$$

The eigenvalues in non-increasing order are $\lambda_1 = 1 + \sqrt{5}$, $\lambda_2 = 0$, $\lambda_3 = 0$, $\lambda_4 = 1 - \sqrt{5}$, $\lambda_5 = -2$, with linearly independent eigenvectors $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4$ and \mathbf{x}_5 , where $\mathbf{x}_1 = (1, 1, 1, 1, -1 + \sqrt{5})^\top$, $\mathbf{x}_2 = (0, 1, 0, -1, 0)^\top$, $\mathbf{x}_3 = (1, 0, -1, 0, 0)^\top$, $\mathbf{x}_4 = (1, 1, 1, 1, -1 - \sqrt{5})^\top$ and $\mathbf{x}_5 = (1, -1, 1, -1, 0)^\top$.

We have $\mathcal{E}(1 + \sqrt{5}) = \langle \mathbf{x}_1 \rangle$, $\mathcal{E}(0) = \langle \mathbf{x}_2, \mathbf{x}_3 \rangle$, $\mathcal{E}(1 - \sqrt{5}) = \langle \mathbf{x}_4 \rangle$ and $\mathcal{E}(-2) = \langle \mathbf{x}_5 \rangle$, where angle brackets denote the subspace spanned by the enclosed vectors. \square

Example 1.1.4. The eigenvalues of an n -cycle are $2\cos\frac{2\pi j}{n}$ ($j = 0, 1, \dots, n-1$). One way to see this is to observe that an adjacency matrix has the form $A = P + P^{-1}$ where P is the permutation matrix determined by a cyclic permutation of length n . If ω is an n -th root of unity then $(1, \omega, \omega^2, \dots, \omega^{n-1})^\top$ is an eigenvector of P with corresponding eigenvalue ω . Hence the eigenvalues of A are the numbers $\omega + \omega^{-1}$, where $\omega^n = 1$. Thus the largest eigenvalue is 2 (with multiplicity 1) and the second largest is $2\cos\frac{2\pi}{n}$ (with multiplicity 2). The least eigenvalue is -2 (with multiplicity 1) if n is even, and $2\cos\frac{(n-1)\pi}{n}$ (with multiplicity 2) if n is odd. \square

Example 1.1.5. The well-known Petersen graph (Fig. 1.2) has spectrum $3^1, 1^5, (-2)^4$. \square

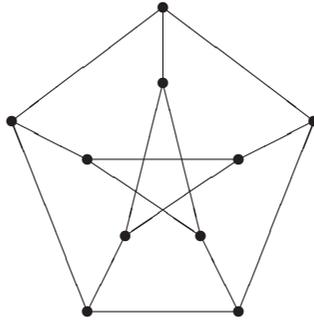


Figure 1.2 The Petersen graph.

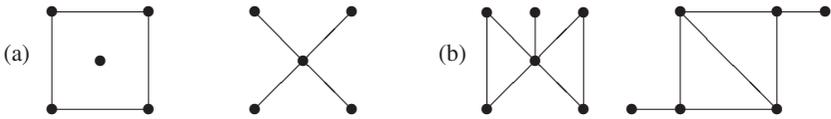


Figure 1.3 Two pairs of non-isomorphic cospectral graphs.

We say that two graphs are *cospectral* if they have the same spectrum; clearly, isomorphic graphs are cospectral (in other words, the spectrum is a graph invariant). However, cospectral graphs are not necessarily isomorphic: the non-isomorphic graphs shown in Fig. 1.3(a) share the spectrum $2^1, 0^3, (-2)^1$. This is an example with fewest vertices. Fig. 1.3(b) shows non-isomorphic cospectral *connected* graphs with fewest vertices: their common characteristic polynomial is $(x-1)(x+1)^2(x^3-x^2-5x+1)$. Various graphs which *are* characterized by their spectrum, or by their spectrum together with related algebraic invariants, are discussed in Chapter 4.

Symmetric matrices other than the $(0, 1)$ -adjacency matrix A can be used to specify a graph, and we mention next the spectra of those that feature in this book. For a graph G with vertex set $\{1, \dots, n\}$, let D be the diagonal matrix $\text{diag}(d_1, \dots, d_n)$, where d_i denotes the degree of vertex i ($i = 1, \dots, n$). The *Laplacian matrix* of a graph G is the matrix $D - A$, and the *signless Laplacian* is the matrix $D + A$; their spectra are discussed in Chapter 7. The *Seidel matrix* of G is the matrix $S = J - I - 2A$, where J denotes the all-1 matrix (of size $n \times n$); thus the (i, j) -entry of S is 0 if $i = j$, -1 if $i \sim j$, and 1 otherwise. As far as regular graphs are concerned, there is little to choose between these matrices from the spectral point of view, for suppose that G is regular of degree r , and that A has eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ in non-increasing order. By Propositions 1.1.1 and 1.1.2, $\lambda_1 = r$ and the all-1 vector may be extended to an orthogonal

basis of \mathbb{R}^n consisting of eigenvectors common to the matrices A , $rI \pm A$ and $J - I - 2A$. Then we find that $D \pm A$ has eigenvalues

$$r \pm r, r \pm \lambda_2, \dots, r \pm \lambda_n,$$

while S has eigenvalues

$$n - 1 - 2r, -1 - 2\lambda_2, \dots, -1 - 2\lambda_n.$$

Similar remarks apply to the generalized adjacency matrix $yJ - A$ discussed in [DamHK]. For non-regular graphs, there is no simple relation between the various spectra; Theorem 1.3.15 will provide some inequalities, but meanwhile we give an explicit example.

Example 1.1.6. For the graph in Fig. 1.1, the eigenvalues of the Laplacian are $5, 5, 3, 3, 0$; the eigenvalues of the signless Laplacian are $\frac{1}{2}(9 + \sqrt{17}), 3, 3, \frac{1}{2}(9 - \sqrt{17}), 1$; and the Seidel eigenvalues are $3, \frac{1}{2}(-1 + \sqrt{17}), -1, -1, \frac{1}{2}(-1 - \sqrt{17})$. \square

The Seidel matrix is of particular relevance to *graph switching* (often called *Seidel switching*): given a subset U of vertices of the graph G , the graph G_U obtained from G by switching with respect to U differs from G as follows. For $u \in U, v \notin U$ the vertices u, v are adjacent in G_U if and only if they are non-adjacent in G . Suppose that G has adjacency matrix $A(G) = \begin{pmatrix} A_U & B^\top \\ B & C \end{pmatrix}$, where A_U is the adjacency matrix of the subgraph induced by U , and B^\top denotes the transpose of B . Then G_U has adjacency matrix $A(G_U) = \begin{pmatrix} A_U & \bar{B}^\top \\ \bar{B} & C \end{pmatrix}$, where \bar{B} is obtained from B by interchanging 0 and 1. When G is regular, this formulation makes it straightforward (Exercise 1.3) to find a necessary and sufficient condition on U for G_U to be regular of the same degree:

Proposition 1.1.7. *Suppose that G is regular with n vertices and degree r . Then G_U is regular of degree r if and only if U induces a regular subgraph of degree k , where $|U| = n - 2(r - k)$.*

Note that switching with respect to the subset U of the vertex-set is the same as switching with respect to its complement. Switching is described easily in terms of the Seidel matrix S of G : the Seidel matrix of G_U is $T^{-1}ST$ where T is the (involutory) diagonal matrix whose i -th diagonal entry is 1 if $i \in U$, -1 if $i \notin U$. Now it is easy to see that switching with respect to U and then with respect to V is the same as switching with respect to $(U \setminus V) \dot{\cup} (V \setminus U)$; it follows that switching determines an equivalence relation on graphs. Note that

switching-equivalent graphs have similar Seidel matrices and hence the same Seidel spectrum. In view of the relation between spectrum and Seidel spectrum for regular graphs, we have the following consequence:

Proposition 1.1.8. *If G and G_U are regular of the same degree, then G and G_U are cospectral.*

1.2 Some more graph-theoretic notions

As usual, K_n , C_n and P_n denote respectively the *complete graph*, the *cycle* and the *path* on n vertices. A connected graph with n vertices is said to be *unicyclic* if it has n edges, for then it contains a unique cycle. If this cycle has odd length, then the graph is said to be *odd-unicyclic*. A connected graph with n vertices and $n + 1$ edges is called a *bicyclic* graph. The *girth* of a graph G is the length of a shortest cycle in G . A complete subgraph of G is called a *clique* of G , while a *coclique* is an induced subgraph without edges. The *complete bipartite* graph with parts of size m and n is denoted by $K_{m,n}$. A graph of the form $K_{1,n}$ is called an *n -claw* or a *star*. (The term ‘star’ is used in different contexts in Sections 3.4 and 5.1.) More generally, K_{n_1, n_2, \dots, n_k} denotes the *complete k -partite graph* with parts (colour classes) of size n_1, n_2, \dots, n_k . The *m -dimensional hypercube* is denoted by Q_m ; its vertices are the 2^m m -tuples of 0s and 1s, and two such m -tuples are adjacent if and only if they differ in just one place.

Vertices, or edges, are said to be *independent* if they are pairwise non-adjacent. In the literature, a set of independent vertices is often referred to as a *stable set*. Any set of independent edges in a graph G is called a *matching* of G . A matching of G is *perfect* if each vertex of G is the endvertex of an edge from the matching; perfect matchings are also called *1-factors*. The *cocktail party graph* $CP(n)$ is the unique regular graph with $2n$ vertices of degree $2n - 2$; it is obtained from K_{2n} by deleting a perfect matching. The degree of a vertex v is denoted by $\deg(v)$ or d_v . The least degree in G is denoted by $\delta(G)$, the largest by $\Delta(G)$. An edge that contains a vertex of degree 1 is called a *pendant edge*.

A regular graph of degree r is said to be *r -regular*, and a 3-regular graph is called a *cubic graph*. A *strongly regular* graph, with parameters (n, r, e, f) , is an r -regular graph with n vertices ($0 < r < n - 1$) such that any two adjacent vertices have e common neighbours and any two non-adjacent vertices have f common neighbours. For example, the Petersen graph (Fig. 1.2) is strongly regular with parameters $(10, 3, 0, 1)$. The restriction $0 < r < n - 1$ simply excludes the complete graphs and their complements.

A graph is called *semi-regular bipartite*, with parameters (n_1, n_2, r_1, r_2) , if it is bipartite (i.e. 2-colourable) and vertices in the same colour class have the same degree (n_1 vertices of degree r_1 and n_2 vertices of degree r_2 , where $n_1 r_1 = n_2 r_2$).

If \mathcal{B} is a collection of subsets of the set S then the *incidence graph* determined by \mathcal{B} and S is the bipartite graph $G_{\mathcal{B}}$ with vertex set $\mathcal{B} \dot{\cup} S$, and with an edge between $x \in S$ and $B \in \mathcal{B}$ whenever $x \in B$. Thus if \mathcal{B} is a design with v points and b blocks, in which each block has k points and each point lies in r blocks, then $G_{\mathcal{B}}$ is a semi-regular bipartite graph with parameters (v, b, r, k) . In this case, we call $G_{\mathcal{B}}$ the graph of the design. Recall that in a t -design with parameters (v, k, λ) , any t points lie in exactly λ blocks; and a *symmetric* design is a 2-design for which $b = v > k$ (equivalently, $r = k < v$).

The *complement* of a graph G is denoted by \overline{G} , while mG denotes the graph consisting of m disjoint copies of G . The *subdivision graph* $S(G)$ is obtained from G by inserting a vertex of degree 2 in each edge of G .

We write $V(G)$ for the vertex set of G , and $E(G)$ for the edge set of G . We say that G is *empty* if $V(G) = \emptyset$, *trivial* if $|V(G)| = 1$, and *null* if $E(G) = \emptyset$. A subgraph H with $V(H) = V(G)$ is called a *spanning* subgraph of G . A spanning cycle is called a *Hamiltonian cycle*, and a graph with such a cycle is said to be *Hamiltonian*.

An *automorphism* of G is a permutation π of $V(G)$ such that $u \sim v$ if and only if $\pi(u) \sim \pi(v)$. Clearly, the automorphisms of G form a group (with respect to composition of functions). We say that G is *vertex-transitive* if, for any $u, v \in V(G)$, there exists an automorphism π of G such that $\pi(u) = v$.

The *union* of disjoint copies of the graphs G and H is denoted by $G \dot{\cup} H$. The *join* $G \nabla H$ of (disjoint) graphs G and H is the graph obtained from $G \dot{\cup} H$ by joining each vertex of G to each vertex of H . The graph $K_1 \nabla H$ is called the *cone* over H , while $K_2 \nabla H (= K_1 \nabla (K_1 \nabla H))$ is called the *double cone* over H . The graph $K_1 \nabla C_n$ ($n \geq 3$) is the *wheel* W_{n+1} with $n + 1$ vertices; thus the graph of Example 1.1.3 is the wheel W_5 .

If uv is an edge of G we write $G - uv$ for the graph obtained from G by deleting uv . More generally, if E is a set of edges of G we write $G - E$ for the graph obtained from G by deleting the edges in E . For $v \in V(G)$, $G - v$ denotes the graph obtained from G by deleting the vertex v and all edges incident with v . For $U \subseteq V(G)$, $G - U$ denotes the subgraph of G induced by $V(G) \setminus U$. If each vertex of $G - U$ is adjacent to a vertex of U then U is called a *dominating set* in G .

If u, v are vertices of a connected graph G then the *distance* between u and v , denoted by $d(u, v)$, is the length of a shortest u - v path in G .

Definition 1.2.1. The line graph $L(H)$ of a graph H is the graph whose vertices are the edges of H , with two vertices in $L(H)$ adjacent whenever the corresponding edges in H have exactly one vertex in common.

If $G = L(H)$ for some graph H , then H is called a *root graph* of G . If $E(H) = \emptyset$ then G is the empty graph. Accordingly, we take a line graph to mean a graph of the form $L(H)$, where $E(H)$ is non-empty; note that we may assume if necessary that H has no isolated vertices. If H is connected, then the same is true of $L(H)$. If H is disconnected, then each non-trivial component of H gives rise to a connected component of $L(H)$.

We mention a simple, but useful, observation (Exercise 1.10):

Proposition 1.2.2. *If H is a connected graph and $L(H)$ is regular, then H is either regular or semi-regular bipartite.*

The *incidence matrix* of the graph H is a matrix B whose rows and columns are indexed by the vertices and edges of H , respectively. The (v, e) -entry of B is

$$b_{ve} = \begin{cases} 0 & \text{if } v \text{ is not incident with } e, \\ 1 & \text{if } v \text{ is incident with } e. \end{cases}$$

Thus the columns of B are the characteristic vectors of the edges of H as subsets of $V(H)$. Now we find easily that

$$B^T B = A(L(H)) + 2I. \quad (1.2)$$

If $A(L(H))\mathbf{x} = \lambda\mathbf{x}$ then $(\lambda + 2)\mathbf{x}^T \mathbf{x} = \mathbf{x}^T B^T B \mathbf{x} \geq 0$. Thus every eigenvalue of $L(H)$ is greater than or equal to -2 ; this is a notable spectral property of line graphs.

The class of graphs with spectrum in the interval $[-2, \infty)$ also contains the *generalized line graphs*, defined as follows. First we say that a *petal* is added to a graph when we add a pendant edge and then duplicate this edge to form a pendant 2-cycle. A *blossom* B_k consists of k petals ($k \geq 0$) attached at a single vertex; thus B_0 is just the trivial graph. A graph with blossoms (possibly empty) at each vertex is called a *B-graph*. Now we extend Definition 1.2.1 to the line graph of a *B-graph* \hat{H} : vertices in $L(\hat{H})$ are adjacent if and only if the corresponding edges in \hat{H} have exactly one vertex in common. In particular, duplicate edges between two vertices of \hat{H} are non-adjacent in $L(\hat{H})$; thus $L(B_k) = CP(k)$. If $G = L(\hat{H})$ then we call the multigraph \hat{H} a *root graph* of G .

Definition 1.2.3. Let H be a graph with vertex set $\{v_1, \dots, v_n\}$, and let a_1, \dots, a_n be non-negative integers. The generalized line graph $G =$

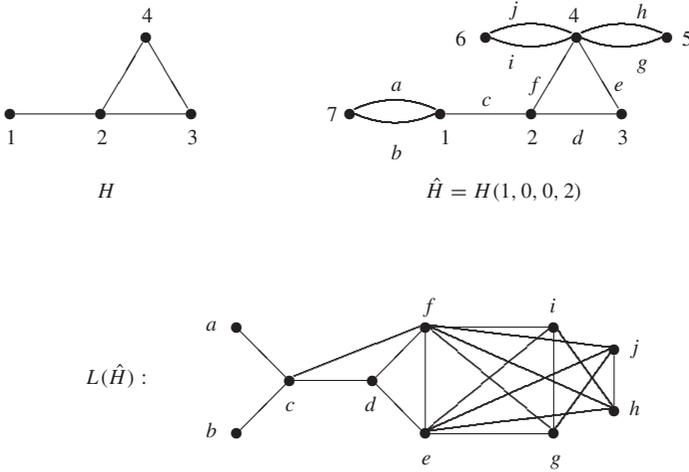


Figure 1.4 Construction of a generalized line graph.

$L(H; a_1, \dots, a_n)$ is the graph $L(\hat{H})$, where \hat{H} is the B -graph $H(a_1, \dots, a_n)$ obtained from H by adding a_i petals at vertex v_i ($i = 1, \dots, n$). If not all a_i are zero, G is called a proper generalized line graph.

This construction of a generalized line graph is illustrated in Fig. 1.4.

An incidence matrix $C = (c_{ve})$ of $\hat{H} = H(a_1, \dots, a_n)$ is defined as for H with the following exception: if e and f are the edges between v and w in a petal at v then $\{c_{ve}, c_{wf}\} = \{-1, 1\}$. (Note that all other entries in row w are zero.) For example, an incidence matrix of the multigraph \hat{H} from Fig. 1.4 is:

$$\begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Here the rows are indexed by $1, 2, \dots, 7$ and the columns are indexed by a, b, \dots, j .

With the incidence matrix C defined above, we have $A(L(\hat{H})) = C^T C - 2I$ and so $\lambda(L(\hat{H})) \geq -2$. Note that the least eigenvalue is strictly greater than -2 if and only if the rank of the matrix C is $|V(\hat{H})|$. Not all connected graphs G with $\lambda(G) \geq -2$ are generalized line graphs; however there are only finitely many exceptions, and they are discussed in Section 3.4.

We conclude this section with several examples to illustrate how various strongly regular graphs can be constructed from line graphs by switching. The relation between the eigenvalues and the parameters of a strongly regular graph will be discussed in Section 3.6. In particular, we shall see that the property of strong regularity can be identified from the spectrum.

Examples 1.2.4. If we switch the graph $L(K_{4,4})$ with respect to four independent vertices, then we obtain another 6-regular graph on 16 vertices, called the *Shrikhande* graph; it is strongly regular with parameters $(16, 6, 2, 2)$. By Proposition 1.1.8, this graph is cospectral with $L(K_{4,4})$. If we switch $L(K_{4,4})$ with respect to the vertices of an induced subgraph $L(K_{4,2})$ then we obtain a 10-regular graph with 16 vertices, called the *Clebsch* graph; it is strongly regular with parameters $(16, 10, 6, 6)$.

These graphs are represented in Fig. 1.5. In Fig. 1.5(a), the vertices of $L(K_{4,4})$ are shown as the points of intersection of four horizontal and four vertical lines, two vertices being adjacent in $L(K_{4,4})$ if and only if the corresponding points are collinear. In Figs. 1.5(b) and 1.5(c), the white vertices are those in switching sets which yield the Shrikhande and Clebsch graphs, respectively. \square

Example 1.2.5. If we switch a graph G with respect to the set of neighbours of a vertex v , we obtain a graph H in which v is an isolated vertex. If $G = L(K_8)$ then $H - v$ is a 16-regular graph on 27 vertices which is called the *Schläfli* graph Sch_{16} ; it is strongly regular with parameters $(27, 16, 10, 8)$. \square

Example 1.2.6. Let S_1, S_2, S_3 be sets of vertices of $L(K_8)$ which induce subgraphs isomorphic to $4K_1, C_5 \dot{\cup} C_3$ and C_8 , respectively. The graphs Ch_1, Ch_2, Ch_3 obtained from $L(K_8)$ by switching with respect to S_1, S_2, S_3 respectively are called the *Chang graphs*. The graphs $L(K_8), Ch_1, Ch_2, Ch_3$ are regular of degree 12, and hence cospectral by Proposition 1.1.8. They are pairwise non-isomorphic, and strongly regular with parameters $(28, 12, 6, 4)$. \square

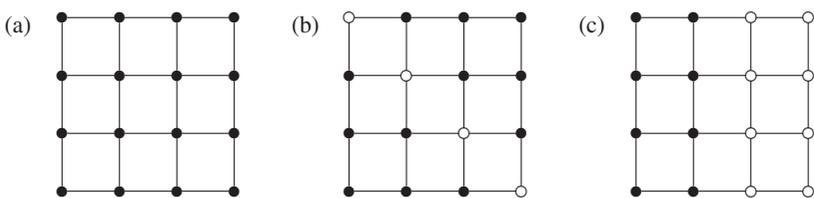


Figure 1.5 Construction of the graphs in Example 1.2.4.

1.3 Some results from linear algebra

First we note that a graph is determined by eigenvalues and corresponding eigenvectors in the following way. Let A be the adjacency matrix of a graph G with vertices $1, 2, \dots, n$ and eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. If $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ are linearly independent eigenvectors of A corresponding to $\lambda_1, \lambda_2, \dots, \lambda_n$ respectively, if $X = (\mathbf{x}_1 | \mathbf{x}_2 | \dots | \mathbf{x}_n)$ and if $E = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$, then $AX = XE$ and so

$$A = XEX^{-1}.$$

Since G is determined by A , we have the following elementary result:

Theorem 1.3.1. *Any graph is determined by its eigenvalues and a basis of corresponding eigenvectors.*

Since A is a symmetric matrix with real entries there exists an orthogonal matrix U such that $U^T A U = E$. Here the columns of U are eigenvectors which form an orthonormal basis of \mathbb{R}^n . If this basis is constructed by stringing together orthonormal bases of the eigenspaces of A then $E = \mu_1 E_1 + \dots + \mu_m E_m$, where μ_1, \dots, μ_m are the distinct eigenvalues of A and each E_i has block diagonal form $\text{diag}(O, \dots, O, I, O, \dots, O)$ ($i = 1, \dots, m$). Then A has the *spectral decomposition*

$$A = \mu_1 P_1 + \dots + \mu_m P_m \quad (1.3)$$

where $P_i = U E_i U^T$ ($i = 1, \dots, m$). For fixed i , if $\mathcal{E}(\mu_i)$ has $\{\mathbf{x}_1, \dots, \mathbf{x}_d\}$ as an orthonormal basis then

$$P_i = \mathbf{x}_1 \mathbf{x}_1^T + \dots + \mathbf{x}_d \mathbf{x}_d^T \quad (1.4)$$

and P_i represents the orthogonal projection of \mathbb{R}^n onto $\mathcal{E}(\mu_i)$ with respect to the standard orthonormal basis $\{\mathbf{e}_1, \dots, \mathbf{e}_n\}$ of \mathbb{R}^n . Moreover, $\sum_{i=1}^m P_i = I$, $P_i^2 = P_i = P_i^T$ ($i = 1, \dots, m$) and $P_i P_j = O$ ($i \neq j$). We shall also need the observation that for any polynomial f , we have

$$f(A) = f(\mu_1) P_1 + \dots + f(\mu_m) P_m.$$

In particular, P_i is a polynomial in A for each i ; explicitly, $P_i = f_i(A)$ where

$$f_i(x) = \frac{\prod_{s \neq i} (x - \mu_s)}{\prod_{s \neq i} (\mu_i - \mu_s)}. \quad (1.5)$$

Next we mention an eigenvector technique which is often employed to find the graphs with maximal or minimal index in a given class of graphs. A *Rayleigh quotient* for A is a scalar of the form $\mathbf{y}^T A \mathbf{y} / \mathbf{y}^T \mathbf{y}$ where \mathbf{y} is a

non-zero vector in \mathbb{R}^n . The supremum of the set of such scalars is the largest eigenvalue λ_1 of A , equivalently

$$\lambda_1 = \sup\{\mathbf{x}^\top A \mathbf{x} : \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\| = 1\}. \quad (1.6)$$

This well-known fact follows immediately from the observation that if $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is an orthonormal basis of eigenvectors of A and if $\mathbf{x} = \alpha_1 \mathbf{x}_1 + \dots + \alpha_n \mathbf{x}_n$ then $\alpha_1^2 + \dots + \alpha_n^2 = 1$, while

$$\mathbf{x}^\top A \mathbf{x} = \lambda_1 \alpha_1^2 + \dots + \lambda_n \alpha_n^2, \quad (1.7)$$

where $A \mathbf{x}_i = \lambda_i \mathbf{x}_i$ ($i = 1, \dots, n$).

Note that for $\mathbf{y} \neq \mathbf{0}$, we have $\mathbf{y}^\top A \mathbf{y} / \mathbf{y}^\top \mathbf{y} \leq \lambda_1$, with equality if and only if $A \mathbf{y} = \lambda_1 \mathbf{y}$. More generally, *Rayleigh's Principle* may be stated as follows:

$$\text{if } \mathbf{0} \neq \mathbf{y} \in \langle \mathbf{x}_i, \dots, \mathbf{x}_n \rangle \text{ then } \lambda_i \geq \mathbf{y}^\top A \mathbf{y} / \mathbf{y}^\top \mathbf{y},$$

with equality if and only if $A \mathbf{y} = \lambda_i \mathbf{y}$; and

$$\text{if } \mathbf{0} \neq \mathbf{y} \in \langle \mathbf{x}_1, \dots, \mathbf{x}_i \rangle \text{ then } \lambda_i \leq \mathbf{y}^\top A \mathbf{y} / \mathbf{y}^\top \mathbf{y},$$

with equality if and only if $A \mathbf{y} = \lambda_i \mathbf{y}$.

Moreover, each eigenvalue λ_i ($i = 1, \dots, n$) can be characterized in terms of subspaces of \mathbb{R}^n as follows. Let U be an $(n - i + 1)$ -dimensional subspace of \mathbb{R}^n , so that $\langle \mathbf{x}_1, \dots, \mathbf{x}_i \rangle \cap U \neq \{\mathbf{0}\}$. If \mathbf{x} is a unit vector in this intersection of subspaces then $\alpha_{i+1} = \dots = \alpha_n = 0$ and so $\mathbf{x}^\top A \mathbf{x} \geq \lambda_i$ by (1.7). It follows that $\sup\{\mathbf{x}^\top A \mathbf{x} : \mathbf{x} \in U, \|\mathbf{x}\| = 1\} \geq \lambda_i$. On the other hand, by (1.7) again, this lower bound is attained when $U = \langle \mathbf{x}_i, \dots, \mathbf{x}_n \rangle$ because in this case $\alpha_1 = \dots = \alpha_{i-1} = 0$ for every vector in U . Hence for each $i \in \{1, \dots, n\}$ we have

$$\lambda_i = \inf\{\sup\{\mathbf{x}^\top A \mathbf{x} : \mathbf{x} \in U, \|\mathbf{x}\| = 1\} : U \in \mathcal{U}_{n-i+1}\}, \quad (1.8)$$

where \mathcal{U}_{n-i+1} denotes the set of all $(n - i + 1)$ -dimensional subspaces of \mathbb{R}^n .

An $n \times n$ symmetric matrix M (with real entries) is said to be *positive semi-definite* if all its eigenvalues are non-negative, equivalently $\mathbf{x}^\top M \mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$.

Theorem 1.3.2. *Let M be a positive semi-definite matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Then*

$$\lambda_1 + \lambda_2 + \dots + \lambda_r = \sup\{\mathbf{u}_1^\top M \mathbf{u}_1 + \mathbf{u}_2^\top M \mathbf{u}_2 + \dots + \mathbf{u}_r^\top M \mathbf{u}_r\} \quad (r = 1, 2, \dots, n),$$

where the supremum is taken over all orthonormal vectors $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r$. In particular, $\lambda_1 + \lambda_2 + \dots + \lambda_r$ is bounded below by the sum of the r largest diagonal entries of M .

Proof. Let $M\mathbf{x}_i = \lambda_i\mathbf{x}_i$ ($i = 1, 2, \dots, n$), where $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ are orthonormal. Let $U = (\mathbf{u}_1|\mathbf{u}_2|\dots|\mathbf{u}_r)$, $X = (\mathbf{x}_1|\mathbf{x}_2|\dots|\mathbf{x}_n)$ and $\mathbf{u}_j = \sum_{i=1}^n c_{ij}\mathbf{x}_i$ ($j = 1, 2, \dots, r$). Then $U = XC$, where $C = (c_{ij})$; moreover, $I = U^\top U = C^\top C$. Using Equation (1.7), we have

$$\sum_{j=1}^r \mathbf{u}_j^\top M \mathbf{u}_j = \sum_{j=1}^r \sum_{i=1}^n c_{ij}^2 \lambda_i = \sum_{i=1}^n \left(\sum_{j=1}^r c_{ij}^2 \right) \lambda_i.$$

Note that $\sum_{j=1}^r c_{ij}^2 = b_i$, where b_i is the i -th diagonal entry of CC^\top . Now CC^\top and $C^\top C$ have the same non-zero eigenvalues and so the spectrum of CC^\top is $1^r, 0^{n-r}$. By (1.7) again, $b_i = \mathbf{e}_i^\top CC^\top \mathbf{e}_i \leq 1$ ($i = 1, 2, \dots, n$). Now we have:

$$\sum_{j=1}^r \mathbf{u}_j^\top M \mathbf{u}_j = \sum_{i=1}^n b_i \lambda_i, \quad 0 \leq b_i \leq 1, \quad \sum_{i=1}^n b_i = \text{tr}(CC^\top) = r,$$

and it follows that $\sum_{j=1}^r \mathbf{u}_j^\top M \mathbf{u}_j \leq \sum_{j=1}^r \lambda_j$. Equality holds when $\mathbf{u}_i = \mathbf{x}_i$ ($i = 1, 2, \dots, r$), and so the first statement of the theorem is proved. For the second statement, we may suppose without loss of generality that the r largest diagonal entries of M are the first r diagonal entries; the assertion follows by taking $\mathbf{u}_i = \mathbf{e}_i$ ($i = 1, 2, \dots, r$). \square

If M is a positive semi-definite matrix of rank r then there exists an orthogonal matrix U such that

$$U^\top M U = \begin{pmatrix} \theta_1 & & & & & \\ & \ddots & & & & \\ & & \theta_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix},$$

where $\theta_1 \geq \dots \geq \theta_r > 0$. Now this matrix can be written as $X^\top X$, where

$$X = \begin{pmatrix} \sqrt{\theta_1} & \dots & 0 & 0 & \dots & 0 \\ 0 & \ddots & 0 & 0 & \dots & 0 \\ 0 & \dots & \sqrt{\theta_r} & 0 & \dots & 0 \end{pmatrix},$$

of size $r \times n$. Thus $M = Q^\top Q$, where $Q = XU^\top$. If $Q = (\mathbf{q}_1 | \cdots | \mathbf{q}_n)$ then each column \mathbf{q}_i lies in \mathbb{R}^r , and the (i, j) -entry of M is the scalar product $\mathbf{q}_i^\top \mathbf{q}_j$. The matrix $Q^\top Q$ is called the *Gram matrix* of the vectors $\mathbf{q}_1, \dots, \mathbf{q}_n$. We shall often make use of Gram matrices in the case that $M = A - \lambda I$ and λ is the least eigenvalue of G ; in this situation, the multiplicity of λ is $n - r$.

Since in general a graph is not determined by its eigenvalues, it is natural to seek further algebraic invariants which might serve to distinguish non-isomorphic cospectral graphs. For our first such definition, recall that $\{\mathbf{e}_1, \dots, \mathbf{e}_n\}$ is the standard orthonormal basis of \mathbb{R}^n . The mn numbers $\alpha_{ij} = \|P_i \mathbf{e}_j\|$ are called the *angles* of G ; they are the cosines of the (acute) angles between axes and eigenspaces. We shall assume that $\mu_1 > \cdots > \mu_m$. If also we order the columns of the matrix (α_{ij}) lexicographically then this matrix is a graph invariant, called the *angle matrix* of G . We shall see in the next chapter that the spectrum of the vertex-deleted subgraph $G - j$ is determined by the spectrum of G and the angles $\alpha_{1j}, \dots, \alpha_{mj}$. The basic relations between angles are the following:

Proposition 1.3.3. *The angles α_{ij} of a graph satisfy the equalities*

$$\sum_{j=1}^n \alpha_{ij}^2 = \dim \mathcal{E}(\mu_i), \quad \sum_{i=1}^m \alpha_{ij}^2 = 1. \quad (1.9)$$

Proof. We have $\alpha_{ij}^2 = \|P_i \mathbf{e}_j\|^2 = \mathbf{e}_j^\top P_i \mathbf{e}_j$, and so the numbers $\alpha_{i1}^2, \alpha_{i2}^2, \dots, \alpha_{in}^2$ appear on the diagonal of P_i . Now $\sum_{j=1}^n \alpha_{ij}^2 = \text{tr}(P_i) = \text{tr}(E_i) = \dim \mathcal{E}(\mu_i)$, and $\sum_{i=1}^m \alpha_{ij}^2 = 1$ because $\sum_{i=1}^m P_i = I$. \square

Next we discuss the relation between eigenvalues, angles and walks in a graph. By a *walk of length k* in a graph we mean any sequence of (not necessarily different) vertices v_0, v_1, \dots, v_k such that for each $i = 1, 2, \dots, k$ there is an edge from v_{i-1} to v_i . The walk is *closed* if $v_k = v_0$. The following result has a straightforward proof by induction on k .

Proposition 1.3.4. *If A is the adjacency matrix of a graph, then the (i, j) -entry $a_{ij}^{(k)}$ of the matrix A^k is equal to the number of walks of length k that start at vertex i and end at vertex j .*

It follows from Proposition 1.3.4 that the number of closed walks of length k is equal to the k -th spectral moment, since $\sum_{j=1}^n a_{jj}^{(k)} = \text{tr}(A^k) = \sum_{j=1}^n \lambda_j^k$. From the spectral decomposition of A we have

$$A^k = \mu_1^k P_1 + \mu_2^k P_2 + \cdots + \mu_m^k P_m \quad (1.10)$$

and so $a_{jj}^{(k)} = \sum_{i=1}^m \mu_i^k \alpha_{ij}^2$, where the α_{ij} are the angles of G . In particular, the vertex degrees $a_{jj}^{(2)}$ are determined by the spectrum and angles.

We write \mathbf{j} (or \mathbf{j}_n) for the all-1 vector in \mathbb{R}^n , and \mathbf{j}^\perp for the subspace of vectors orthogonal to \mathbf{j} . It follows from (1.10) that the number N_k of all walks of length k in G is given by

$$N_k = \sum_{u,v} a_{uv}^{(k)} = \mathbf{j}^\top A^k \mathbf{j} = \sum_{i=1}^n \mu_i^k \|P_i \mathbf{j}\|^2, \quad (1.11)$$

The numbers $\beta_i = \|P_i \mathbf{j}\|/\sqrt{n}$ ($i = 1, \dots, m$) are called the *main angles* of G ; they are the cosines of the (acute) angles between eigenspaces and \mathbf{j} . Note that $\sum_{i=1}^m \beta_i^2 = 1$ because $\mathbf{j} = \sum_{i=1}^m P_i \mathbf{j}$. The eigenvalue μ_i is said to be a *main eigenvalue* if $\mathcal{E}(\mu_i) \not\subseteq \mathbf{j}^\perp$, equivalently $P_i \mathbf{j} \neq \mathbf{0}$. In view of (1.11) we have the following result.

Theorem 1.3.5. *The total number N_k of walks of length k in a graph G is given by*

$$N_k = n \sum' \mu_i^k \beta_i^2, \quad (1.12)$$

where the sum \sum' is taken over all main eigenvalues μ_i .

We shall see in Chapter 2 that the spectrum of the complement \overline{G} , the spectrum of the cone $K_1 \nabla G$ and the Seidel spectrum of G are all determined by the spectrum and main angles of G . A means of calculating main angles is described in Section 6.7.

Now we turn to some more general results from matrix theory that have implications for the spectra of graphs.

A symmetric matrix M is *reducible* if there exists a permutation matrix P such that $P^{-1}MP$ is of the form $\begin{pmatrix} X & O \\ O & Y \end{pmatrix}$, where X and Y are square matrices. Otherwise, M is called *irreducible*. If $M = (m_{ij})$, of size $n \times n$, then we define the graph G^M as follows. The vertices of G^M are $1, \dots, n$, and distinct vertices i, j are adjacent if and only if $m_{ij} \neq 0$. Thus G^M is connected if and only if M is irreducible.

Theorem 1.3.6. *Let M be an irreducible symmetric matrix with non-negative entries. Then the largest eigenvalue λ_1 of M is simple, with a corresponding eigenvector whose entries are all positive. Moreover, $|\lambda| \leq \lambda_1$ for all eigenvalues λ of M .*

Proof. Let $\mathbf{x} = (x_1, \dots, x_n)^\top$ be a unit eigenvector corresponding to λ_1 . Let $\mathbf{y} = (y_1, \dots, y_n)^\top$, where $y_i = |x_i|$ ($i = 1, \dots, n$). Then $\mathbf{y}^\top \mathbf{y} = 1$ and $\mathbf{y}^\top M \mathbf{y} \geq \mathbf{x}^\top M \mathbf{x} = \lambda_1$. Hence \mathbf{y} is also an eigenvector corresponding to λ_1 .

We show that no y_i (and hence no x_i) is zero by considering adjacencies in G^M . The eigenvalue equations may be written:

$$\lambda_1 y_i = m_{ii} y_i + \sum_{j \sim i} m_{ij} y_j \quad (i = 1, \dots, n). \quad (1.13)$$

If $y_i = 0$ then by (1.10), $y_j = 0$ for all $j \sim i$. Since G^M is connected, $y_j = 0$ for all j , a contradiction. Now λ_1 is a simple eigenvalue, for if $\dim \mathcal{E}(\lambda_1) > 1$ then there exists an eigenvector with a zero entry in any chosen position. In particular, $\mathcal{E}(\lambda_1)$ is spanned by \mathbf{y} (and $\mathbf{x} = \pm \mathbf{y}$). Finally, if $M\mathbf{z} = \lambda\mathbf{z}$ where $\mathbf{z}^\top \mathbf{z} = 1$ and $\mathbf{z} = (z_1, \dots, z_n)^\top$ then

$$|\lambda| = |\mathbf{z}^\top M\mathbf{z}| = \left| \sum_{i,j} z_i m_{ij} z_j \right| \leq \sum_{i,j} |z_i| m_{ij} |z_j| \leq \lambda_1.$$

□

We say that a vector $\mathbf{x} = (x_1, \dots, x_n)^\top$ is non-negative (positive) if each x_i is non-negative (positive); we write $\mathbf{x} \geq \mathbf{0}$, $\mathbf{x} > \mathbf{0}$ respectively. In the situation of Theorem 1.3.6, M has a unique positive unit eigenvector corresponding to λ_1 , and this is called the *principal* eigenvector of M . In the case that M is the adjacency matrix of a (labelled) connected graph G , we refer to this vector as the *principal eigenvector* of G .

Corollary 1.3.7. *Let M be an irreducible symmetric $n \times n$ matrix with non-negative entries m_{ij} , and let λ_1 be the largest eigenvalue of M . For any positive vector $\mathbf{y} = (y_1, y_2, \dots, y_n)^\top$, we have*

$$\min_{1 \leq i \leq n} \sum_{j=1}^n \frac{m_{ij} y_j}{y_i} \leq \lambda_1 \leq \max_{1 \leq i \leq n} \sum_{j=1}^n \frac{m_{ij} y_j}{y_i}. \quad (1.14)$$

Either equality holds if and only if \mathbf{y} is an eigenvector of M corresponding to λ_1 .

Proof. Let $\mathbf{x} = (x_1, x_2, \dots, x_n)^\top$ be the principal eigenvector of M . Then

$$\lambda_1 \sum_{i=1}^n x_i y_i = \mathbf{y}^\top M\mathbf{x} = \mathbf{x}^\top M\mathbf{y} = \sum_{i=1}^n x_i y_i \left(\frac{\sum_{j=1}^n m_{ij} y_j}{y_i} \right). \quad (1.15)$$

The inequalities follow, since $\sum_{i=1}^n x_i y_i > 0$. Let $z_i = \lambda_1 y_i - \sum_{j=1}^n m_{ij} y_j$ ($i = 1, \dots, n$). If an equality holds in (1.14) then either all z_i are non-negative or all z_i are non-positive. From (1.15), we have $\sum_{i=1}^n x_i z_i = 0$, and so all z_i are zero. In this situation, \mathbf{y} is an eigenvector of M corresponding to λ_1 , as required. □

If we apply Theorem 1.3.6 to the adjacency matrix of a graph, we obtain:

Corollary 1.3.8. *A graph is connected if and only if its index is a simple eigenvalue with a positive eigenvector.*

We can also use Theorem 1.3.6 to prove:

Proposition 1.3.9. *For any vertex u of a connected graph G , we have $\lambda_1(G - u) < \lambda_1(G)$.*

Proof. Let $A = \begin{pmatrix} A' & \mathbf{r} \\ \mathbf{r}^\top & 0 \end{pmatrix}$, where $A' = A(G - u)$, and let \mathbf{x} be a unit eigenvector of A' corresponding to $\lambda_1(G - u)$. If $\mathbf{y} = \begin{pmatrix} \mathbf{x} \\ 0 \end{pmatrix}$ then $\mathbf{y}^\top \mathbf{y} = 1$ and $\lambda_1(G - u) = \mathbf{y}^\top A \mathbf{y} \leq \lambda_1(G)$. If equality holds then \mathbf{y} is an eigenvector of A corresponding to $\lambda_1(G)$; but this is a contradiction because \mathbf{y} has a zero entry. \square

If we apply Corollary 1.3.8 to each component of an arbitrary graph G which has index $\lambda_1(G)$, we can see that there is a non-negative eigenvector corresponding to $\lambda_1(G)$. This vector may also be used in Rayleigh quotients to obtain bounds for the index of modified graphs, as for example in the following:

Proposition 1.3.10. *If $G - uv$ is the graph obtained from a connected graph G by deleting the edge uv , then $\lambda_1(G - uv) < \lambda_1(G)$.*

Proof. Let $\mathbf{x} = (x_1, \dots, x_n)^\top$ be a non-negative unit eigenvector of $G - uv$ corresponding to $\lambda_1(G - uv)$. Then

$$\lambda_1(G - uv) = \mathbf{x}^\top A(G - uv) \mathbf{x} \leq \mathbf{x}^\top A(G) \mathbf{x} \leq \lambda_1(G).$$

If $\lambda_1(G - uv) = \lambda_1(G)$ then \mathbf{x} is the principal eigenvector of G and hence has no zero entries. Now $\mathbf{x}^\top A(G - uv) \mathbf{x} = \mathbf{x}^\top A(G) \mathbf{x} - 2x_u x_v < \lambda_1(G - uv)$, a contradiction. \square

Next we consider interlacing of eigenvalues.

Theorem 1.3.11. *Let Q be a real $n \times m$ matrix such that $Q^\top Q = I$, and let A be an $n \times n$ real symmetric matrix with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. If the eigenvalues of $Q^\top A Q$ are $\mu_1 \geq \dots \geq \mu_m$ then*

$$\lambda_{n-m+i} \leq \mu_i \leq \lambda_i \quad (i = 1, \dots, m). \quad (1.16)$$

Proof. Let $\mathbf{x}_1, \dots, \mathbf{x}_n$ be orthonormal eigenvectors of A , and let $\mathbf{y}_1, \dots, \mathbf{y}_m$ be orthonormal eigenvectors of $Q^\top A Q$, taken in order. For each $i \in \{1, \dots, m\}$, let \mathbf{z}_i be a non-zero vector in the subspace

$$\langle \mathbf{y}_1, \dots, \mathbf{y}_i \rangle \cap \langle Q^\top \mathbf{x}_1, \dots, Q^\top \mathbf{x}_{i-1} \rangle^\perp.$$

Then $Q\mathbf{z}_i \in \langle \mathbf{x}_1, \dots, \mathbf{x}_{i-1} \rangle^\perp$, and so (by Rayleigh's Principle)

$$\lambda_i \geq \frac{(Q\mathbf{z}_i)^\top A(Q\mathbf{z}_i)}{(Q\mathbf{z}_i)^\top (Q\mathbf{z}_i)} = \frac{\mathbf{z}_i^\top Q^\top A Q \mathbf{z}_i}{\mathbf{z}_i^\top \mathbf{z}_i} \geq \mu_i.$$

The second inequality in (1.16) is obtained by applying the above argument to $-A$ and $-Q^\top A Q$. \square

When the inequalities (1.16) are satisfied, we say that the eigenvalues μ_i *interlace* the eigenvalues λ_j .

Corollary 1.3.12. *Let G be a graph with n vertices and eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, and let H be an induced subgraph of G with m vertices. If the eigenvalues of H are $\mu_1 \geq \mu_2 \geq \dots \geq \mu_m$ then $\lambda_{n-m+i} \leq \mu_i \leq \lambda_i$ ($i = 1, \dots, m$).*

Proof. Let $V(G) = \{1, \dots, n\}$ and $V(H) = \{1, \dots, m\}$. Then $A(H) = Q^\top A(G)Q$, where Q^\top has the form $(I \mid O)$, and so the result follows from Theorem 1.3.11. \square

The inequalities in Corollary 1.3.12 are known as *Cauchy's inequalities* and this result is generally known as the *Interlacing Theorem*. It is used frequently as a spectral technique in graph theory. In particular, when H is a vertex-deleted subgraph we have $m = n - 1$ and:

$$\lambda_n \leq \mu_{n-1} \leq \lambda_{n-1} \leq \dots \leq \lambda_2 \leq \mu_1 \leq \lambda_1.$$

The next result is a further consequence of Theorem 1.3.11.

Corollary 1.3.13. *Let A be a real symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Given a partition $\{1, 2, \dots, n\} = \Delta_1 \dot{\cup} \Delta_2 \dot{\cup} \dots \dot{\cup} \Delta_m$ with $|\Delta_i| = n_i > 0$, consider the corresponding blocking $A = (A_{ij})$, where A_{ij} is an $n_i \times n_j$ block. Let e_{ij} be the sum of the entries in A_{ij} and set $B = (e_{ij}/n_i)$ (Note that e_{ij}/n_i is the average row sum in A_{ij} .) Then the eigenvalues of B interlace those of A .*

Proof. Suppose that the vertex-block incidence matrix has columns $\mathbf{c}_1, \dots, \mathbf{c}_m$, and let Q be the matrix with columns $\frac{1}{\sqrt{n_1}}\mathbf{c}_1, \dots, \frac{1}{\sqrt{n_m}}\mathbf{c}_m$. Then $Q^\top Q = I$, $Q^\top A Q = B$ and the result follows from Theorem 1.3.11. \square

If we assume that in each block A_{ij} from Corollary 1.3.13 all row sums are equal then we can say more:

Theorem 1.3.14. *Let A be any matrix partitioned into blocks as in Corollary 1.3.13. Suppose that the block A_{ij} has constant row sums b_{ij} , and*

let $B = (b_{ij})$. Then the spectrum of B is contained in the spectrum of A (taking into account the multiplicities of the eigenvalues).

Proof. It is straightforward to check that if $(x_1, \dots, x_m)^\top$ is an eigenvector of B then $\begin{pmatrix} x_1 \mathbf{j}_{n_1} \\ \vdots \\ x_m \mathbf{j}_{n_m} \end{pmatrix}$ is an eigenvector of A corresponding to the same eigenvalue. \square

Theorem 1.3.12 will be used in Section 3.9 to provide a link between spectral and structural properties of a graph. Next we establish the Courant–Weyl inequalities, embodied in the following result; as usual, the eigenvalues here are in non-increasing order.

Theorem 1.3.15. *Let A and B be $n \times n$ Hermitian matrices. Then*

$$\lambda_i(A + B) \leq \lambda_j(A) + \lambda_{i-j+1}(B) \quad (n \geq i \geq j \geq 1),$$

$$\lambda_i(A + B) \geq \lambda_j(A) + \lambda_{i-j+n}(B) \quad (1 \leq i \leq j \leq n).$$

Proof. Let $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$, $\{\mathbf{y}_1, \dots, \mathbf{y}_n\}$, $\{\mathbf{z}_1, \dots, \mathbf{z}_n\}$ be orthonormal bases of eigenvectors for A , B , $A + B$ respectively. Suppose first that $i \geq j$, and consider the subspaces

$$V_1 = \langle \mathbf{x}_j, \dots, \mathbf{x}_n \rangle, \quad V_2 = \langle \mathbf{y}_{i-j+1}, \dots, \mathbf{y}_n \rangle, \quad V_3 = \langle \mathbf{z}_1, \dots, \mathbf{z}_i \rangle.$$

Since $\dim(V_1 \cap V_2) \geq \dim V_1 + \dim V_2 - n$, we have

$$\dim((V_1 \cap V_2) \cap V_3) \geq \dim V_1 + \dim V_2 + \dim V_3 - 2n = 1,$$

and so $V_1 \cap V_2 \cap V_3$ contains a unit vector \mathbf{x} . Applying Rayleigh's Principle, we have:

$$\lambda_j(A) + \lambda_{i-j+1}(B) \geq \mathbf{x}^\top A \mathbf{x} + \mathbf{x}^\top B \mathbf{x} = \mathbf{x}^\top (A + B) \mathbf{x} \geq \lambda_i(A + B).$$

When $i \leq j$, we obtain the second inequality of the theorem by applying the first inequality to $-A$ and $-B$. \square

Theorem 1.3.15 applies to a graph on n vertices specified as the edge-disjoint union of two spanning subgraphs. For example, if A and B are the adjacency matrices of G and \overline{G} then $A + B = J - I$ and so (for $n \geq 2$) $\lambda_2(G) + \lambda_{n-1}(\overline{G}) \geq \lambda_n(K_n) = -1$, $\lambda_2(G) + \lambda_n(\overline{G}) \leq \lambda_2(K_n) = -1$. We can also use Theorem 1.3.15 to obtain inequalities that relate the spectrum of an adjacency matrix A to the spectra of the Laplacian $D - A$, the signless Laplacian $D + A$ and the Seidel matrix $J - I - 2A$: we apply the theorem to A and $D - A$,

to $-A$ and $D + A$, and to $2A$ and $J - I - 2A$ respectively. For example, $\lambda_k(D \pm A) \geq \lambda_n(A) \pm \lambda_{n-k+1}(A)$ and $\lambda_k(J - I - 2A) \geq -2\lambda_{n-k+1}(A) - 1$.

Proposition 1.3.16. *Let M be a symmetric $n \times n$ matrix with real entries. If*

$$M = \begin{bmatrix} P & Q \\ Q^\top & R \end{bmatrix},$$

then

$$\lambda_1(M) + \lambda_n(M) \leq \lambda_1(P) + \lambda_1(R).$$

Proof. Let $\lambda = \lambda_n(M)$. Then we have $M - \lambda I = S + T$, where

$$S = \begin{pmatrix} P - \lambda I & O \\ Q^\top & O \end{pmatrix}, \quad T = \begin{pmatrix} O & Q \\ O & R - \lambda I \end{pmatrix}.$$

Any non-zero eigenvalue of S is an eigenvalue of $P - \lambda I$, and so the eigenvalues of S are real. Similarly, the eigenvalues of T are real. Using Theorem 1.3.15, we have

$$\begin{aligned} \lambda_1(M) - \lambda &= \lambda_1(S + T) \leq \lambda_1(S) + \lambda_1(T) = \\ &\lambda_1(P - \lambda I) + \lambda_1(R - \lambda I) = \lambda_1(P) - \lambda + \lambda_1(R) - \lambda, \end{aligned}$$

and the result follows. \square

Using an induction argument, we obtain the following:

Corollary 1.3.17. *Let M be a symmetric $n \times n$ matrix with real entries. If M is partitioned into k^2 blocks M_{ij} (of size $n_i \times n_j$) then*

$$\lambda_1(M) + (k - 1)\lambda_n(M) \leq \sum_{i=1}^k \lambda_1(M_{ii}).$$

Finally we prove a result on determinants required in Chapter 7. For an $n \times m$ matrix R ($n \leq m$), we write R_{k_1, \dots, k_n} for the matrix consisting of rows k_1, \dots, k_n of R ; and for an $m \times n$ matrix S ($n \leq m$) we write S^{k_1, \dots, k_n} for the matrix consisting of columns k_1, \dots, k_n of S . (Here, k_1, \dots, k_n are not necessarily distinct.) If F is an n -element subset of $\{1, \dots, m\}$, say $F = \{k_1, \dots, k_n\}$ where $k_1 < k_2 < \dots < k_n$, then we write $R_F = R_{k_1, \dots, k_n}$ and $S^F = S^{k_1, \dots, k_n}$.

Theorem 1.3.18 (The Binet–Cauchy Theorem). *If R is an $n \times m$ matrix and S is an $m \times n$ matrix ($n \leq m$), then*

$$\det(RS) = \sum_{|F|=n} \det(R_F) \det(S^F).$$

Proof. Let $R = (r_{ij})$ and $S = (s_{ij})$. We have

$$\begin{aligned} \det(RS) &= \sum_{\sigma} \operatorname{sgn}(\sigma) \prod_{i=1}^n \left(\sum_{k=1}^n r_{ik} s_{k\sigma(i)} \right) \\ &= \sum_{\sigma} \operatorname{sgn}(\sigma) \left(\sum_{k_1=1}^m r_{1k_1} s_{k_1\sigma(1)} \right) \left(\sum_{k_2=1}^m r_{2k_2} s_{k_2\sigma(2)} \right) \cdots \left(\sum_{k_n=1}^m r_{nk_n} s_{k_n\sigma(n)} \right) \\ &= \sum_{k_1=1}^m \sum_{k_2=1}^m \cdots \sum_{k_n=1}^m r_{1k_1} r_{2k_2} \cdots r_{nk_n} \sum_{\sigma} \operatorname{sgn}(\sigma) s_{k_1\sigma(1)} s_{k_2\sigma(2)} \cdots s_{k_n\sigma(n)} \\ &= \sum_{k_1=1}^m \sum_{k_2=1}^m \cdots \sum_{k_n=1}^m r_{1k_1} r_{2k_2} \cdots r_{nk_n} \det(S^{\{k_1, \dots, k_n\}}). \end{aligned}$$

Now $\det(S^{\{k_1, \dots, k_n\}}) = 0$ when k_1, \dots, k_n are not distinct, and so we may take the sum over n -element subsets $\{k_1, \dots, k_n\}$ of $\{1, \dots, m\}$. Then $\det(S^{\{\tau(k_1), \dots, \tau(k_n)\}}) = \operatorname{sgn}(\tau) \det(S^{\{k_1, \dots, k_n\}})$ for any permutation τ of k_1, \dots, k_n , and so

$$\begin{aligned} &\sum_{k_1=1}^m \sum_{k_2=1}^m \cdots \sum_{k_n=1}^m r_{1k_1} r_{2k_2} \cdots r_{nk_n} \det(S^{\{k_1, \dots, k_n\}}) \\ &= \sum_{\tau} \sum_{k_1 < k_2 < \dots < k_n} \operatorname{sgn}(\tau) r_{1\tau(1)} r_{2\tau(2)} \cdots r_{n\tau(n)} \det(S^{\{k_1, \dots, k_n\}}) \\ &= \sum_{|F|=n} \det(R_F) \det(S^F). \end{aligned}$$

□

Exercises

- 1.1 Prove Proposition 1.1.2.
- 1.2 By considering the nullspace of an all-1 matrix, or otherwise, show that K_n ($n > 1$) has spectrum $(n-1)^1, (-1)^{n-1}$.
- 1.3 Prove Proposition 1.1.7.
- 1.4 Show that $L(K_{4,4})$ has spectrum $6^1, 2^6, (-2)^9$.
- 1.5 Let G be a graph with n vertices. Show that $\lambda_1(G) \leq n-1$, with equality if and only if $G = K_n$.
- 1.6 Let G be a bipartite graph, with each edge joining a vertex in $\{1, \dots, k\}$ to a vertex in $\{k+1, \dots, n\}$. Show that if $(x_1, \dots, x_n)^{\top}$ is an eigenvector of G corresponding to λ , then $(x_1, \dots, x_k, -x_{k+1}, \dots, -x_n)^{\top}$ is an

- eigenvector of G corresponding to $-\lambda$. Deduce that the spectrum of a bipartite graph is symmetric about 0.
- 1.7 Let G be a graph with p vertices of odd degree and q vertices of even degree, where p and q have the same parity. Show that if G' is switching equivalent to G then either G' has p vertices of odd degree and q vertices of even degree, or G' has q vertices of odd degree and p vertices of even degree [Sei2].
 - 1.8 Show that for any graph G and any vertex v of G there exists a unique switching-equivalent graph G' which has v as an isolated vertex [Sei3].
 - 1.9 Let $I(G)$ be the collection of graphs obtained by isolating in turn the vertices of the graph G . Show that the graphs G_1 and G_2 are switching equivalent if and only if $I(G_1) = I(G_2)$ [BuCS1].
 - 1.10 Prove Proposition 1.2.2.
 - 1.11 Show that a regular connected generalized line graph is either a line graph or a cocktail party graph.
 - 1.12 Prove Proposition 1.3.4.
 - 1.13 Suppose that G, \overline{G} have adjacency matrices A, \overline{A} . Show that if μ is a non-main eigenvalue of G then $\mathcal{E}_A(\mu) \subseteq \mathcal{E}_{\overline{A}}(-\mu - 1)$. Provide an example of proper inclusion.
 - 1.14 Let G be a graph with adjacency matrix A and vertex degrees d_1, \dots, d_n . Let $\mathbf{d} = (d_1, \dots, d_n)$. Then G is said to be *harmonic* if \mathbf{d} is an eigenvector of A . Show that both G and \overline{G} are harmonic if and only if G is regular.
 - 1.15 With the notation of Section 1.1, show that the vector $(d_1, \dots, d_n)^\top$ is orthogonal to (i) $\mathcal{E}(0)$, and (ii) $\mathcal{E}(\lambda)$ for every non-main eigenvalue λ .
 - 1.16 Show that no line graph has -2 as a main eigenvalue.
 - 1.17 Show that if G is a strongly regular graph then each vertex-deleted subgraph $G - v$ ($v \in V(G)$) has exactly two main eigenvalues.
 - 1.18 Show that in a connected graph G , the minimum degree of a vertex is bounded above by the index of G .
 - 1.19 Show that if (α_{ij}) is the angle matrix of the connected graph G then $(\alpha_{11}, \dots, \alpha_{1n})^\top$ is the principal eigenvector of G .
 - 1.20 Show that if the graphs G, G' differ in only one edge then $|\lambda_1(G) - \lambda_1(G')| \leq 1$.
 - 1.21 Use Theorem 1.3.15 to show that if the adjacency matrix of G has eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ and the Laplacian of G has eigenvalues $\nu_1 \geq \dots \geq \nu_n$ then

$$\delta(G) - \lambda_i \leq \nu_{n-i+1} \leq \Delta(G) - \lambda_i \quad (i = 1, \dots, n).$$

State and prove an analogous result relating the eigenvalues of the signless Laplacian to $\lambda_1, \dots, \lambda_n$.

1.22 Show that if A is a symmetric matrix with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ then

$$\lambda_1 - \lambda_n = \sup\{\mathbf{u}^\top A \mathbf{u} - \mathbf{v}^\top A \mathbf{v}\},$$

where the supremum is taken over all pairs of orthonormal vectors \mathbf{u}, \mathbf{v} [Mir].

Notes

For a background in graph theory and linear algebra, the reader is referred to the monographs [Mer5] and [Str] respectively; earlier texts are [Har2] and [Hal]. Most undergraduate texts on linear algebra discuss the orthogonal diagonalization of a matrix with real entries; a more advanced text is [Pra]. For results on matrices (not necessarily symmetric) with non-negative entries, [Gan, Vol. 2] is a standard reference. The interlacing property of the eigenvalues arising in Theorem 1.3.11 is taken from [Hae2]; Corollary 1.3.13 appears in the earlier paper [Hae1]. Theorem 1.3.14 appears in [Hay] and [PeSa1]. The proofs of Theorems 1.3.15 and 1.3.18 are taken from [Pra].

Line graphs are characterized by a collection of 9 forbidden induced subgraphs; see [Har2, Chapter 8] or the original proof by L. W. Beineke [Bei]. The concept of a strongly regular graph was introduced in 1963 by R. C. Bose [Bos], and there is now an extensive literature on graphs of this type; see, for example, [BroLi]. Generalized line graphs were introduced by A. J. Hoffman [Hof5] in 1970, and studied extensively by D. Cvetković, M. Doob and S. Simić [CvDS1, CvDS2] in 1980. They were characterized by a collection of 31 forbidden induced subgraphs in [CvDS1, CvDS2], and independently by S. B. Rao, N. M. Singhi and K. S. Vijayan in [RaoSV]; a recent proof appears in [CvRS8] and the monograph [CvRS7]. A survey of results concerning main eigenvalues, together with an explanation of their relation to harmonic graphs (Exercise 1.14), can be found in [Row16].

The modifications $G - u$, $G - uv$ may be regarded as perturbations of G ; other perturbations are considered in Section 8.1.

2

Graph operations and modifications

In this chapter we describe some procedures for determining characteristic polynomials of graphs derived from simpler graphs by certain operations or modifications. Typically, we define an n -ary operation on graphs G_1, G_2, \dots, G_n ($n = 1, 2, \dots$) to obtain a graph G , and then describe relations between the spectra of G_1, G_2, \dots, G_n and the spectrum of G . In some important cases, the spectrum of G is determined by the spectra of G_1, G_2, \dots, G_n ; in other cases, additional invariants of G_1, G_2, \dots, G_n are required in the form of graph angles or walk generating functions. The modifications considered include the deletion and addition of a vertex.

Naturally, several proofs rely simply on determinantal expansions, but others require an interpretation of the coefficients in a characteristic polynomial, and this is presented in Section 2.4. At the end of the chapter, in Section 2.6, we use the theory we have developed to derive the spectra, or characteristic polynomials, of several special classes of graphs.

2.1 Complement, union and join of graphs

The operations of complement, union and join are connected by the relation

$$\overline{G \nabla H} = \overline{G} \dot{\cup} \overline{H}.$$

First we consider the (disjoint) union of graphs. If G has adjacency matrix A and H has adjacency matrix B , then the adjacency matrix of $G \dot{\cup} H$ is the direct sum

$$A \dot{+} B = \begin{pmatrix} A & O \\ O & B \end{pmatrix}.$$

Consideration of determinants leads immediately to the following result.