





图的谱半径

[塞尔维亚] Stevanović, D. (斯特万诺维奇) 著





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Spectral Radius of Graphs

Dragan Stevanović

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DEDICATION

To my wife Sanja and to my mentor Dragoš, both of whom, independently of each other, forced me to write this book

PREFACE

The aim of this book is to provide an overview of important developments on the spectral radius λ_1 of adjacency matrix of simple graphs, obtained in the last 10 years or so. Most of the presented results are related to the Brualdi-Solheid problem [24], which asks to characterize graphs with extremal values of the spectral radius in a given class of graphs. As a careful reader will easily find out, this usually means characterizing graphs with the maximum spectral radius—prevailing reason being that the Rayleigh quotient, the basic building block of most proofs, allows one to check whether the spectral radius has increased after transforming a graph, but not whether it has decreased. Despite the scarcity of lemmas on the decrease of the spectral radius, increase of interest in graphs with the minimum spectral radius is motivated by the recently discovered relation [156]

$$\tau_{\rm c} = \frac{1}{\lambda_1}$$

between the epidemic threshold τ_c for the effective infection rate of a SIS-type network infection and the network's spectral radius. As the network becomes virus-free in the steady state if the effective infection rate is smaller than τ_c , the task of constructing a more resistant network obviously translates to the task of constructing a network with λ_1 as small as possible, giving impetus to the minimum part of the Brualdi-Solheid problem.

The book is primarily intended for a fellow research mathematician, aiming to make new contributions to the spectral radius of graphs. The focus of presentation is not only on the overview of recent results, but also on proof techniques, conjectures, and open problems. For the impatient reader, perhaps the best starting points are the entries "conjecture" and "open problem" in the index at the end of the book. Otherwise, Chapter 2 is devoted to the study of properties of the components of the principal eigenvector corresponding to λ_1 that will be used in several occasions later in the book. Chapters 3 and 4 deal with the instances of the Brualdi-Solheid problem. Chapter 3 presents the results on the spectral radius of graphs belonging to standard graph classes, such as graphs with a given degree sequence or planar graphs. On the other hand, graph classes in Chapter 4

are mostly defined as the set of graphs having the same value of an integervalued graph invariant, such as the diameter or the domination number.

The book is reasonably self-contained, with necessary preliminary results collected in a short, introductory chapter, but do note that it assumes some prior familiarity with graph theory (more) and linear algebra (less). It could be used in teaching, as part of a beginning graduate course or an advanced undergraduate course, including also courses within the research experience for undergraduates programs, but do also note that it lacks exercises (unless you treat conjectures and open problems as exercises).

I hope it is understandable that in a book of this size, one cannot possibly cover all the interesting new developments in the theory of graph spectra (and not even everything that has been published on the spectral radius of graphs!) in the last 10 years or so. For the reader looking forward to expand his/her knowledge of graph spectra, some further reading may be suggested. Results on the spectral properties of directed graphs are well covered in a survey paper by Brualdi [22]. Nikiforov has surveyed his results on extremal spectral graph theory [114], although some of his results are covered here as well. Results on the spectral radius of weighted graphs are more oriented toward the spectral theory of nonnegative matrices than to graph theory; the reader is, thus, referred to Chapter 6 of Friedland's manuscript on matrices [63]. If the reader is looking for a textbook covering a wider array of topics in spectral graph theory, then good choices are the books by Cvetković et al. [47], by Van Mieghem [155], or by Brouwer and Haemers [21].

At the end, I would like to acknowledge kind hospitality of the Max Planck Institute for Mathematics in Sciences in Leipzig during the final stages of writing this book. I am grateful to Türker Bıyıkoğlu, Josef Leydold, Sebastian Cioabă, and Kelly Thomas for permissions to use some of the proofs from [17, 31, 33, 64] without significant change. I am also very much grateful to my family—Sanja, Djordje, and Milica—for all their love, support, and patience while this book was being materialized from an idea to a reality.

Dragan Stevanović Niš & Leipzig, June 2014

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CHAPTER $\it I$

Introduction

This short, introductory chapter contains definitions and tools necessary to follow the results presented in the forthcoming chapters. We will cover various graph notions and invariants, adjacency matrix, its eigenvalues and its characteristic polynomial, and some standard matrix theory tools that will be used later in proofs.

1.1 GRAPHS AND THEIR INVARIANTS

A simple graph is the pair G = (V, E) consisting of the vertex set V with n = |V| vertices and the edge set $E \subseteq \binom{V}{2}$ with m = |E| edges. Often in the literature, n is called the order and m the size of G. Simple graphs contain neither directed nor parallel edges, so that an edge $e \in E$ may be identified with the pair $\{u, v\}$ of its distinct endvertices $u, v \in V$. We will write shortly uv for the set $\{u, v\}$. We will also use V(G) and E(G) to denote the vertex set and the edge set of G, if they have not been named already. To simplify notation, we will omit graph name (usually G), whenever it can be understood from the context.

For a vertex $u \in V$, the set of its neighbors in G is denoted as

$$N_u = \{ v \in V : uv \in E \}.$$

The degree of u is the number of its neighbors, i.e., $\deg_u = |N_u|$. The maximum vertex degree Δ and the minimum vertex degree δ for G are defined as

$$\Delta = \max_{u \in V} \deg_u, \qquad \delta = \min_{u \in V} \deg_u.$$

Graph G is said to be d-regular graph, or just regular, if all of its vertices have degree equal to d.

A sequence $W: u = u_0, u_1, \dots, u_k = v$ of vertices from V such that $u_i u_{i+1} \in E$, $i = 0, \dots, k-1$, is called a walk between u and v in G of length k. Two vertices $u, v \in V$ are connected in G if there exists a walk between them in G, and the whole graph G is connected if there exists a walk between any two of its vertices.

The distance d(u, v) between two vertices u, v of a connected graph G is the length of the shortest walk between u and v in G. The eccentricity ecc_u of a vertex $u \in V$ is the maximum distance from u to other vertices of G, i.e.,

$$\mathrm{ecc}_{u} = \max_{v \in V} d(u, v).$$

The diameter D and the radius r of G are then defined as

$$D = \max_{u \in V} ecc_u, \qquad r = \min_{u \in V} ecc_u.$$

Graph H=(V',E') is a subgraph of G=(V,E) if $V'\subseteq V$ and $E'\subseteq E$. If V'=V, we say that H is the spanning subgrah of G. On the other hand, if $E'=\binom{V'}{2}\cap E$, i.e., if H contains all edges of G whose both endpoints are in H, we say that H is the induced subgraph of G. If G is a subset of vertices of G=(V,E), we will use G-G (or just G-G induced by G (or just G induced by G induced by G induced by G is a subset of edges of G, we will use G-G (or just G induced by G is a subset of edges of G).

A subset $C \subseteq V$ is said to be a clique in G if $uv \in E$ holds for any two distinct vertices $u, v \in C$. The clique number ω of G is the maximum cardinality of a clique in G.

A subset $S \subseteq V$ is said to be an independent set in G if $uv \notin E$ holds for any two distinct vertices $u, v \in S$. The independence number α of G is the maximum cardinality of an independent set in G.

A function $f: V \to Z$, for arbitrary set Z, is said to be a coloring of G if $f(u) \neq f(v)$ whenever $uv \in E$. The chromatic number χ is the smallest cardinality of a set Z for which there exists a coloring $f: V \to Z$. Alternatively, as $f^{-1}(z)$, $z \in Z$, is necessarily an independent set, the chromatic number χ may be equivalently defined as the smallest number of parts into which V can be partitioned such that any two adjacent vertices belong to distinct parts.

A set D of vertices of a graph G is a dominating set if every vertex of $V(G) \setminus D$ is adjacent to a vertex of S. The domination number γ of G is the minimum cardinality of a dominating set in G.

A set M of disjoint edges of G is a matching in G. The matching number ν of G is the maximum cardinality of a matching in G.

Given two graphs G = (V, E) and G' = (V', E'), the function $f: V \to V'$ is an isomorphism between G and G' if f is bijection and for each $u, v \in V$

holds $\{u, v\} \in E$ if and only if $\{f(u), f(v)\} \in E'$. If there is an isomorphism between G and G', we say that G and G' are isomorphic and denote it as $G \cong G'$. In case G and G' are the one and the same graph, then we have an automorphism.

Further, a function $i: G \to \mathbb{R}$ is a graph invariant if i(G) = i(G') holds whenever $G \cong G'$. In other words, the value of i depends on the structure of a graph, and not on the way its vertices are labeled. All the values mentioned above

$$n, m, \Delta, \delta, D, r, \omega, \alpha, \chi, \gamma, \nu$$

are examples of graph invariants. Graph theory, actually, represents a study of graph invariants and in this book the focus will be on yet another graph invariant—the spectral radius of a graph, which is defined in the next section.

We will now define several types of graphs that will appear throughout the book. The path P_n has vertices $1, \ldots, n$ and edges of the form $\{i, i+1\}$ for $i=1,\ldots,n-1$. The cycle C_n is the graph obtained from P_n by adding edge $\{n,1\}$ to it. The complete graph K_n has vertices $1,\ldots,n$ and contains all edges ij for $1 \le i < j \le n$. The complete bipartite graph K_{n_1,n_2} consists of two disjoint sets of vertices V_1 , $|V_1| = n_1$, and V_2 , $|V_2| = n_2$, and all edges v_1v_2 for $v_1 \in V_1$ and $v_2 \in V_2$. The star S_n is a shortcut for the complete bipartite graph $K_{1,n-1}$. The complete multipartite graph K_{n_1,\ldots,n_p} consists of disjoint sets of vertices V_i , $|V_i| = n_i$, $i = 1,\ldots,p$, and all edges v_iv_j , $v_i \in V_i$, $v_j \in V_j$, for $i \ne j$. The Turán graph $T_{n,p} \cong K_{\lceil n/p \rceil,\ldots,\lceil n/p \rceil,\lfloor n/p \rfloor,\ldots,\lfloor n/p \rfloor}$ is the (p+1)-clique-free graph with the maximum number of edges [151]. The complete split graph $CS_{n,p} = K_{n-p,1,\ldots,1}$ consists of an independent set of n-p vertices and a clique of p vertices, such that each vertex of the independent set is adjacent to each vertex of the clique.

The coalescence $G \cdot H$ of two graphs G and H with disjoint vertex sets is obtained by selecting a vertex u in G and a vertex v in H and then identifying u and v. The kite $KP_{s,r}$ is a coalescence of the complete graph K_s and the path P_r , where one endpoint of P_r is identified with an arbitrary vertex of K_s . The lollipop $CP_{s,r}$ is a coalescence of the cycle C_s and the path P_r , where one endpoint of P_r is identified with an arbitrary vertex of C_s . The bug Bug_{p,q_1,q_2} is obtained from the complete graph K_p by deleting its edge uv, and then by identifying u with an endpoint of P_{q_1} and v with an endpoint of P_{q_2} . The bag $Bag_{p,q}$ is obtained from the complete graph K_p by replacing its edge uv with a path P_q . The pineapple $PA_{n,q}$ is a graph with n vertices consisting of a

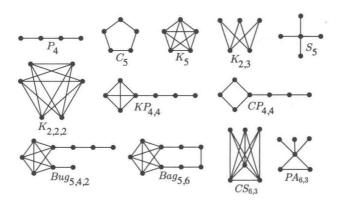


Figure 1.1 Examples of graph drawings.

clique on q vertices and an independent set on the remaining n-q vertices, such that each vertex of the independent set is adjacent to the same clique vertex.

The complement of a graph G = (V, E) is the graph $\overline{G} = \left(V, \binom{V}{2} \setminus E\right)$, so that each pair $\{u, v\}$, $u \neq v$, appears as an edge in exactly one of G and \overline{G} . Further, for two graphs G = (V, E) and G' = (V', E'), their union $G \cup G'$ is a graph with the vertex set $V \cup V'$ and the edge set $E \cup E'$. kG is a shortcut for $G \cup G \cup \cdots \cup G$. The join $G \vee G'$ of two graphs G = (V, E) and G' = (V', E') is a graph with the vertex set $V \cup V'$ and the edge set $E \cup E' \cup \{st : s \in V, t \in V'\}$.

Graphs are often depicted as drawings in which vertices are represented as points (actually, as circles with small diameter), and edges between them as simple curves (most often, as straight segments). Examples of such drawings are given in Fig. 1.1.

For other undefined notions, and for further study of the basics of graph theory, the reader is referred to [50], a modern "classical" textbook in graph theory.

1.2 ADJACENCY MATRIX, ITS EIGENVALUES, AND ITS CHARACTERISTIC POLYNOMIAL

The adjacency matrix of G = (V, E) is the $n \times n$ matrix A indexed by V, whose (u, v)-entry is defined as

$$A_{uv} = \begin{cases} 1 & \text{if } uv \in E, \\ 0 & \text{if } uv \notin E. \end{cases}$$

Recall that a matrix is said to be reducible if it can be transformed to the form

$$A = \begin{bmatrix} A' & B \\ 0 & A'' \end{bmatrix},$$

where A' and A'' are square matrices, by simultaneous row/column permutations. Otherwise, A is said to be irreducible. It is easy to see that the adjacency matrix A is irreducible if and only if G is a connected graph.

Adjacency matrix is closely related to the numbers of walks between vertices of G. Namely,

Theorem 1.1. The number of walks of length $k, k \ge 0$, between vertices u and v in G is equal to $(A^k)_{u,v}$.

Proof. By induction on k. For k = 0, the unit matrix $A^0 = I$ has entries 1 and 0, equal to the numbers of walks of length 0, as these are the walks which consist of a single vertex only (so 1s for the diagonal entries and 0s for nondiagonal entries).

Assume now that the inductive hypothesis holds for some $k \ge 0$. Any walk of length k between u and v consists of an edge uz for some neighbor $z \in N_u$ and a walk of length k-1 between z and v, so that, by the inductive hypothesis, the number of walks of length k between u and v is equal to

$$\sum_{z \in N_u} (A^{k-1})_{z,v} = \sum_{z \in V} A_{u,z} (A^{k-1})_{z,v} = (A^k)_{u,v}.$$

The adjacency matrix A is a real, symmetric matrix, so that A is diagonalizable and has n real eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

and *n* real, linearly independent, unit eigenvectors $x_1, x_2, ..., x_n \in \mathbb{R}^n$ satisfying the eigenvalue equation

$$Ax_i = \lambda_i x_i, \qquad i = 1, \dots, n.$$

The eigenvectors, in addition, can be chosen so as to form the orthonormal basis of \mathbb{R}^n , i.e., such that $x_i^T x_i = 0$ for $i \neq j$.

The family of eigenvalues $\lambda_1, \ldots, \lambda_n$ is the spectrum of G. The multiplicity of an eigenvalue λ is the number of times it appears in the spectrum, i.e., it is the dimension of the subspace of eigenvectors corresponding to λ (this subspace is also called the eigenspace of λ). An eigenvalue is simple if its multiplicity is 1. The rank of a matrix is the maximum number of linearly independent columns of A. By the rank-nullity theorem [101, p. 199], the rank of A is n minus the multiplicity of eigenvalue zero.

The eigenvalues and orthonormal eigenvectors provide the spectral decomposition of A:

$$A = \sum_{i=1}^{n} \lambda_i x_i x_i^{\mathrm{T}}.$$
 (1.1)

It is easy to see why this holds: let $B = A - \sum_{i=1}^{n} \lambda_i x_i x_i^T$. Due to $x_i^T x_k = 0$ for $i \neq k$, and $x_k^T x_k = 1$, we have that for each x_k

$$Bx_k = (A - \sum_{i=1}^n \lambda_i x_i x_i^{\mathrm{T}}) x_k = \lambda_k x_k - \lambda_k x_k x_k^{\mathrm{T}} x_k = 0.$$

As B maps each basis vector to 0, we conclude that B = 0 holds.

Further, the entries of the adjacency matrix are 0s and 1s only, so that for $u \in V$,

$$(Ax_i)_u = \sum_{v \in N_u} (x_i)_v.$$

Thus, the eigenvalue equation for $i \in \{1, ..., n\}$ and $u \in V$ can also be written as

$$\lambda_i(x_i)_u = \sum_{v \in N_u} (x_i)_v. \tag{1.2}$$

One of important early properties of graph eigenvalues is their characterization of bipartiteness.

Theorem 1.2 ([128]). A connected graph is bipartite if and only if $-\lambda_1$ is an eigenvalue of G, in which case the whole spectrum is symmetric with respect to 0. If G is bipartite, then the eigenvector of $-\lambda_1$ is obtained from

its principal eigenvector by changing signs of the components in one part of the bipartition.

See [53] for more details and further extensions of Sachs' theorem.

The characteristic polynomial of G is the characteristic polynomial of A:

$$P_G(\lambda) = \det(\lambda I - A) = \lambda^n + a_1 \lambda^{n-1} + \dots + a_n.$$

The eigenvalues of G are the roots of its characteristic polynomial $P_G(\lambda)$. The coefficients of the characteristic polynomial count, in a way, appearances of basic figures in G. An elementary figure is either an edge K_2 or a cycle C_q , $q \geq 3$, and a basic figure is any graph whose all connected components are elementary figures. Let p(U) and c(U) denote the number of components and the number of cycles contained in a basic figure U. If U_i denotes the set all basic figures contained in G having exactly i vertices, then, for $1 \leq i \leq n$,

$$a_i = \sum_{U \in \mathcal{U}_i} (-1)^{p(U)} 2^{c(U)}.$$

See, e.g., [43, p. 32] for the proof of this formula.

There are many formulas relating characteristic polynomial of a graph to those of its special subgraphs. Two most often encountered ones concern cut edges and coalescence.

Theorem 1.3 ([76]). If uv is a cut edge of a connected graph G and G_1 and G_2 are the connected components of G – uv, such that u belongs to G_1 and v belongs to G_2 , then

$$P_G(\lambda) = P_{G_1}(\lambda)P_{G_2}(\lambda) - P_{G_1-u}(\lambda)P_{G_2-v}(\lambda).$$

Theorem 1.4 ([130]). If $G \cdot H$ is the coalescence of G and H obtained by identifying a vertex u of G with a vertex v of H, then

$$P_{G \cdot H}(\lambda) = P_G(\lambda)P_{H-\nu}(\lambda) + P_{G-\nu}(\lambda)P_H(\lambda) - \lambda P_{G-\nu}(\lambda)P_{H-\nu}(\lambda).$$

For further characteristic polynomial reduction formulas, see [47, Chapter 2].

We list here the spectra of some of the graphs defined in the previous section:

• The path P_n has eigenvalues $2\cos\frac{\pi i}{n+1}$, $i=0,\ldots,n-1$. Its characteristic polynomial is $U_n(\lambda/2)$, where

$$U_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \binom{n-k}{k} x^{n-2k}$$

is the Chebyshev polynomial of the second kind;

• The cycle C_n has eigenvalues $2\cos\frac{2\pi i}{n}$, i = 0, ..., n-1. Its characteristic polynomial is $2T_n(\lambda/2) - 2$, where

$$T_n(x) = \frac{n}{2} \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k}{n-k} \binom{n-k}{k} (2x)^{n-2k}$$

is the Chebyshev polynomial of the first kind;

- The complete graph K_n has a simple eigenvalue n-1 and eigenvalue -1 of multiplicity n-1. Hence, $P_{K_n}(\lambda) = (\lambda n + 1)(\lambda + 1)^{n-1}$;
- The complete bipartite graph K_{n_1,n_2} has two simple eigenvalues $\pm \sqrt{n_1 n_2}$ and eigenvalue 0 of multiplicity n-2. Hence, $P_{K_{n_1,n_2}}(\lambda) = (\lambda^2 n_1 n_2) \lambda^{n-2}$.

The characteristic polynomials of some other graph types, such as kites, lollipops, and bugs, can be obtained using Theorems 1.3 and 1.4. Nevertheless, their eigenvalues are not easily identifiable from their characteristic polynomials.

1.3 SOME USEFUL TOOLS FROM MATRIX THEORY

The celebrated Perron-Frobenius theorem can be applied to adjacency matrices of connected graphs.

Theorem 1.5 (The Perron-Frobenius theorem). *An irreducible, nonnegative* $n \times n$ *matrix* A *always has a real, positive eigenvalue* λ_1 , *so that:*

- 1) $|\lambda_i| \leq \lambda_1$ holds for all other (possibly complex) eigenvalues λ_i , i = 2, ..., n,
- 2) λ_1 is a simple zero of the characteristic polynomial $\det(\lambda I A)$, and
- 3) the eigenvector x_1 corresponding to λ_1 has positive components.

In addition, if A has a total of h eigenvalues whose moduli are equal to λ_1 , then these eigenvalues are obtained by rotating λ_1 for multiples of angle

 $2\pi/h$ in the complex plane, i.e., these eigenvalues are equal to $\lambda_1 e^{\frac{2\pi j}{h}}$ for $j = 0, \ldots, h-1$.

For the proof of the Perron-Frobenius theorem see, e.g., [65, Chapter XIII].

Hence, the largest eigenvalue λ_1 of the adjacency matrix A of connected graph G is, at the same time, the spectral radius of A. The corresponding positive unit eigenvector x_1 is called the principal eigenvector of A.

Note that the principal eigenvector is the only positive eigenvector of A: if we would suppose that x' is another positive eigenvector of A, then we would have both $x_1^T x' = 0$ due to orthogonality, and $x_1^T x' > 0$ due to positivity of components of both eigenvectors.

Another useful result concerns the Rayleigh quotient:

$$\lambda_1 = \sup_{x \neq 0} \frac{x^{\mathrm{T}} A x}{x^{\mathrm{T}} x}.\tag{1.3}$$

Let the eigenvalues of A be ordered as $\lambda_1 \ge \cdots \ge \lambda_n$, and choose the orthonormal basis x_1, \ldots, x_n such that x_i is the eigenvector corresponding to λ_i , $i = 1, \ldots, n$. Hence, if $x = \sum_{i=1}^n \alpha_i x_i$, then $x^T x_i = \alpha_i$, and from the spectral decomposition (1.1) follows that

$$\frac{x^{T}Ax}{x^{T}x} = \frac{\sum_{i=1}^{n} \lambda_{i} x^{T} x_{i} x_{i}^{T} x}{x^{T}x} = \frac{\sum_{i=1}^{n} \lambda_{i} \alpha_{i}^{2}}{\sum_{i=1}^{n} \alpha_{i}^{2}} \le \frac{\sum_{i=1}^{n} \lambda_{1} \alpha_{i}^{2}}{\sum_{i=1}^{n} \alpha_{i}^{2}} = \lambda_{1}.$$

Equality is attained above for $x = x_1$, so that (1.3) holds.

As an immediate consequence of the Rayleigh quotient, we have that addition of an edge e = uv to connected graph G strictly increases its spectral radius. Namely, if x is the principal eigenvector of G, then by (1.3)

$$\lambda_1(G+e) \ge \frac{x^T A x + 2x_u x_v}{x^T x} > \frac{x^T A x}{x^T x} = \lambda_1(G).$$
 (1.4)

Of course, this also means that deletion of an edge from a connected graph strictly decreases its spectral radius.

The Rayleigh quotient also enables the use of edge rotations and switching in order to increase the spectral radius of a graph.