14 Spectral Analysis

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A graph can be associated with several matrices, whose eigenvalues reflect structural properties of the graph. The adjacency matrix, the Laplacian, and the normalized Laplacian are in the main focus of spectral studies. How can the spectrum be used to analyze a graph? In particular, the following questions will be of interest:

- What can the spectrum tell us about subgraphs? Can we prove the existence or nonexistence of certain subgraphs by looking at the spectrum?
- Can certain eigenvalues be related to other global statistics (also called graph parameters), such as diameter, isoperimetric number or chromatic number?
- How can spectra help in classifying graphs?

This chapter is organized as follows: In the first section, we review facts from linear algebra and point out some fundamental properties of graph spectra. In the next section, we summarize what methods we know to compute the spectrum. In the sections that follow, we give some answers and ideas regarding the above questions.

14.1 Fundamental Properties

We define the different spectra and point out some fundamental properties. We show why it makes sense to consider more than the adjacency spectrum and list the three spectra for some basic graph classes (Table 14.1).

14.1.1 Basics from Linear Algebra

Let $M = (m_{i,j}) \in \mathbb{C}^{n \times n}$ be an $n \times n$ matrix with complex numbers as entries. A non-zero vector $x \in \mathbb{C}^n$ is an *eigenvector* of M with corresponding *eigenvalue* $\lambda \in \mathbb{C}$ if x and λ satisfy the equation

$$Mx = \lambda x. \tag{14.1}$$

The vector $\mathbf{0}_n$ is excluded from the set of possible eigenvectors since *every* $\lambda \in \mathbb{C}$ is a solution to $M\mathbf{0}_n = \lambda\mathbf{0}_n$. Equation (14.1) has a non-zero solution if and only if $\operatorname{rank}(M - \lambda I_n) < n$, which is equivalent to $\det(M - \lambda I_n) = 0$. Hence we can characterize the eigenvalues of M as roots of the polynomial $p_M(\lambda) := \det(M -$

U. Brandes and T. Erlebach (Eds.): Network Analysis, LNCS 3418, pp. 373–417, 2005.

λI_n). This *characteristic polynomial* p_M does not change if M is replaced by $Q^{-1}MQ$ for some arbitrary non-singular matrix Q. So M and $Q^{-1}MQ$ have the same eigenvalues. The *spectrum* of M is defined as the multiset of all eigenvalues of M, where the multiplicity of an eigenvalue λ is its (algebraic) multiplicity as a root of p_M.

From now on we shall assume that M is a symmetric matrix, i.e. $M = M^\top$, with real valued entries. One can show that there exists a non-singular matrix Q such that $M' := Q^{-1}MQ$ has diagonal form and $Q^{-1} = Q^\top$. Clearly, each vector e_i from the standard basis of $\mathbb{R}^n$ is an eigenvector of M' with $\lambda_i := m'_{i,i}$, the ith entry on the diagonal of M', as its corresponding eigenvalue. Since the characteristic polynomial is unchanged,

$$\det(M - \lambda I_n) = \det(M' - \lambda I_n) = \prod_{i=1}^{n}(\lambda_i - \lambda). \tag{14.2}$$

So the spectrum of M consists of n (not necessarily distinct) eigenvalues $\lambda_1, \ldots, \lambda_n \in \mathbb{R}$, and we have $\det(M) = \prod_{i=1}^n \lambda_i$. From the definition of the determinant as

$$\det M = \sum_{\pi \in S_n} \operatorname{sign}(\pi) \cdot m_{1,\pi(1)} \cdot \cdots \cdot m_{n,\pi(n)}$$

we see that $\det(M - \lambda I_n) = \prod_{i=1}^n (m_{i,i} - \lambda) + R(\lambda)$, where $R(\lambda)$ is the sum corresponding to permutations from $S_n \setminus \{\mathrm{id}\}$ and thus has degree $\leq n-2$. Hence the coefficient of λ^{n-1} in the characteristic polynomial is $\sum_{i=1}^n m_{i,i}$, the *trace* of M, and by comparison with (14.2) we infer that $\operatorname{trace}(M) = \sum_{i=1}^n \lambda_i$. Defining $v_i := Qe_i$ for all $i \in \{1, \ldots, n\}$, we have

$$\begin{aligned} Mv_i &= MQe_i = QQ^{-1}MQe_i = Q\lambda_i e_i = \lambda_i v_i \\ v_i^\top v_j &= (Qe_i)^\top Qe_j = e_i^\top Q^\top Qe_j = e_i^\top e_j, \end{aligned}$$

i.e., $v_1, \ldots, v_n$ are orthonormal eigenvectors of M. Consequently, $\{v_1, \ldots, v_n\}$ is a basis of $\mathbb{R}^n$, and the multiplicity of λ_i as an eigenvalue equals the maximum cardinality of a corresponding set of linearly independent eigenvectors.

In sum we have observed the following facts.

Theorem 14.1.1 ([135, 247, 576]). *Let $M \in \mathbb{R}^{n\times n}$ be a matrix with $M = M^\top$, then*

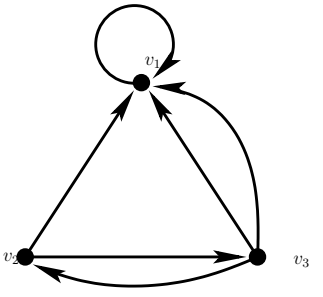
1. *M has real eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ and n orthonormal eigenvectors forming a basis of $\mathbb{R}^n$ [Spectral Theorem],*
2. *multiplicity of λ_i as an eigenvalue := multiplicity of λ_i as a root of the characteristic polynomial $\det(M - \lambda I_n)$ = cardinality of a maximum linearly independent set of eigenvectors corresponding to λ_i,*
3. *there is a matrix Q with $Q^\top = Q^{-1}$ such that $Q^\top MQ = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}$,*
4. *$\det(M) = \prod_{i=1}^n \lambda_i$, trace$(M) = \sum_{i=1}^n \lambda_i$.*

14.1.2 The Spectrum of a Graph

Given a multi-digraph $G = (V, E)$ with labeled vertices $v_1, \ldots, v_n$, we define the *adjacency matrix* $A = (a_{i,j})$ by

$$a_{i,j} := \text{multiplicity of edge } (v_i, v_j) \text{ in } E,$$

i.e., $a_{i,j}$ is equal to the number of arcs starting at vertex v_i and terminating at vertex v_j (for loops $(v_i, v_i) \in E$ it is sometimes useful to define $a_{i,i}$ as 2 instead of 1). The spectrum of G is the spectrum of the adjacency matrix of G (see Figure 14.1 for an example).



$$A = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}$$

Fig. 14.1. Example of an adjacency matrix

Note that though A depends on the order of labeling, the spectrum does not, since exchanging the labels of vertices v_i and v_j corresponds to exchanging row i with row j and column i with column j in A, which does not affect $\det(A)$ nor $\det(A - \lambda I_n)$. For the rest of this chapter we will identify V with the set of labels, i.e., we will assume that $V = \{1, \ldots, n\}$. Moreover we shall mainly focus on simple undirected graphs without loops. So, any graph $G = (V, E)$ will be assumed as simple, loopless, and undirected, unless explicitly stated otherwise. Hence the adjacency matrix A will (almost always) be a symmetric 0/1 matrix with a real spectrum of n eigenvalues λ_i, where we assume for convenience that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$.

Notation. We will use both, spectrum(A) and spectrum(G) to denote the eigenvalues of an adjacency matrix A corresponding to a graph G. Moreover, when speaking of the spectrum of a graph, we will always have the adjacency spectrum in mind (unless stated otherwise).

Let $w \in \mathbb{C}^n$ be an arbitrary vector and let $\omega : V \to \mathbb{C}$ map each $i \in V$ on w_i. Since A represents a graph, the ith component of Aw, $\sum_{j=1}^{n} a_{i,j} w_j$, can be written as $\sum_{j \in N(i)} \omega(j)$. Now the equation $Ax = \lambda x$ has the following useful interpretation.

Remark 14.1.2. 1. A has eigenvalue λ if and only if there exists a non-zero weight function $\omega : V \to \mathbb{C}$ such that for all $i \in V$, $\lambda\omega(i) = \sum_{j \in N(i)} \omega(j)$.

2. The Spectral Theorem 14.1.1.1. ensures that we can restrict ourselves to considering real-valued weight functions. Moreover, we can assume the maximum weight to be non-negative (if $\max\{\omega(i);\ i \in V\} < 0$ then $\omega(i) < 0$ for all $i \in V$ and we can consider $-\omega$ instead of ω).

Consider an assignment of weights to the vertices of a triangle as depicted in Figure 14.2. From

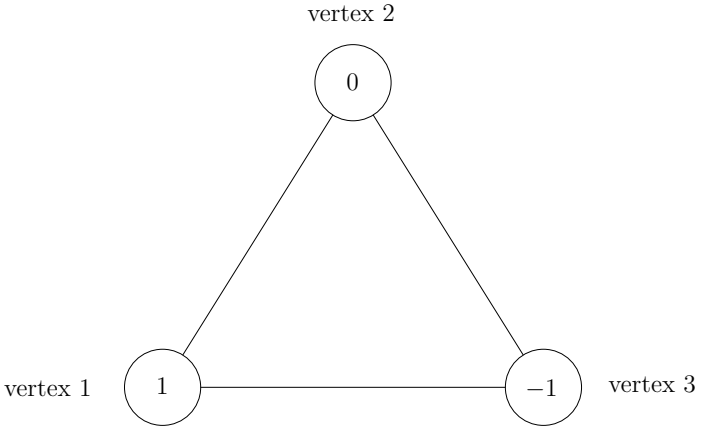


Fig. 14.2. A triangle with eigenvector components as weights

$$\begin{aligned}
\omega(1) = 1 &= -(0 + (-1)) = -(\omega(2) + \omega(3)),\\
\omega(2) = 0 &= -(1 + (-1)) = -(\omega(1) + \omega(3)),\\
\omega(3) = -1 &= -(1 + 0) = -(\omega(1) + \omega(2)),
\end{aligned}$$

we can conclude that -1 is an eigenvalue. Similarly, by assigning a weight of 1 to all vertices we can check that 2 is in the spectrum of the triangle. For another example, have a look at Figure 14.3, which proves that 2 is an eigenvalue of a star on 5 vertices.

Remark 14.1.2 enables us to prove the following claims.

Lemma 14.1.3 ([576]). *Let $G = (V, E)$ be a graph on n vertices with adjacency matrix A and eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$. Let Δ be the maximum vertex degree of G.*

1. *$\lambda_n \leq \Delta$.*
2. *If $G = G_1 \dot\cup G_2$ is the union of two disjoint graphs G_1 and G_2 then spectrum(G) = spectrum$(G_1) \cup$ spectrum(G_2).*
3. *If G is bipartite then $\lambda \in$ spectrum$(G) \Leftrightarrow -\lambda \in$ spectrum(G).*
4. *If G is a simple cycle then spectrum$(G) = \left\{ 2\cos\left(\frac{2\pi k}{n}\right);\ k \in \{1, \ldots, n\} \right\}$.*

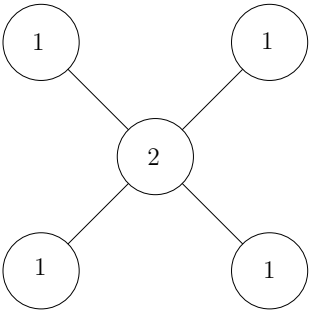


Fig. 14.3. A star with eigenvector components as weights

Proof. 1. Let ω be a non-zero weight function on the vertices such that $\lambda_n \omega(i) = \sum_{j \in N(i)} \omega(j)$ for all $i \in V$ and let i_0 be a vertex of maximum weight. Then $\lambda_n \omega(i_0) = \sum_{j \in N(i_0)} \omega(j) \leq \Delta \omega(i_0)$ implies $\lambda_n \leq \Delta$.

2. Let ω be a non-zero weight function for $\lambda_i \in \text{spectrum}(G)$. Since ω is not identically zero, either $\omega|_{V(G_1)}$ or $\omega|_{V(G_2)}$ must not be identically zero and hence is a weight function for λ_i on G_1 or G_2. On the other hand, if ω is a weight function for $\lambda \in \text{spectrum}(G_j)$ for $j = 1$ (or $j = 2$) then extending ω by defining $\omega(i) := 0$ for all $i \in V \setminus V(G_j)$, yields a non-zero weight function for λ on G.

3. Let ω be a weight function for λ on G. Let V_1, V_2 denote the partition classes of V. Define $\omega' : V \to \mathbb{R}$ by

$$i \mapsto \begin{cases} \omega(i), & \text{if } i \in V_1 \\ -\omega(i), & \text{if } i \in V_2. \end{cases}$$

Then for all $i \in V_1$,

$$-\lambda \omega'(i) = -\lambda \omega(i) = -\sum_{j \in N(i)} \omega(j) = \sum_{j \in N(i)} \omega'(j),$$

and for all $i \in V_2$,

$$-\lambda \omega'(i) = \lambda \omega(i) = \sum_{j \in N(i)} \omega(j) = \sum_{j \in N(i)} \omega'(j).$$

4. For the proof of this claim we will use complex weights. Assume that the edges of the cycle are $\{1, n\}$ and $\{i, i+1\}$, for all $i \in \{1, \ldots, n-1\}$. For each $k \in \{1, \ldots, n\}$ let $\tau_k := \exp(2\pi \mathbf{i} k/n)$ be an nth root of unity and put $\omega(j) := \tau_k^{j-1}$. (Here, $\mathbf{i}$ denotes the complex number $\mathbf{i}$ with $\mathbf{i}^2 = -1$ and *not* a vertex.) Then for all $j \in V$,

$$\sum_{l \in N(j)} \omega(l) = (\tau_k^{-1} + \tau_k) \cdot \tau_k^{j-1},$$

and thus $\tau_k^{-1} + \tau_k = \exp(-2\pi \mathbf{i} k/n) + \exp(2\pi \mathbf{i} k/n) = 2 \cos\left(\frac{2\pi k}{n}\right)$ is an eigenvalue of G. □

We mention two further results on the adjacency spectrum (see [135] for a proof): it can be shown that $\lambda_n = \Delta$ if and only if G has a Δ-regular component. For the smallest eigenvalue of G one can prove the lower bound $\lambda_1 \geq -\lambda_n$, where equality holds if and only if G has a bipartite component whose largest eigenvalue is equal to λ_n.

Let us determine the spectra of the complete bipartite graph K_{n_1,n_2} and the complete graph K_n.

Lemma 14.1.4 ([576]). *Let n_1, n_2, and n be positive integers.*

1. *For $G = K_{n_1,n_2}$, $\lambda_1 = -\sqrt{n_1 n_2}$, $\lambda_2 = \cdots = \lambda_{n-1} = 0$, and $\lambda_n = \sqrt{n_1 n_2}$.*
2. *For $G = K_n$, $\lambda_1 = \cdots = \lambda_{n-1} = -1$, $\lambda_n = n - 1$.*

Proof. 1. Since A is diagonalizable with eigenvalues as diagonal entries, the rank of A is equal to the number of non-zero eigenvalues. For K_{n_1,n_2}, the rank is 2, so A has two non-zero eigenvalues λ_i and λ_j. Note that the trace of A is both the sum of the eigenvalues and the number of loops in G. Hence, $\lambda_i + \lambda_j = 0$, and we conclude that the spectrum of G is $\lambda_1 = -c, \lambda_2 = \cdots = \lambda_{n-1} = 0, \lambda_n = c$ for some $c \in \mathbb{R}_{>0}$. Let us look at the characteristic polynomial, $\det(A - \lambda I_n) = (-c - \lambda)\lambda^{n-2}(c - \lambda) = \lambda^n - c^2\lambda^{n-2}$. Since λ appears only on the diagonal of $A - \lambda I_n$, terms in the permutation expansion that contribute to λ^{n-2} arise from those permutations that select $n - 2$ diagonal elements and 2 non-diagonal elements, $a_{i,j} = a_{j,i} = 1$. Choosing i and j completely determines the permutation, so there are exactly $n_1 \cdot n_2$ permutations contributing to λ^{n-2}, each with negative sign. Consequently, $c^2 = n_1 n_2$ and thus $\lambda_1 = -\sqrt{n_1 n_2}$, $\lambda_n = \sqrt{n_1 n_2}$.

2. For K_n, the adjacency matrix is $J - I_n$, where J is the matrix of all ones. Subtracting c from the diagonal of a matrix M shifts its eigenvalues by $-c$, since $Mx = \lambda x$ is equivalent to $(M - cI_n)x = (\lambda - c)x$. By induction on n it can be shown that the spectrum of J consists of a single eigenvalue being n and $n - 1$ eigenvalues equal to zero. Thus the spectrum of K_n is $\lambda_1 = \cdots = \lambda_{n-1} = -1$, $\lambda_n = n - 1$. □

The adjacency matrix is also useful for counting paths of length k in a graph.

Lemma 14.1.5 ([576]). *Let G be a multi-digraph possibly with loops. The (i,j)th entry of A^k counts the $i \to j$-paths of length k. The eigenvalues of A^k are λ_i^k.*

Proof. The first claim can be shown by induction on k. For the second claim, note that for every eigenvector x with corresponding eigenvalue λ, $A^k x = A^{k-1}(Ax) = \lambda A^{k-1}x = \cdots = \lambda^k x$. □

Corollary 14.1.6. *1. $\sum_{i=1}^n \lambda_i =$ number of loops in G.*
2. $\sum_{i=1}^n \lambda_i^2 = 2 \cdot |E|$.
3. $\sum_{i=1}^n \lambda_i^3 = 6 \cdot$ number of triangles in G.

Now we can prove that the converse of the third claim in Lemma 14.1.3 is also true.

Lemma 14.1.7 ([576]). *G is bipartite if and only if the eigenvalues of G occur in pairs λ, λ' such that $\lambda = -\lambda'$.*

Proof. One direction of the claim has been shown in the proof of Lemma 14.1.3. For the other direction, note that $\lambda_i = -\lambda_j$ implies $\lambda_i^k = -\lambda_j^k$ for every odd k. Since $\text{trace}(A^k) = \sum_{i=1}^{k} \lambda_i^k = 0$ counts the number of cycles of length k in G, we infer that in particular there are no odd simple cycles which means that G is bipartite. □

We have seen that it is possible to retrieve certain structural properties of a graph (e.g. number of edges, number of triangles, whether or not it is bipartite) from its spectrum. However, the spectrum does not reflect all of the graph's structure. Take for example the graphs in Figure 14.4.

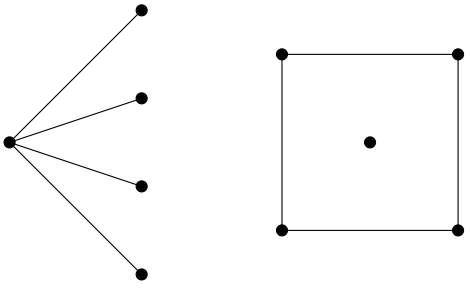


Fig. 14.4. Two non-isomorphic graphs with identical adjacency spectrum

Both have eigenvalues $\lambda_1 = -2,\ \lambda_2 = \lambda_3 = \lambda_4 = 0$, and $\lambda_5 = 2$, but they are not isomorphic. Such graphs are called *cospectral*. Obviously, we can not even determine from the spectrum if a graph is connected. Nevertheless, this can be achieved by looking at eigenvalues of another graph matrix, the Laplacian.

14.1.3 The Laplacian Spectrum

Let $G = (V, E)$ be an undirected multigraph (possibly with loops) with adjacency matrix A. Let $D = \text{diag}(d(1), \ldots, d(n))$ be the diagonal matrix of vertex degrees. The *Laplacian* matrix $L = (l_{i,j})$ is defined as $L := D - A$, so if G is a simple undirected graph, then

$$l_{i,j} = \begin{cases} -1, & \text{if } \{i,j\} \in E \\ d(i), & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

Another way of defining the Laplacian of an undirected simple graph is the following. Consider an arbitrary *orientation* of G, i.e. a mapping assigning each edge $e = \{i, j\}$ a direction by indicating whether i or j is to be viewed as the

head of e. The *incidence matrix* $B = (b_{i,e})$ of the oriented graph (G, σ) is a $\{0, 1, -1\}$ matrix with rows and columns indexed by the vertices and edges of G, respectively, such that

$$b_{i,e} := \begin{cases} 1, & \text{if } i \text{ is the head of } e \\ -1, & \text{if } i \text{ is the tail of } e \\ 0 & \text{otherwise.} \end{cases}$$

It can be shown that independently of the choice of σ, $L = BB^\top$. Consequently, we obtain the following result.

Lemma 14.1.8. *For each* $x \in \mathbb{C}^n$, $x^\top Lx = x^\top BB^\top x = \sum_{\{i,j\} \in E} (x_i - x_j)^2$.

Since A is real and symmetric, $L = D - A$ is also symmetric, and hence the Laplacian spectrum consists of n real eigenvalues $\lambda_1(L) \leq \cdots \leq \lambda_n(L)$. Again, we may interpret an eigenvector $x \in \mathbb{R}^n$ as an assignment of weights $\omega : V \to \mathbb{R}$, $i \mapsto x_i$. From this point of view, λ is an eigenvalue of L if there exists a non-zero (and not completely negative) weight function $\omega : V \to \mathbb{R}$ such that

$$\lambda\omega(i) = \sum_{j \in N(i)} (\omega(i) - \omega(j))$$

for all $i \in V$. Considering this equation for $i \in V$ with maximum weight, we see that $\lambda\omega(i) = \sum_{j \in N(i)} (\omega(i) - \omega(j)) \geq 0$, so all eigenvalues are non-negative. For $\omega \equiv 1$ we have $\lambda = \lambda\omega(i) = \sum_{j \in N(i)} (\omega(i) - \omega(j)) = 0$, hence the vector $\mathbf{1}_n$ is an eigenvector of L with eigenvalue 0.

Lemma 14.1.9 ([247]). *A graph G consists of k connected components if and only if $\lambda_1(L) = \cdots = \lambda_k(L) = 0$ and $\lambda_{k+1}(L) > 0$.*

Proof. Let B be the incidence matrix of an arbitrary orientation of G. For each component C of G define $z(C) \in \mathbb{R}^n$ by

$$z(C)_i := \begin{cases} 1, & \text{if } i \in V(C) \\ 0 & \text{otherwise.} \end{cases}$$

Then, $Z := \{z(C);\ C \text{ component of } G\}$ is linearly independent and $Lz(C) = BB^\top z(C) = \mathbf{0}_n$. Hence the connected component can be injectively mapped into a linearly independent set of eigenvectors with eigenvalue 0. On the other hand, if $z \in \mathbb{R}^n$ is a vector such that $Lz = BB^\top z = \mathbf{0}_n$, then $z^\top BB^\top z = 0$ implies $B^\top z = \mathbf{0}_n$, meaning that z must be constant on each connected component. Thus, z is a linear combination of elements from Z, and consequently we have exactly as many components as there are linearly independent eigenvectors corresponding to eigenvalue 0. □

The Laplacian is useful for counting the number of spanning trees of a graph.

Theorem 14.1.10 (Matrix-Tree Theorem [135, 247, 427]). *The Laplacian matrix L of a graph G is related to spanning trees in the following way.*

1. *For every* $i \in \{1, \ldots, n\}$ *the number of spanning trees in* G *is equal to* $|det(L_i)|$*, where* L_i *is obtained from the Laplacian* L *by deleting row* i *and column* i*.*
2. *Moreover, the number of spanning trees is equal to* $\frac{1}{n}\prod_{i\geq 2}\lambda_i(L)$*.*

While the Laplacian spectrum has the advantage over the adjacency spectrum of indicating the number of connected components of a graph, it fails to identify bipartite structures, as can be seen from the graphs in Figure 14.5 which are cospectral with respect to L.

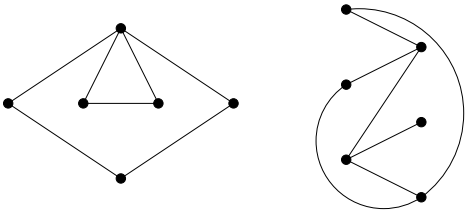


Fig. 14.5. Two cospectral graph with respect to the Laplacian

14.1.4 The Normalized Laplacian

A matrix whose spectrum enables us to recognize both, bipartite structure and connected components, can be obtained by multiplying L from left and right with the diagonal matrix $D^{-1/2}$, where the ith entry in the diagonal is $d(i)^{-1/2}$ if $d(i) > 0$ and 0 otherwise. This matrix is called the *normalized Laplacian* $\mathcal{L} = D^{-1/2}LD^{-1/2}$. For simple graphs, $\mathcal{L} = (\bar{l}_{i,j})$ satisfies

$$\bar{l}_{i,j} = \begin{cases} 1, & \text{if } i = j \text{ and } d(i) > 0 \\ -\frac{1}{\sqrt{d(i)d(j)}}, & \text{if } \{i,j\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

λ is an eigenvalue of $\mathcal{L}$ if there is a non-zero weight function $\omega : V \to \mathbb{C}$, such that

$$\lambda\omega(i) = \frac{1}{\sqrt{d(i)}} \sum_{j \in N(i)} \left(\frac{\omega(i)}{\sqrt{d(i)}} - \frac{\omega(j)}{\sqrt{d(j)}} \right).$$

Again, $\mathcal{L}$ is symmetric with real valued entries, and we can order its n eigenvalues in the sequence $\lambda_1(\mathcal{L}) \leq \cdots \leq \lambda_n(\mathcal{L})$.

The following claims are proved in [125].

Lemma 14.1.11 ([125]). *Let* G *be a graph with normalized Laplacian matrix* $\mathcal{L}$*.*

1. $\lambda_1(\mathcal{L}) = 0$, $\lambda_n(\mathcal{L}) \leq 2$.
2. *G is bipartite if and only if for each $\lambda(\mathcal{L})$, the value $2 - \lambda(\mathcal{L})$ is also an eigenvalue of $\mathcal{L}$.*
3. *If $\lambda_1(\mathcal{L}) = \cdots = \lambda_i(\mathcal{L}) = 0$ and $\lambda_{i+1}(\mathcal{L}) \neq 0$, then G has exactly i connected components.*

14.1.5 Comparison of Spectra

If G is graph where each vertex has exactly d neighbors, then $L = dI_n - A$ and $\mathcal{L} = I - D^{-1/2}AD^{-1/2}$. This implies that for d-regular graphs, the three spectra are equivalent. In particular, if $d > 0$ and

$$\begin{aligned} \text{spectrum}(A) &= (\lambda_1, \ldots\ldots\ldots, \lambda_n) \quad \text{then} \\ \text{spectrum}(L) &= (d - \lambda_n, \ldots, d - \lambda_1) \quad \text{and} \\ \text{spectrum}(\mathcal{L}) &= \left(1 - \frac{\lambda_n}{d}, \ldots, 1 - \frac{\lambda_1}{d}\right). \end{aligned}$$

In general, there is no simple relationship between the three spectra. Nevertheless, we can bound the eigenvalues of the adjacency matrix in terms of the Laplacian eigenvalues and the maximum and minimum vertex degrees.

Lemma 14.1.12 ([425]). *Let G be a graph with adjacency matrix A and Laplacian matrix L. If Δ and δ are the maximum and the minimum vertex degrees of G, respectively, then the kth smallest eigenvalue $\lambda_k(A)$ of A and the kth largest eigenvalue $\lambda_{n+1-k}(L)$ of L are related by*

$$\delta - \lambda_k(A) \leq \lambda_{n+1-k}(L) \leq \Delta - \lambda_k(A).$$

We will show this claim with the help of Courant-Fischer's characterization of the eigenvalues. This is a well-known theorem from linear algebra, however we include a proof for completeness.

Theorem 14.1.13 ([587]). *Let $M \in \mathbb{R}^{n \times n}$ be a real symmetric matrix with eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$. Then, for all $k \in \{1, \ldots, n\}$,*

$$\lambda_k = \min_{\substack{U \leq \mathbb{R}^n \\ \dim(U) = k}} \max_{\substack{x \in U \\ x \neq \mathbf{0}_n}} \frac{x^\top M x}{x^\top x}.$$

Proof. Let $\{v_1, \ldots, v_n\}$ be an orthonormal basis of eigenvectors of M for $\mathbb{R}^n$ such that $Mv_i = \lambda_i v_i$ for all $i \in \{1, \ldots, n\}$. For each $x \in \mathbb{R}^n$, $x \neq \mathbf{0}_n$, let $i_0(x) \in \{1, \ldots, n\}$ be maximal subject to the condition

$$x \perp v_i \text{ for all } i < i_0(x).$$

In other words, $i_0(x)$ is the first index for which $x \not\perp v_{i_0(x)}$. (x cannot be orthogonal to all vectors from the basis, because $x \neq \mathbf{0}_n$.) Therefore, there exist scalars $\mu_{i_0(x)}, \ldots, \mu_n \in \mathbb{R}$ such that

$$x = \sum_{i=i_0(x)}^{n} \mu_i v_i.$$

Consequently,

$$\begin{aligned} x^\top M x &= x^\top M \sum_{i=i_0(x)}^{n} \mu_i v_i = x^\top \sum_{i=i_0(x)}^{n} \mu_i M v_i \\ &= x^\top \sum_{i=i_0(x)}^{n} \mu_i \lambda_i v_i = \sum_{i=i_0(x)}^{n} \mu_i \lambda_i \underbrace{x^\top v_i}_{=\mu_i} \\ &\geq \lambda_{i_0(x)} \sum_{i=i_0(x)}^{n} \mu_i^2 = \lambda_{i_0(x)} x^\top x. \end{aligned} \tag{14.3}$$

Obviously, equality holds for $x = v_k$, i.e., for all $k \in \{1, \ldots, n\}$ we have,

$$v_k{}^\top M v_k = \lambda_k v_k{}^\top v_k. \tag{14.4}$$

We now make the following claim:

For every k-dimensional subspace $U \leq \mathbb{R}^n$ there exists $x \in U$, $x \neq \mathbf{0}_n$, such that $i_0(x) \geq k$. (14.5)

First, we explain how to prove the theorem from this claim. From (14.3) it follows that for every k-dimensional subspace U,

$$\max_{\substack{x \in U \\ x \neq \mathbf{0}_n}} \frac{x^\top M x}{x^\top x} \geq \lambda_k$$

On the other hand, because $\langle v_1, \ldots, v_k \rangle$ *is* a k-dimensional subspace, it follows from (14.4) that

$$\min_{\substack{U \leq \mathbb{R}^n \\ \dim(U) = k}} \max_{\substack{x \in U \\ x \neq \mathbf{0}_n}} \frac{x^\top M x}{x^\top x} = \lambda_k.$$

We now have to prove (14.5). For a contradiction, assume that for all $x \in U$, we have $i_0(x) < k$. By the definition of i_0 this means that for every $x \in U$ there exists an $i < k$ such that $x \not\perp v_i$ or equivalently, [1]

$$\langle v_1, \ldots, v_{k-1} \rangle^\perp \cap U = \mathbf{0}_n.$$

On the other hand

$$\dim \langle v_1, \ldots, v_{k-1} \rangle^\perp + \dim U = n - (k-1) + k = n + 1,$$

a contradiction. □

[1] Here, $\langle W \rangle$ denotes the linear hull of a subset $W \subseteq \mathbb{R}^n$, and $W^\perp$ denotes the set of all vectors that are orthogonal to each vector from W.

For later use, we state a simple corollary from this theorem.

Corollary 14.1.14. *(a) The largest eigenvalue λ_n of a real symmetric matrix $M \in \mathbb{R}^{n\times n}$ satisfies*

$$\lambda_n = \max_{\substack{x\in\mathbb{R}^n \\ x\neq \mathbf{0}_n}} \frac{x^\top M x}{x^\top x}.$$

(b) The second smallest eigenvalue of the Laplacian matrix satisfies

$$\lambda_2(L) = \min_{x\perp \mathbf{1}_n} \frac{x^\top L x}{x^\top x}.$$

Later, we will also use another characterization of Laplacian eigenvalues, which we cite without a proof. Let us call a vector $x \in \mathbb{R}^n$ *constant*, if all its entries are the same, i.e., if it is a multiple of $\mathbf{1}_n$.

Theorem 14.1.15 (Fiedler [211]).

$$\lambda_2(L) = n \min \left\{ \frac{\sum_{\{i,j\}\in E}(x_i - x_j)^2}{\sum_{\{i,j\}\in \binom{V}{2}}(x_i - x_j)^2};\ x \in \mathbb{R}^n \text{ non-constant} \right\} \tag{14.6}$$

$$\lambda_n(L) = n \max \left\{ \frac{\sum_{\{i,j\}\in E}(x_i - x_j)^2}{\sum_{\{i,j\}\in \binom{V}{2}}(x_i - x_j)^2};\ x \in \mathbb{R}^n \text{ non-constant} \right\} \tag{14.7}$$

Now, we turn to the proof of Lemma 14.1.12.

Proof (of Lemma 14.1.12). Since $\lambda_{n+1-k}(L)$ is the kth largest eigenvalue of L, $\delta - \lambda_{n+1-k}(L)$ is the kth smallest eigenvalue of the matrix $\delta I_n - L = A - (D - \delta I_n)$ which differs from A only on the diagonal, where the non-negative values $d(i) - \delta$ are subtracted. We have $\frac{x^\top (A-(D-\delta I_n))x}{x^\top x} = x^\top A x - r(x)$ for $r(x) := \frac{x^\top (D-\delta I_n)x}{x^\top x} \in \mathbb{R}_{\geq 0}$, and Theorem 14.1.13 gives

$$\begin{aligned}
\delta - \lambda_{n+1-k}(L) &= \lambda_k(\delta I_n - L) \\
&= \lambda_k(A - (D - \delta I_n)) \\
&= \min_{\substack{U\leq\mathbb{R}^n \\ \dim(U)=k}} \max_{\substack{x\in U \\ x\neq \mathbf{0}_n}} \frac{x^\top \left(A - (D - \delta I_n)\right) x}{x^\top x} \\
&= \min_{\substack{U\leq\mathbb{R}^n \\ \dim(U)=k}} \max_{\substack{x\in U \\ x\neq \mathbf{0}_n}} \left(\frac{x^\top A x}{x^\top x} - r(x) \right) \\
&\leq \min_{\substack{U\leq\mathbb{R}^n \\ \dim(U)=k}} \max_{\substack{x\in U \\ x\neq \mathbf{0}_n}} \frac{x^\top A x}{x^\top x} \\
&= \lambda_k(A).
\end{aligned}$$

The other inequality is obtained in a similar way. □

Figure 14.6 shows two non-isomorphic graphs that are cospectral with respect to all three matrices.

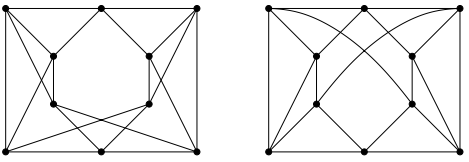


Fig. 14.6. Two graphs that are cospectral with respect to A, L, and $\mathcal{L}$

14.1.6 Examples

Table 14.1 lists the spectrum of the adjacency matrix A, the Laplacian L, and the normalized Laplacian $\mathcal{L}$ for some elementary graph classes. All graphs are assumed to have n vertices.

Table 14.1. Spectra of some elementary graph classes

graph class	spectrum(A)	spectrum(L)	spectrum($\mathcal{L}$)
simple path $G = P_n$	$2\cos\left(\frac{\pi k}{n+1}\right)$, $k \in \{1, \ldots, n\}$	$2 - 2\cos\left(\frac{\pi(k-1)}{n}\right)$, $k \in \{1, \ldots, n\}$	$1 - \cos\left(\frac{\pi(k-1)}{n-1}\right)$, $k \in \{1, \ldots, n\}$
simple cycle $G = C_n$	$2\cos\left(\frac{2\pi k}{n}\right)$, $k \in \{1, \ldots, n\}$	$2 - 2\cos\left(\frac{2\pi k}{n}\right)$, $k \in \{1, \ldots, n\}$	$1 - \cos\left(\frac{2\pi k}{n}\right)$, $k \in \{1, \ldots, n\}$
star $G = K_{1,n}$	$-\sqrt{n}, \sqrt{n}$, 0 ($n-2$ times)	$0, n$, 1 ($n-2$ times)	$0, 2$, 1 ($n-2$ times)
$G = K_{n_1,n_2}$	$-\sqrt{n_1 n_2}, \sqrt{n_1 n_2}$, $0 (n-2$ times)	$0, n_1$ ($n_2 - 1$ times) n_2 ($n_1 - 1$ times), n	$0, 2$ 1 ($n-2$ times)
$G = K_n$	$1, -1$ ($n-1$ times)	$0, n$ ($n-1$ times)	$0, \frac{n}{n-1}$ ($n-1$ times)

14.2 Numerical Methods

To use the spectrum of a graph for analysis, we have to compute it (or parts of it) first. What methods are available? What are their running times and other characteristics?

14.2.1 Methods for Computing the Whole Spectrum of Small Dense Matrices

It is not at all obvious how to compute the spectrum of a matrix M efficiently, since already a straightforward evaluation of the characteristic polynomial as $\det(M - \lambda I_n)$ takes $\mathcal{O}(n!)$ steps. A better strategy is to utilize the fact that as a graph matrix, M is real and (in case of undirected graphs) symmetric and thus can be transformed into a diagonal matrix by means of a similarity transformation $M \to P^{-1}MP$. If we are interested only in eigenvalues, not eigenvectors, it is enough to transform the matrix M to be triangular, with all elements below (or above) the diagonal equal to zero. In this case the diagonal elements are already the eigenvalues.
There is a two-stage technique for implementing the diagonalization strategy. In the first stage we iteratively approximate P (and P^{-1}) as a product of certain 'atomic' transformations P_i designed for zeroing a particular off-diagonal element (Jacobi transformation [482]) or a whole particular row or column (Householder transformation [482], elimination method [482]). We stop after $\mathcal{O}(n^3)$ steps with a matrix $\tilde{P}$ such that $M_1 = (m_{i,j}) := \tilde{P}^{-1}M\tilde{P}$ has tridiagonal form (i.e., $m_{i,j} = 0$ whenever $|i - j| > 1$). Now the second stage starts, where we perform a QL- (or QR-) decomposition: the basic idea is that any real matrix M' can be decomposed in the form $M' = QL$ (or QR), such that Q is orthogonal (i.e., $Q^T = Q^{-1}$) and L (R) is lower (upper) triangular. Writing these factors in opposite order we get $M'' := LQ = Q^TQLQ = Q^TM'L$, where properties such as symmetry and tridiagonal form are preserved. The QL-algorithm consists of a sequence of transformations

$$\begin{aligned} M_i &:= Q_iL_i, \\ M_{i+1} &:= L_iQ_i = Q_i^TM_iQ_i, \end{aligned}$$

and relies on the following theorem [535].

Theorem 14.2.1 ([535]). *1. If M has eigenvalues of different absolute value $|\lambda_i|$ then M_s converts to lower triangular form as $s \to \infty$.*
2. If M has an eigenvalue $|\lambda_i|$ of multiplicity p then M_s converts to lower triangular form as $s \to \infty$, except for a diagonal block matrix of order p, whose eigenvalues converge to λ_i.

Note that if M has an eigenvalue with multiplicity greater than one, then the second part of Theorem 14.2.1 allows us to split the matrix into submatrices that can be diagonalized separately. For tridiagonal matrices, one iteration of the QL-algorithm can be performed in $\mathcal{O}(n)$ steps. With the technique of implicit shifts [482] a reasonably good convergence is achieved in $\mathcal{O}(n)$ steps, resulting in a total number of $\mathcal{O}(n^2)$ steps for the second stage. Thus the overall complexity of computing all eigenvalues with 'good precision' is $\mathcal{O}(n^3)$.

14.2.2 Methods for Computing Part of the Spectrum of Large Sparse Matrices

When our given matrix M is very large, the computational and storage costs required for the diagonalization strategy of the previous section become prohibitive. However, in many situations M is sparse and it suffices to determine a small subset of (extremal) eigenvalues. Suppose, we are interested in the largest eigenvalue of M. The eigenvalue equation $Mx = \lambda x$ is clearly equivalent to $\lambda = \frac{x^\top Mx}{x^\top x}$. In fact, we have observed in Corollary 14.1.14 that

$$\lambda_n = \max\left\{\frac{x^\top Mx}{x^\top x};\ x \in \mathbb{R}^n \setminus \{\mathbf{0}_n\}\right\}.$$

This suggests a simple algorithm: Choose an arbitrary starting vector x_1 with $x_1^\top x_1 = 1$, and then follow the direction of steepest ascend to successively obtain an improved approximation to λ_n. The *Lanczos algorithm* is a run-time and storage cost efficient algorithm that uses this idea to approximate extremal eigenvalues of M. It proceeds as follows: a given initial vector x_1 is normalized to length one. Then at each step i an orthonormal basis $(x_1, x_2, \ldots, x_i)$ for the space spanned by $(x_1, Mx_1, \ldots, M^{i-1}x_1)$ is constructed (this space is called 'Krylov space'). Let X_i denote the $n \times i$-matrix with $x_1, x_2, \ldots, x_i$ as column vectors. The matrix $T = X_i^\top MX_i$ has tridiagonal form. Its eigenvalues — which are easy to calculate (see [2]) — provide approximations to i eigenvalues of M. The method favors convergence to eigenvalues in the outermost part of the spectrum of A. The process is restarted every k steps for some fixed $k \ll n$ until sufficiently good convergence is achieved. We state the Lanczos method in its simplest form as Algorithm 29.

Algorithm 29: The Lanczos algorithm

1. Initialization: Choose the number of steps k, the desired number of eigenvalues r and an initial vector x_1; let $\beta_0 := x_1^\top x_1$,. $x_1 := x_1/\beta_0$

2. Lanczos steps:
for $i = 1$ *to* k **do**
  (i) $y := Mx_i$
  (ii) $\alpha_i := x_i^\top y$
  (iii) $x_{i+1} := y - \alpha_i x_i - \beta_{i-1}x_{i-1}$
  (iv) $\beta_i := x_{i+1}^\top x_{i+1}$
  (v) $x_{i+1} := x_{i+1}/\beta_i$;
Set $X_i :=$Mat$(x_1, \ldots, x_i)$

3. Eigenvalue computation: Compute the eigenvalues of $T := X_i^\top MX_i$.

4. Convergence test and restart: If the first r columns of T satisfy the convergence criteria then accept the corresponding eigenvalues and stop. Otherwise restart with a suitable new x_1.

By replacing M with $(M - \mu I_n)^{-1}$ in step 2(i) of the algorithm, this scheme is capable of approximating eigenvalues in the vicinity of any given value μ. In general, the minimum number of Lanczos iterations necessary to compute a desired set of eigenvalues is unknown. In practice, a fast convergence can be achieved via a restarting scheme (see [591]). Farkas et al. [198] were able to compute the spectrum of graphs with up to 40,000 vertices and 200,000 edges with the 'thick-restart' version of the Lanczos algorithm. The *Arnoldi Method* differs from the Lanczos algorithm in replacing steps (ii)–(iv) with

(ii)' $h_{i,j} := x_j^\top y$ for all $j \in \{1, \ldots, i\}$
(iii)' $x_{i+1} := y - \sum_{j+1}^{i} x_j h_{j,i}$
(iv)' $h_{i,i+1} := x_{i+1}^\top x_{i+1},\ \beta_i := h_{i,i+1}$.

For symmetrical matrices, Arnoldi's and Lanczos' methods are mathematically equivalent, but the Lanczos algorithm uses fewer arithmetic operations per step by explicitly taking advantage of the symmetry of M. The advantage of Arnoldi's method is that it can be applied to treat asymmetric matrices. In that case, $H = X_i^\top M X_i$ is an upper Hessenberg matrix that can be reduced to block triangular form, allowing for an efficient computation of eigenvalues (see [509]).

14.3 Subgraphs and Operations on Graphs

What can the spectrum tell us about subgraphs in a graph? Do eigenvalues of subgraphs show up in the spectrum? Can we conclude that a certain graph is not a subgraph (or at least not an induced subgraph) by looking at the spectrum? What happens to the spectra of two graphs that are joined by taking the Cartesian product or the sum?

In this section, we will show some directions for answering these questions. We only consider the adjacency spectrum here, although many results also hold for the Laplacian spectra.

14.3.1 Interlacing Theorem

How do induced subgraphs manifest themselves in the spectrum? Obviously, not every induced subgraph inserts its eigenvalues or some of its eigenvalues into the spectrum of the whole graph. For example, the complete graph K_2 on two vertices has eigenvalues -1 and 1. But many graphs containing K_2 as an induced subgraph, i.e., an edge, do not have -1 or 1 in their spectrum. See Table 14.1 in Section 14.1.6 for examples.

However, there is an *interlacing* of the eigenvalues of induced subgraphs. Let $G = (V, E)$ be a graph on n vertices and let H be an induced subgraph of G with $n - 1$ vertices. (In other words: H is obtained from G be removing one vertex.) If, in our usual notation, $\lambda_1 \leq \ldots \leq \lambda_n$ are the eigenvalues of the adjacency matrix of G and $\mu_1 \leq \ldots \leq \mu_{n-1}$ are those of H, we have

$$\lambda_i \leq \mu_i \leq \lambda_{i+1} \quad \forall i \in \{1, \ldots, n-1\},$$

i.e., between two eigenvalues of G there lies exactly one eigenvalue of H. Consequently, if G has an eigenvalue with multiplicity k, then H has this eigenvalue with multiplicity $k-1$.

For an induced subgraph on m vertices, by induction (over the number of vertices removed to obtain H from G) the interlacing generalizes to

$$\lambda_i \leq \mu_i \leq \lambda_{i+(n-m)} \quad \forall i \in \{1,\dots,m\}. \tag{14.8}$$

We will now prove an even more general result than this, from which we will get (14.8) directly.

Theorem 14.3.1. *Let $n, m \in \mathbb{N}$ and $S \in \mathbb{R}^{n\times m}$ such that $S^\top S = \mathrm{Id}_m$. Let $A \in \mathbb{R}^{n\times n}$ be symmetric and $B := S^\top AS$. Then, for the eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ of A and the eigenvalues $\mu_1 \leq \ldots \leq \mu_m$ of B we have the interlacing property* (14.8)*, i.e.,*

$$\lambda_i \leq \mu_i \leq \lambda_{i+(n-m)} \quad \forall i \in \{1,\dots,m\}. \tag{14.9}$$

The interlacing property of the adjacency spectrum follows from this. To see this, let A be the adjacency matrix of G. The adjacency matrix of an induced subgraph H is a principal submatrix of A, i.e., a matrix that is obtained by deleting the ith row and ith column of A for every vertex $i \in V \setminus V(H)$. Such a principal submatrix can be obtained from A in the same way as B is obtained from A in the above theorem. If $i_1,\dots,i_k$ are the vertices removed from G to get H, we have to choose S to be the identity matrix with the i_jth row deleted, $j = 1,\dots,k$.

Proof (of Theorem 14.3.1). The matrix S defines an injective mapping from $\mathbb{R}^m$ to $\mathbb{R}^n$. For a subset $U \subseteq \mathbb{R}^m$ we as usually denote by $S(U)$ the image of U under that mapping, i.e.,

$$S(U) := \{Su;\ u \in U\}.$$

If $U \leq \mathbb{R}^m$ is an i-dimensional subspace ($i \leq m$), then $S(U)$ is an i-dimensional subspace of $\mathbb{R}^n$, because S is injective.

Remember the characterization of eigenvalues given in Theorem 14.1.13. For every $i \in \{1,\dots,m\}$ we have

$$\begin{aligned}
\lambda_i &= \min_{\substack{U\leq\mathbb{R}^n\\ \dim(U)=i}} \max_{\substack{x\in U\\ x\neq 0}} \frac{x^\top Ax}{x^\top x} \leq \min_{\substack{U\leq S(\mathbb{R}^m)\\ \dim(U)=i}} \max_{\substack{x\in U\\ x\neq 0}} \frac{x^\top Ax}{x^\top x} \\
&= \min_{\substack{U\leq\mathbb{R}^m\\ \dim(U)=i}} \max_{\substack{x\in S(U)\\ x\neq 0}} \frac{x^\top Ax}{x^\top x} = \min_{\substack{U\leq\mathbb{R}^m\\ \dim(U)=i}} \max_{\substack{x\in U\\ x\neq 0}} \frac{(Sx)^\top A(Sx)}{(Sx)^\top (Sx)} \\
&= \min_{\substack{U\leq\mathbb{R}^m\\ \dim(U)=i}} \max_{\substack{x\in U\\ x\neq 0}} \frac{x^\top (S^\top AS)x}{x^\top x} = \min_{\substack{U\leq\mathbb{R}^m\\ \dim(U)=i}} \max_{\substack{x\in U\\ x\neq 0}} \frac{x^\top Bx}{x^\top x} \\
&= \mu_i.
\end{aligned}$$

This is the first inequality of (14.9).

Applying the same argument to $-A$ instead of A, we get for every $k \in \{0, \ldots, m-1\}$ that $-\lambda_{n-k} \leq -\mu_{m-k}$, which means

$$\lambda_{n-k} \geq \mu_{m-k}.$$

Setting $k := m - i$ yields the second inequality of (14.9). □

From the Interlacing Theorem we immediately get the following corollary.

Corollary 14.3.2. *Let G and H be two graphs with eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ and $\mu_1 \leq \ldots \leq \mu_m$ respectively. If $\mu_1 < \lambda_1$ or $\lambda_n < \mu_n$, then H does not occur as an induced subgraph of G.*

For example, let G be a graph with all eigenvalues smaller than 2.

The graphs C_j, $j \in \mathbb{N}$, all have 2 as their largest eigenvalue (see Table 14.1 in Section 14.1.6). Hence, G does not contain a cycle as an induced subgraph. Because in every cycle, we can find a simple cycle, in which in turn we can find an induced simple cycle, G even is cycle-free.

We also know that G has no vertices of degree larger than 3. Otherwise, G would have a $K_{1,j}$, $j \geq 4$, as an induced subgraph, which has $\sqrt{j}$ (as largest eigenvalue) in its spectrum.

14.3.2 Grafting

Let us now approach the question about the role of subgraphs from a different direction. Suppose you have a graph G and another graph H and would like to modify G in a way that gives G some of the eigenvalues of H.

For a disconnected graph the spectrum is the union of the spectra of its components. This is easy to see. It also gives us a straightforward method for accomplishing our goal in the given setup: Simply add H to G as a separate component. However this is not a suitable approach in case one has to preserve the connectivity of the graph.

Let λ be an eigenvalue of H which we would like to add to the spectrum of G. Let us first consider the special case that the eigenvector x corresponding to λ has an entry equal to zero, say, $x_{i_0} = 0$. Think of the graph G' as the union of G and H where the vertex i_0 of H has been identified with some arbitrary vertex of G. Formally, we define G' from $G = (V(G), E(G))$ and $H = (V(H), E(H))$ by picking a vertex $j_0 \in V(G)$ and setting

$$V(G') := V(G) \cup (V(H) \setminus \{i_0\}) \text{ and}$$
$$E(G') := E(G) \cup E(H - i_0) \cup \{\{j_0, i\};\ i \in V(H), \{i_0, i\} \in E(H)\}.$$

We say that H is *grafted* onto G along i_0 and j_0.

To get an eigenvector for λ, assign 0 to all vertices of G in G'. To the vertices of $H - i_0$ in G' assign the values given by the eigenvector x. Using the combinatorial interpretation of eigenvectors (Remark 14.1.2), one easily verifies that this yields an eigenvector of G' for eigenvalue λ. See Figure 14.7 for an example.

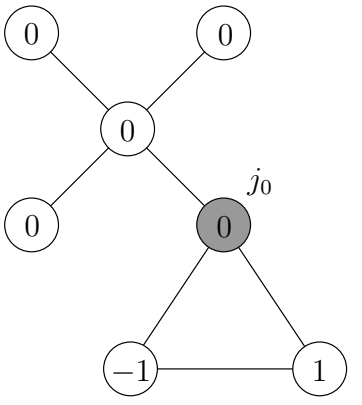


Fig. 14.7. A triangle grafted on a star of five vertices. The new graph has an eigenvalue -1, which the star alone did not have

But what if we do not have an eigenvector of H for λ with an entry equal to zero? We can still do a similar trick. We pick a vertex $i_0 \in V(H)$ and make two copies H^+ and H^- of H. The copies of a vertex $i \in V(H)$ are called i^+ and i^- respectively. We then take a new vertex i_1 and connect H^+ with H^- via two new edges $\{i_0^+, i_1\}$ and $\{i_1, i_0^-\}$. Call the resulting graph $\tilde{H}$.

Let λ be an eigenvalue of H and x a corresponding eigenvector. Then the following vector $\tilde{x}$ is an eigenvector of $\tilde{H}$ with the same eigenvalue λ.

$$\tilde{x}_{i^+} := x_i \text{ and } \tilde{x}_{i^-} := -x_i \quad \forall i \in V(H)$$

and

$$\tilde{x}_{i_1} := 0.$$

Now, $\tilde{H}$ can be grafted onto G along i_1 and an arbitrary vertex $j_0 \in V(G)$. We call such a construction a *symmetric graft*. Note, that if H is a tree, $\tilde{H}$ will be a tree as well. Symmetric grafts of trees play an important role in the analysis of spectra of random graphs [49]; see also the notes about sparse random graphs in 14.5.2.

As an example, consider the path on three vertices, P_3. This graph has an eigenvalue $\sqrt{2}$ with eigenvector $(1/\sqrt{2}, 1, 1/\sqrt{2})^\top$. Take the middle vertex as i_0. Figure 14.8 shows the symmetric construction ready to be grafted along i_1.

Finally we remark that grafting along one vertex can be extended in a natural way to grafting along several vertices.

14.3.3 Operations on Graphs

Consider two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$. The *sum* $G_1 + G_2$ is a graph on $V_1 \times V_2$ where two vertices $(i_1, i_2), (j_1, j_2) \in V_1 \times V_2$ are connected if either (but not both!) $\{i_1, j_1\} \in E_1$ or $\{i_2, j_2\} \in E_2$. On the other hand, letting

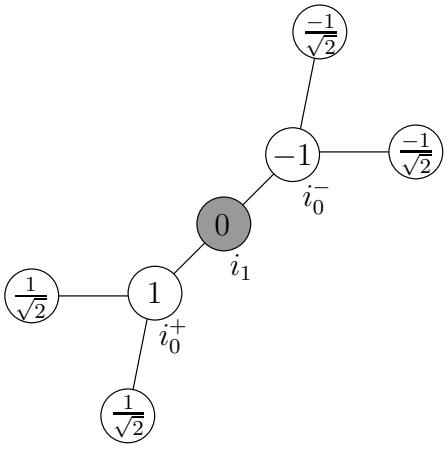


Fig. 14.8. A symmetric construction from two copies of P_3, ready to be grafted

(i_1, i_2) and (j_1, j_2) share an edge if and only if $\{i_1, j_1\} \in E_1$ and $\{i_2, j_2\} \in E_2$ defines the *Cartesian product* graph $G_1 \times G_2$. Figure 14.9 depicts the sum and the product of a simple path on four vertices with itself.

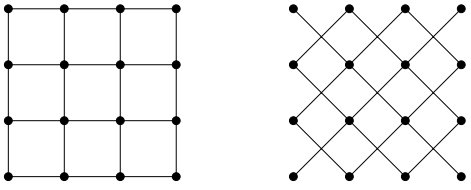


Fig. 14.9. The sum and the Cartesian product of a 4-vertex simple path with itself

It is easy to compute the eigenvalues of $G_1 + G_2$ and $G_1 \times G_2$ from the spectra of G_1 and G_2.

Lemma 14.3.3. *(a) spectrum*$(G + H) =$ *spectrum*$(G) +$ *spectrum*(H)*.*
(b) spectrum$(G \times H) =$ *spectrum*$(G) \cdot$ *spectrum*(H)*.*

More general, the spectrum of any *non-complete extended p-sum* of graphs is determined by the individual spectra.

Definition 14.3.4 ([135]). *Let $p \in \mathbb{N}_{\geq 2}$ and let $\mathcal{B} \subseteq \{0,1\}^p \setminus \mathbf{0}_p$. The non-complete extended p-sum of graphs $G_1 = (V_1, E_1), \ldots, G_p = (V_p, E_p)$ with basis $\mathcal{B}$ is the graph $NEpS(G_k)_{k=1}^p$ with vertex set $V_1 \times \cdots \times V_p$, in which two vertices $(i_1, \ldots, i_p), (j_1, \ldots, j_p)$ are adjacent if and only if there exists $\beta \in \mathcal{B}$ such that $i_k = j_k$ whenever $\beta_k = 0$ and $\{i_k, j_k\} \in E_k$ whenever $\beta_k = 1$.*

Theorem 14.3.5 ([135]). *Let $p \in \mathbb{N}_{\geq 2}$. For each $k \in \{1, \ldots, p\}$ let G_k be a graph on n_k vertices with spectrum $\lambda_{k1}, \ldots, \lambda_{kn_k}$. Then*

$$\mathit{spectrum}(\mathit{NEpS}(G_k)_{k=1}^{p}) = \left\{ \sum_{\beta \in \mathcal{B}} \lambda_{1i_1}^{\beta_1} \cdot \ldots \cdot \lambda_{pi_p}^{\beta_p};\ (i_1, \ldots, i_k) \in I \right\},$$

where

$$I := \{1, \ldots, n_1\} \times \ldots \times \{1, \ldots, n_k\}.$$

Note that the sum and the Cartesian product of graphs are NEpS with $p = 2$ and basis $\mathcal{B} = \{(1,0),(0,1)\}$ resp. $\mathcal{B} = \{(1,1)\}$.

14.4 Bounds on Global Statistics

Certain eigenvalues, especially the extreme eigenvalues, give bounds for global statistics. Recall from Section 11.7 in Chapter 11 that a global statistic assigns to each graph (from some class of graphs) a single value. These statistics are sometimes also called *graph parameters*.

We will study a selection of eigenvalue bounds on graph parameters.

Average Degree

Recall that the degree $d(i)$ of a vertex i is the number of edges incident with i. Denote the *average degree* by $\bar{d}$, i.e.,

$$\bar{d} := \frac{1}{n} \sum_{i \in V} d(i). \tag{14.10}$$

The average degree is related to the largest eigenvalue of the adjacency matrix, as seen in the following observation.

Lemma 14.4.1. *Let G be a graph and $\bar{d}$ its average degree. Then*

$$\bar{d} \leq \lambda_n.$$

Proof. Let $x := \mathbf{1}_n$ be the n-dimensional vector with all entries equal to 1. Then by Corollary 14.1.14 we have

$$\lambda_n \geq \frac{x^\top A x}{x^\top x} = \frac{\sum_{i \in V} d(i)}{n} = \bar{d}.$$

□

Diameter and Mean Distance

We only cite some results in this section. Recall that the diameter is the largest distance between two vertices. Eigenvalues of the Laplacian provide bounds on the diameter of a connected graph.

Theorem 14.4.2 ([126, 426]). *Let $\alpha > 1$. Then*

$$\operatorname{diam}(G) \leq 2 \left\lfloor \frac{\cosh^{-1}(n-1)}{\cosh^{-1}\left(\frac{\lambda_n(L)+\lambda_2(L)}{\lambda_n(L)-\lambda_2(L)}\right)} \right\rfloor + 1$$

and

$$\operatorname{diam}(G) \geq \left\lceil \frac{4}{n\lambda_2(L)} \right\rceil.$$

Recall that the mean distance $\bar{\rho}$ is the average over all distances between distinct vertices.

Theorem 14.4.3 ([426]). *The mean distance is bounded by Laplacian eigenvalues in the following way:*

$$\frac{1}{n-1}\left(\frac{2}{\lambda_2(L)} + \frac{n-2}{2}\right) \leq \bar{\rho}(G) \leq \frac{n}{n-1}\left\lceil \frac{\Delta + \lambda_2(L)}{4\lambda_2(L)} \ln(n-1) \right\rceil.$$

Connectivity

We already know that $\lambda_2(L)$ is non-zero if and only if the graph is connected. Fiedler [210] noticed more relations between $\lambda_2(L)$ and connectivity properties. $\lambda_2(L)$ is therefore also called the *algebraic connectivity*. We only cite his results.

Theorem 14.4.4 ([210]). *Let G be a graph and $\omega = \frac{\pi}{n}$. Let $\kappa(G)$ and $\eta(G)$ denote the minimum number of nodes and edges, respectively that have to be removed in order to make G disconnected. Then,*

1. $\lambda_2(L) \leq \kappa(G) \leq \eta(G)$,
2. $\lambda_2(L) \geq 2\eta(G)(1-\cos\omega)$, *and*
3. $\lambda_2(L) \geq 2(\cos\omega - \cos 2\omega)\eta(G) - 2\cos\omega(1-\cos\omega)\Delta(G)$.

Isoperimetric Number

The isoperimetric number is defined as follows:

$$i(G) := \min\left\{ \frac{|E(X,Y)|}{\min\{|X|,|Y|\}};\ \emptyset \neq X \underset{\neq}{\subset} V,\ Y = V \setminus X \right\},$$

where $E(X,Y)$ denotes the set of edges connecting X with Y. The definition characterizes $i(G)$ as the size of a smallest possible edge-cut separating as large a subset X as possible from the remaining larger part Y (we assume $|X| \leq |Y|$

w.l.o.g.). Hence, $i(G)$ is a measure of how many edges we have to remove from a network to isolate a large portion of nodes. This relates $i(G)$ to both, network connectivity and the min-bisection problem, which has important applications in VLSI design.

Obviously, by choosing $X = \{v\}$ with $d(v) = \delta(G)$, we see that

$$i(G) \leq \delta(G). \tag{14.11}$$

If G is disconnected, we have $i(G) = 0$.

A well-known relationship between the isoperimetric number and $\lambda_2(L)$ states that $i(G) \geq \frac{\lambda_2(L)}{2}$. For the case of $\lambda_2(L) \leq 2$, this bound is outperformed by the following result.

Theorem 14.4.5 ([176]). *The isoperimetric number is bounded from below by Laplacian eigenvalues in the following way:*

$$i(G) \geq \min\left\{1, \frac{\lambda_2(L)\lambda_n(L)}{2(\lambda_n(L) + \lambda_2(L) - 2)}\right\}.$$

We will now look at an upper bound following [425].

Proposition 14.4.6. *Let G be a graph with maximum degree Δ that is not a complete graph. Then,*

$$\lambda_2(L) \leq \Delta.$$

Proof. If G is disconnected, then $\lambda_2(L) = 0 \leq \Delta$. So let G be connected. Then G contains a path on three vertices P_3 as an induced subgraph. (Otherwise, G would be complete: Take two vertices i and j and by induction on the length of the shortest i-j path show that there exists an edge $\{i, j\}$.) By the examples in Table 14.1 in Section 14.1.6 we know that $\lambda_2(A(P_3)) = 0$. Hence, by the Interlacing Theorem, see (14.8), we get

$$0 = \lambda_2(A(P_3)) \leq \lambda_{n-1}(A).$$

We also know from Lemma 14.1.12 that

$$\lambda_2(L) \leq \Delta - \lambda_{n-1}(A) \leq \Delta.$$

□

With the help of the preceding proposition, we can prove:

Theorem 14.4.7. *Let $G = (V, E)$ be a graph not equal to K_1, K_2 or K_3 with n vertices and m edges. Then*

$$i(G) \leq \sqrt{\lambda_2(L)(2\Delta - \lambda_2(L))}. \tag{14.12}$$

The proof takes up several pages and includes some more technical details. Nevertheless it is a nice proof and an interesting example, how we can obtain non-trivial bounds from Laplacian eigenvalues. It is therefore presented in an extra section 14.4.1 at the end of this section.

Expansion

Many times a good vertex expansion is a desired property of a network. One common definition capturing this property that 'all small sets of nodes have large neighborhoods' is the following.

$$c_V := \min\left\{\frac{|N(S)\setminus S|}{|S|};\ S\subseteq V,\ |S|\leq\frac{n}{2}\right\}.$$

A large vertex expansion c_V is crucial, e.g. for the construction of parallel sorting networks, superconcentrators, fault-tolerant networks, and networks for simulating random generators, the latter being an important means for derandomization via small sample spaces. Using probabilistic methods, one can generate a random network that will have good expansion properties almost surely, but it is hard to measure the expansion properties from the definition. Therefore the following bounds are very useful.

Theorem 14.4.8 ([19]). $\frac{\lambda_2(L)}{\frac{\Delta}{2}+\lambda_2(L)}\leq c_V=\mathcal{O}(\sqrt{\lambda_2(L)})$.

A graph with expansion at least α is called an *α-magnifier*.

Let us prove a weak version of Theorem 14.4.8 for regular graphs.

Theorem 14.4.9 ([576]). *A d-regular graph is a $\frac{\lambda_2(L)}{2d}$-magnifier.*

Proof. Let $G=(V,E)$ be a d-regular graph on $V=\{1,\ldots,n\}$. Take a subset S of V of cardinality $s\leq n/2$. Define a vector $x\in\{s-n,s\}^n$ by

$$x_i := \begin{cases} s-n, & i\in S \\ s, & i\in V\setminus S. \end{cases}$$

By definition of L, $x^\top Lx = x^\top(D-A)x = d\sum_{i=1}^n x_i^2 - \sum_{i=1}^n x_i\sum_{\{i,j\}\in E}x_j = \sum_{\{i,j\}\in E}(x_i-x_j)^2 = n^2\cdot|E(S,V\setminus S)|$, where $E(S,V\setminus S)$ is the set of edges with exactly one end point in S. Since $\sum_i x_i = s(s-n)+(n-s)s = 0$, we see that x is perpendicular to the eigenvector $\mathbf{1}_n$ of L which corresponds to the eigenvalue 0. From Corollary 14.1.14 we conclude that $n^2|(S,\bar{S})| = x^\top Lx \geq \lambda_2(L)x^\top x = \lambda_2(L)sn(n-s)$, and consequently $|N(S)|\geq\frac{|(S,\bar{S})|}{d}\geq\frac{\lambda_2(L)s(n-s)}{dn}\geq\frac{\lambda_2(L)|S|}{2d}$ as claimed. □

For results on the closely related Cheeger constants see [125].

Routing Number

Consider a set of (distinguishable) 'pebbles'. Initially, each pebble is located on a distinct vertex of the connected graph $G=(V,E)$, $|V|=n$. We are given a permutation π on V. The goal is to move each pebble which at the start is on vertex $i\in V$ to vertex $\pi(i)$. This has to be done in a number of steps of the following form. At each step, choose a set of disjoint edges $E_0\subseteq E$ and interchange the pebbles at the endpoints of each edge in E_0.

The minimum number of steps required to accomplish the goal is denoted by $rt(G, \pi)$. The *routing number* $rt(G)$ of G is

$$rt(G) := \max_{\pi \in S_n} rt(G, \pi).$$

Now let G be connected and d-regular. We can upper bound the routing number in terms of λ_{n-1}. We only cite the following result.

Theorem 14.4.10 ([21]). *Let G be a d-regular connected graph. Then we have $\lambda_{n-1} < d$ and*

$$rt(G) = \mathcal{O}\left(\frac{d^2}{(d - \lambda_{n-1})^2} \log^2 n\right).$$

Chromatic Number

A *coloring* of a graph is an assignment of colors, e.g., natural numbers, to the vertices such that adjacent vertices have different colors. We speak of a *k-coloring* if the graph is assigned k different colors. The *chromatic number* of a graph is the minimum number of colors required for a coloring. We denote the chromatic number by $\chi(G)$.

It is well-known that computing the chromatic number is $\mathcal{NP}$-hard. However, eigenvalues provide us with lower and upper bounds. We consider only eigenvalues of the adjacency matrix.

Theorem 14.4.11 ([428]). *Let G be a graph. Then*

$$\chi(G) \leq 1 + \lambda_n.$$

Proof. Let H be a subgraph of G without isolated vertices and such that

$$\chi(H) = \chi(G) \text{ and for every edge } e \text{ in } H \text{ we have } \chi(H - e) < \chi(H). \quad (14.13)$$

It is easy to show that such a subgraph always exists and that in fact $\chi(H - e) = \chi(H) - 1$. We have $\chi(H) \leq \delta(H) + 1$. To see this, assume $\chi(H) > \delta(H) + 1$ and let $i \in V(H)$ be a vertex with $d_H(i) = \delta(H)$. Let $j \in N(i)$ and $e = \{i, j\}$. Then $k := \chi(H - e) = \chi(H) - 1 > \delta(H)$. Because $d_H(i) = \delta(H)$, we can construct a k-coloring of H from a k-coloring of $H - e$. This is a contradiction to (14.13).

From Lemma 14.4.1 and the Interlacing Theorem (14.8), we derive

$$\chi(G) - 1 = \chi(H) - 1 \leq \delta(H) \leq \lambda_n(H) \leq \lambda_n(G).$$

□

It is possible to actually find a $1 + \lambda_n$–coloring in polynomial time; see [428] for details.

Theorem 14.4.12 ([246, 268]). *Let G be a graph. Then*

$$1 - \frac{\lambda_n}{\lambda_1} \leq \chi(G).$$

Theorem 14.4.13 ([135]). *Let G be a graph. Then*

$$\frac{n}{n - \lambda_n} \leq \chi(G).$$

Independence Number

An *independent set* is a set of vertices such that none of them is adjacent to another vertex from that set. Independent sets are also called *stable sets*. For a graph G, the *independence number* $\alpha(G)$ is the cardinality of an independent set of maximal cardinality among all independent sets of G.

We will follow [427] in extending the following result due to Hoffman and Lovász [397].

Theorem 14.4.14. *Let G be a d-regular graph. Then*

$$\alpha(G) \leq n\left(1 - \frac{d}{\lambda_n(L)}\right).$$

Now, let $G = (V, E)$ be a graph with n vertices and degrees

$$d_1 \leq d_2 \ldots \leq d_n.$$

Set

$$\bar{d}_s := \frac{1}{s} \sum_{i \in \{1,\ldots,s\}} d_i \text{ for all } s \in \{1, \ldots, n\}.$$

Then the sequence $\bar{d}_1, \bar{d}_2, \ldots, \bar{d}_n$ is non-decreasing and for a d-regular graph $\bar{d}_s = d$ for all $s \in \{1, \ldots, n\}$.

Theorem 14.4.15. *Let s_0 be the smallest integer such that*

$$\bar{d}_{s_0} > \frac{\lambda_n(L)(n - s_0)}{n}.$$

Then

$$\alpha(G) \leq s_0 - 1,$$

and consequently

$$\alpha(G) \leq n\left(1 - \frac{\bar{d}_{s_0-1}}{\lambda_n(L)}\right).$$

Proof. We will show that

$$\frac{\lambda_n(L)(n - s)}{n} \geq \bar{d}_s \tag{14.14}$$

whenever there is a stable set of size $s > 1$ in G. To this end, let $S \subseteq V$ be a stable set of size $s := |S| > 1$. Equation (14.14) is true for $s = n$, since then $\bar{d}_i = 0$ for all $i \in \{1, \ldots, n\}$. So let $s < n$. Define $x \in \mathbb{R}^n$ by

$$x_i := \begin{cases} 0 & \text{if } i \in S \\ 1 & \text{otherwise} \end{cases}.$$

Then x is non-constant, i.e., not a multiple of $\mathbf{1}$. By Fiedler's characterization, Theorem 14.1.15, equation (14.7), we have

$$\lambda_n(L) \geq n \frac{\sum_{\{i,j\}\in E}(x_i - x_j)^2}{\sum_{\{i,j\}\in\binom{V}{2}}(x_i - x_j)^2} = n\frac{|E(S, V \setminus S)|}{s(n-s)}.$$

Because S contains no edges, we have $|E(S, V \setminus S)| \geq s\bar{d}_s$, and so

$$\lambda_n(L) \geq n\frac{s\bar{d}_s}{s(n-s)} = n\frac{\bar{d}_s}{n-s}.$$

This yields (14.14).

Now let s_0 be the first integer that violates (14.14). Then, there is no stable set of cardinality s_0. Because $(\bar{d}_s)_{s=1,\ldots,n}$ is non-decreasing, all $s \geq s_0$ violate (14.14) as well, and so there cannot be a stable set larger than $s_0 - 1$. □

Bisection Width

Given a graph with an even number of vertices, the Minimum Bisection problem aims at partitioning the vertices into two classes of equal size that are connected by as few edges as possible. The minimum number of edges between the two classes is called the *bisection width* of the graph. The decision version of the Minimum Bisection problem is $\mathcal{NP}$-complete [241], and the currently best polynomial approximation algorithm is guaranteed only to stay within a multiplicative error of $\mathcal{O}(\log^2 n)$ [203]. The following bound on the bisection width is a special case of a result of Alon and Milman [23].

Lemma 14.4.16. *Let $G = (V, E)$ be a graph on $\{1, \ldots, n\}$, where n is an even positive integer, then*

$$bw(G) \geq \frac{n}{4}\lambda_2(L).$$

Proof. Let S be an arbitrary subset of V of cardinality $\frac{n}{2}$ and define

$$x_i := \begin{cases} 1, & i \in S \\ -1, & i \notin S \end{cases}$$

for all $i \in V$. Then $\sum_{i\in V} x_i = 0$. Hence $x \perp \mathbf{1}_n$ and by Corollary 14.1.14 and Lemma 14.1.8 we have $n\lambda_2(L) = x^\top x\lambda_2(L) \leq x^\top Lx = \sum_{\{i,j\}\in E}(x_i - x_j)^2 = \sum_{\{i,j\}\in E(S,V\setminus S)}(x_i - x_j)^2 = 4 \cdot |E(S, V \setminus S)|$. Choosing S as one class of a minimum bisection yields the claim. □

Bezrukow et al. [60] have shown that this bound is tight if and only if all vertices are incident with exactly $\frac{\lambda_2(L)}{2}$ cut edges, which is true, e.g., for complete graphs, complete bipartite graphs, hypercubes, and the Petersen graph. However, for the $\sqrt{n} \times \sqrt{n}$ grid graph, the bisection width is $\sqrt{n}$ while $\lambda_2(L) = 2 - 2\cos(\pi/\sqrt{n}) \approx \pi^2/n$ [60] and hence $\frac{n}{4} \cdot \lambda_2(L) \approx \frac{\pi^2}{4}$. So the gap between the optimal bisection width and the bound of Lemma 14.4.16 can be large.

As mentioned earlier, the bisection width is closely related to the isoperimetric number: directly from the definition of $i(G)$ and $\mathrm{bw}(G)$ we obtain $i(G) \leq \frac{2\mathrm{bw}(G)}{n}$. Hence, lower bounds on $i(G)$ yield lower bounds on $\mathrm{bw}(G)$.

14.4.1 Proof of Theorem 14.4.7

Recall that $G = (V, E)$ is a graph not equal to K_1, K_2 or K_3 with n vertices and m edges. We have to prove

$$i(G) \leq \sqrt{\lambda_2(L)(2\Delta - \lambda_2(L))}. \tag{14.15}$$

For the proof, let us write $\lambda := \lambda_2(L)$, $\delta := \delta(G)$, and $\Delta := \Delta(G)$.

If $\lambda = 0$, then G is disconnected and so $i(G) = 0$, and we are done. The case that G is a complete graph on $n \geq 4$ vertices or more can be dealt with easily by using $\lambda = n$, see 14.1.6.

Hence we may assume that G is not a complete graph. Then by Proposition 14.4.6, we have $\lambda \leq \Delta$. If $\delta < \lambda$, we have

$$\lambda(2\Delta - \lambda) > \delta(2\Delta - \lambda) \geq \delta(2\Delta - \Delta) = \delta\Delta \geq \delta^2 \underset{(14.11)}{\geq} i(G)^2.$$

This is (14.15). We now may assume that

$$\lambda \leq \delta. \tag{14.16}$$

Let $y \in \mathbb{R}^n$ be an eigenvector for λ and set $W := \{i \in V;\ y_i > 0\}$. Then, perhaps after switching from y to $-y$, we have $|W| = \min\{|W|, |V \setminus W|\}$. Define

$$g_i := \begin{cases} y_i & \text{if } i \in W \\ 0 & \text{otherwise} \end{cases}.$$

Let $E(W) \subseteq E$ be the edges between vertices from W. We have

$$\begin{aligned}
&\sum_{i \in W} \Big(d(i) y_i \pm \sum_{j:\, \{i,j\} \in E} y_j \Big) y_i \\
&= \sum_{i \in W} \sum_{j:\, \{i,j\} \in E} (y_i \pm y_j) y_i \\
&= \sum_{\{i,j\} \in E(W)} ((y_i \pm y_j) y_i + (y_j \pm y_i) y_j) + \sum_{\{i,j\} \in E(W, V \setminus W)} (y_i \pm y_j) y_i \\
&= \sum_{\{i,j\} \in E(W)} (y_i \pm y_j)^2 + \sum_{\{i,j\} \in E(W, V \setminus W)} (y_i \pm y_j) y_i \\
&= \sum_{\{i,j\} \in E(W)} (y_i \pm y_j)^2 + \sum_{i \in W} d(i) y_i^2 \pm \sum_{\{i,j\} \in E(W, V \setminus W)} y_j y_i \\
&= \sum_{\{i,j\} \in E} (g_i \pm g_j)^2 - \sum_{i \in W} d(i) g_i^2 + \sum_{i \in W} d(i) y_i^2 \pm \sum_{\{i,j\} \in E(W, V \setminus W)} y_j y_i \\
&= \sum_{\{i,j\} \in E} (g_i \pm g_j)^2 \pm \sum_{\{i,j\} \in E(W, V \setminus W)} y_j y_i.
\end{aligned} \tag{14.17}$$

Keep in mind that when summing over all edges $\{i,j\} \in E$, the terms must not depend on which end of the edge actually is i and which is j. Observe that this is always the case here, e.g., in the preceding calculation because $(g_i \pm g_j)^2 = (g_j \pm g_i)^2$ for all $i, j \in V$.

Using the eigenvalue property of y we get

$$\lambda y_i = d(i) y_i - \sum_{j:\, \{i,j\} \in E} y_j \quad \forall i \in V. \tag{14.18}$$

This, together with the '$-$' version of (14.17), yields

$$\begin{aligned} \lambda \sum_{i \in W} y_i^2 &= \sum_{i \in W} \Big(d(i) y_i - \sum_{j:\, \{i,j\} \in E} y_j \Big) y_i \\ &\underset{(14.17)}{=} \sum_{\{i,j\} \in E} (g_i - g_j)^2 - \sum_{\{i,j\} \in E(W, V \setminus W)} y_j y_i, \end{aligned} \tag{14.19}$$

and using the '$+$' version of (14.17)

$$\begin{aligned} &(2\Delta - \lambda) \sum_{i \in W} y_i^2 \\ &= 2\Delta \sum_{i \in W} y_i^2 - \sum_{i \in W} d(i) y_i^2 + \sum_{i \in W} \sum_{j:\, \{i,j\} \in E} y_j y_i \\ &\geq \sum_{i \in W} d(i) y_i^2 + \sum_{i \in W} \sum_{j:\, \{i,j\} \in E} y_j y_i \\ &\underset{(14.17)}{=} \sum_{\{i,j\} \in E} (g_i + g_j)^2 + \sum_{\{i,j\} \in E(W, V \setminus W)} y_j y_i. \end{aligned} \tag{14.20}$$

Set $\alpha := \sum_{\{i,j\} \in E(W, V \setminus W)} y_i y_j$. Because the left and right hand sides of (14.19) are not negative, using (14.20) we derive

$$\begin{aligned} &\lambda(2\Delta - \lambda) \Big(\sum_{i \in W} y_i^2 \Big)^2 \\ &\geq \sum_{\{i,j\} \in E} (g_i + g_j)^2 \sum_{\{i,j\} \in E} (g_i - g_j)^2 \\ &\quad + \alpha \Big(\sum_{\{i,j\} \in E} (g_i - g_j)^2 - \sum_{\{i,j\} \in E} (g_i + g_j)^2 \Big) - \alpha^2 \\ &= \sum_{\{i,j\} \in E} (g_i + g_j)^2 \sum_{\{i,j\} \in E} (g_i - g_j)^2 - \alpha \Big(4 \sum_{\{i,j\} \in E(W)} y_i y_j + \alpha \Big). \end{aligned} \tag{14.21}$$

We would like to drop the 'α' term completely in this equation. To this end, observe that by the definition of W we have $\alpha \leq 0$. Furthermore, using again the eigenvalue property of λ (see also (14.18)), we have

$$
\begin{aligned}
& 4 \sum_{\{i,j\} \in E(W)} y_i y_j + \alpha \\
&= 2 \sum_{\{i,j\} \in E(W)} y_i y_j + 2 \sum_{\{i,j\} \in E(W)} y_i y_j + \sum_{\{i,j\} \in E(W, V \setminus W)} y_i y_j \\
&= 2 \sum_{\{i,j\} \in E(W)} y_i y_j + \sum_{i \in W} y_i \sum_{j \colon \{i,j\} \in E} y_j \\
&= 2 \sum_{\{i,j\} \in E(W)} \underbrace{y_i y_j}_{\geq 0} + \sum_{i \in W} \underbrace{(d(i) - \lambda)}_{\geq 0} y_i^2 \\
&\geq 0,
\end{aligned}
$$

because of the definition of W and (14.16). We thus have by (14.21)

$$
\lambda(2\Delta - \lambda) \Big(\sum_{i \in W} y_i^2 \Big)^2 \geq \sum_{\{i,j\} \in E} (g_i + g_j)^2 \sum_{\{i,j\} \in E} (g_i - g_j)^2. \tag{14.22}
$$

Define $v, w \in \mathbb{R}^m$ by $v_{\{i,j\}} := g_i + g_j$ and $w_{\{i,j\}} := |g_i - g_j|$. We apply the Cauchy-Schwartz inequality to v and w, getting

$$
\begin{aligned}
& \Big(\sum_{\{i,j\} \in E} \left| g_i^2 - g_j^2 \right| \Big)^2 \\
&= \Big(\sum_{\{i,j\} \in E} (g_i + g_j) \left| g_i - g_j \right| \Big)^2 \\
&= \langle v, w \rangle^2 \\
&\leq \|v\|^2 \, \|w\|^2 \\
&= \sum_{\{i,j\} \in E} (g_i + g_j)^2 \sum_{\{i,j\} \in E} (g_i - g_j)^2 \\
&\underset{(14.22)}{\leq} \lambda(2\Delta - \lambda) \Big(\sum_{i \in W} y_i^2 \Big)^2 .
\end{aligned} \tag{14.23}
$$

We will now bound this from below. Let $0 = t_0 < t_1 < \ldots < t_N$ be all the different values of the components of g. Define $V_k := \{i \in V;\, g_i \geq t_k\}$ for $k \in \{0, \ldots, N\}$ and for convenience $V_{N+1} := \emptyset$. Then, for $k \in \{1, \ldots, N+1\}$ we have $V_k \subseteq W$ and therefore $|V_k| \leq |W|$, hence $|V_k| = \min\{|V_k|, |V \setminus V_k|\}$. It also holds that $V_N \subseteq V_{N-1} \subseteq \ldots V_1 = W \subseteq V_0 = V$ and that $|V_k| - |V_{k+1}|$ is the number of entries in g equal to t_k for all $k \in \{0, \ldots, N\}$.

We will later show that we can express the sum $\sum_{\{i,j\} \in E} \left| g_i^2 - g_j^2 \right|$ in a convenient way:

$$\sum_{\{i,j\}\in E} \left|g_i^2 - g_j^2\right| = \sum_{k=1}^{N} \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_k}} (g_j^2 - g_i^2)$$

$$= \sum_{k=1}^{N} \sum_{\{i,j\}\in E(V_k, V\setminus V_k)} (t_k^2 - t_{k-1}^2) = \sum_{k=1}^{N} |E(V_k, V\setminus V_k)|\,(t_k^2 - t_{k-1}^2)$$

see below

$$\geq i(G) \sum_{k=1}^{N} |V_k|\,(t_k^2 - t_{k-1}^2) = i(G) \sum_{k=0}^{N} t_k^2 (|V_k| - |V_{k+1}|),$$

since $V_{N+1} = \emptyset$ and $t_0 = 0$. Now we can conclude that $\sum_{\{i,j\}\in E} \left|g_i^2 - g_j^2\right| \geq i(G) \sum_{i\in V} g_i^2 = i(G) \sum_{i\in W} y_i^2$. This together with (14.23) yields the claim of the theorem.

We now only have left to prove the validity of the transformation of the sum, i.e.,

$$\sum_{k=1}^{N} \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_k}} (g_j^2 - g_i^2) = \sum_{k=1}^{N} \sum_{\{i,j\}\in E(V_k, V\setminus V_k)} (t_k^2 - t_{k-1}^2). \tag{14.24}$$

This will be done by induction on N. The case $N = 1$ is clear. So let $N > 1$ and assume that (14.24) has already been proven for instances with $N-1$ instead of N, i.e., instances where we have a vector $\tilde{g}$ on a graph $\tilde{G} = (\tilde{V}, \tilde{E})$ assuming only N different values $0 = \tilde{t_0} < \ldots < \tilde{t}_{N-1}$ on its components and where subsets $\tilde{V}_{N-1} \subseteq \tilde{V}_{N-2} \subseteq \ldots \tilde{V}_1 = \tilde{W} \subseteq \tilde{V}_0 = \tilde{V}$ are defined accordingly.

We will make use of this for the following instance. Define $\tilde{G} := G - V_N$ (the vertices and edges of $\tilde{G}$ are $\tilde{V}$ and $\tilde{E}$, respectively) and let $\tilde{g}$ be the restriction of g on $\tilde{V}$. We then have $\tilde{t}_k = t_k$ for all $k \in \{0, \ldots, N-1\}$. If we then define the sets $\tilde{V}_k$ accordingly, we also have $\tilde{V}_k = V_k \setminus V_N$ for all $k \in \{0, \ldots, N-1\}$. Note that $V_N \subseteq V_k$ for all $k \in \{0, \ldots, N-1\}$, so the sets $\tilde{V}_k$ differ from the sets V_k exactly by the vertices in V_N.

By induction, we have

$$
\begin{aligned}
&\sum_{k=1}^{N} \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_k}} (g_j^2 - g_i^2) \\
&= \sum_{k=1}^{N-1} \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_k}} (g_j^2 - g_i^2) + \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_N}} (g_j^2 - g_i^2) \\
&= \sum_{k=1}^{N-1} \sum_{\substack{\{i,j\}\in E \\ \tilde{g}_i<\tilde{g}_j=t_k}} (\tilde{g}_j^2 - \tilde{g}_i^2) + \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_N}} (g_j^2 - g_i^2) \qquad (14.25) \\
&\underset{\text{induction}}{=} \sum_{k=1}^{N-1} \sum_{\{i,j\}\in E_{\tilde{G}}(\tilde{V}_k,\tilde{V}\setminus\tilde{V}_k)} (\tilde{t}_k^2 - \tilde{t}_{k-1}^2) + \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_N}} (g_j^2 - g_i^2) \\
&= \underbrace{\sum_{k=1}^{N-1} \sum_{\{i,j\}\in E_{\tilde{G}}(\tilde{V}_k,\tilde{V}\setminus\tilde{V}_k)} (t_k^2 - t_{k-1}^2)}_{(*)} + \sum_{\substack{\{i,j\}\in E \\ g_i<g_j=t_N}} (g_j^2 - g_i^2).
\end{aligned}
$$

Observe that the cuts $E_{\tilde{G}}(\tilde{V}_k, \tilde{V} \setminus \tilde{V}_k)$ only consist of edges in $\tilde{E}$. If we switch to cuts in G, we have to subtract some edges afterwards, namely those with one end in V_N. This way, we get for the sum $(*)$ the following:

$$
\begin{aligned}
&\sum_{k=1}^{N-1} \sum_{\{i,j\}\in E_{\tilde{G}}(\tilde{V}_k,\tilde{V}\setminus\tilde{V}_k)} (t_k^2 - t_{k-1}^2) \\
&= \sum_{k=1}^{N-1} \sum_{\{i,j\}\in E(V_k,V\setminus V_k)} (t_k^2 - t_{k-1}^2) - \underbrace{\sum_{k=1}^{N-1} \sum_{\substack{\{i,j\}\in E(V_k,V\setminus V_k) \\ j\in V_N}} (t_k^2 - t_{k-1}^2)}_{(+)}. \qquad (14.26)
\end{aligned}
$$

We will inspect the 'corrective' term $(+)$ closer. To this end, for each $i \in V$ let $k(i)$ be the smallest index such that $i \in V \setminus V_{k(i)}$. We then have $g_i = t_{k(i)-1}$ for all $i \in V$ and

$$\begin{aligned}
&\sum_{k=1}^{N-1} \sum_{\substack{\{i,j\}\in E(V_k, V\setminus V_k)\\ j\in V_N}} (t_k^2 - t_{k-1}^2) \\
&= \sum_{\substack{\{i,j\}\in E(V_N, V\setminus V_N)\\ j\in V_N}} \sum_{\substack{k\in\{1,\dots,N-1\}\\ i\in V\setminus V_k}} (t_k^2 - t_{k-1}^2) \\
&= \sum_{\substack{\{i,j\}\in E(V_N, V\setminus V_N)\\ j\in V_N}} \sum_{k=k(i)}^{N-1} (t_k^2 - t_{k-1}^2) \qquad (14.27)\\
&\underset{\text{telescope}}{=} \sum_{\substack{\{i,j\}\in E(V_N, V\setminus V_N)\\ j\in V_N}} (t_{N-1}^2 - t_{k(i)-1}^2) \\
&= \sum_{\substack{\{i,j\}\in E(V_N, V\setminus V_N)\\ j\in V_N}} (t_{N-1}^2 - g_i^2).
\end{aligned}$$

We can now continue our work on (14.25). Note that

$$\begin{aligned}
&\{(i,j);\, \{i,j\}\in E(V_N, V\setminus V_N), j\in V_N\} \\
=&\{(i,j);\, \{i,j\}\in E, g_i < g_j = t_N\}\,.
\end{aligned} \qquad (14.28)$$

This will later allow us to combine the last sum from (14.25) and that from (14.27).

Putting everything together, we see:

$$\begin{aligned}
&\sum_{k=1}^{N} \sum_{\substack{\{i,j\}\in E\\ g_i<g_j=t_k}} (g_j^2 - g_i^2) \\
&\underset{(14.25)}{=} \underbrace{\sum_{k=1}^{N-1} \sum_{\{i,j\}\in E_{\tilde G}(\tilde V_k, \tilde V\setminus\tilde V_k)} (t_k^2 - t_{k-1}^2)}_{(*)} + \sum_{\substack{\{i,j\}\in E\\ g_i<g_j=t_N}} (g_j^2 - g_i^2) \\
&\underset{(14.26)}{=} \sum_{k=1}^{N-1} \sum_{\{i,j\}\in E(V_k, V\setminus V_k)} (t_k^2 - t_{k-1}^2) - \underbrace{\sum_{k=1}^{N-1} \sum_{\substack{\{i,j\}\in E(V_k, V\setminus V_k)\\ i\in V_N}} (t_k^2 - t_{k-1}^2)}_{(+)} \\
&\qquad + \sum_{\substack{\{i,j\}\in E\\ g_i<g_j=t_N}} (g_j^2 - g_i^2).
\end{aligned}$$

Apply (14.27) to the (+) term and get

$$
\begin{aligned}
\ldots &= \sum_{k=1}^{N-1} \sum_{\{i,j\} \in E(V_k, V \setminus V_k)} (t_k^2 - t_{k-1}^2) - \sum_{\substack{\{i,j\} \in E(V_N, V \setminus V_N) \\ j \in V_N}} (t_{N-1}^2 - g_i^2) \\
&\quad + \sum_{\substack{\{i,j\} \in E \\ g_i < g_j = t_N}} (\underbrace{g_j^2}_{=t_N^2} - g_i^2) \\
&\underset{(14.28)}{=} \sum_{k=1}^{N-1} \sum_{\{i,j\} \in E(V_k, V \setminus V_k)} (t_k^2 - t_{k-1}^2) \\
&\quad + \sum_{\substack{\{i,j\} \in E(V_N, V \setminus V_N) \\ j \in V_N}} (t_N^2 - g_i^2 - t_{N-1}^2 + g_i^2) \\
&= \sum_{k=1}^{N-1} \sum_{\{i,j\} \in E(V_k, V \setminus V_k)} (t_k^2 - t_{k-1}^2) + \sum_{\substack{\{i,j\} \in E(V_N, V \setminus V_N) \\ j \in V_N}} (t_N^2 - t_{N-1}^2) \\
&= \sum_{k=1}^{N} \sum_{\{i,j\} \in E(V_k, V \setminus V_k)} (t_k^2 - t_{k-1}^2).
\end{aligned}
$$

This is (14.24). □

14.5 Heuristics for Graph Identification

We know several models for random graphs from Chapter 13. Given some graph, which one of these models describes it best? In this chapter, we will point out some ideas for using spectral methods to recognize graphs from different random graph models.

We will only consider the adjacency spectrum in this chapter. In the first section we will define some new graph parameters based on this spectrum. In the subsequent sections we will look at histogram plots of the spectrum and at the behavior of these new parameters for different models of random graphs.

In a final section, we briefly review some analytical results concerning the adjacency spectrum of random power law graphs.

14.5.1 New Graph Statistics

The spectrum of a graph as well as the set of its eigenvectors are graph statistics, more precisely they are global distributions. See Section 11.7 in Chapter 11 for a general discussion of graph statistics.

A multigraph is — up to isomorphy — fully determined by its spectrum plus eigenvectors [135, Theorem 1.8, p. 44]. It seems reasonable to define new statistics which store only selected parts of that information in order to retrieve relevant characteristics.

Inverse Participation Ratio. Recall that we can interpret an eigenvector as an assignment of weights to the vertices; see Remark 14.1.2. We will ask, how these weights are distributed. Are there a few vertices that have relatively large weights compared to the rest (we also speak of a high localization in this case), or are the weights very similar for all vertices?

Let G be a graph and let $w_1, \ldots, w_n$ be the *normalized* eigenvectors of its adjacency matrix. We define the *inverse participation ratio* [198] of the jth eigenvector as

$$I_j(G) := \sum_{k=1}^{n} \left((w_j)_k\right)^4. \tag{14.29}$$

We also write I_j when dealing with only one graph at a time.

Because the eigenvectors are normalized, we have $I_j(G) \in [\frac{1}{n}, 1]$ for all $j \in \{1, \ldots, n\}$. The inverse participation ratio measures an eigenvector's extent of localization. This becomes clear by considering extreme cases. First let w_j define perfectly evenly distributed weights on the graph, i.e., $(w_j)_k := \frac{1}{\sqrt{n}}$ for all $k \in \{1, \ldots, n\}$. Then, $I_j = \frac{1}{n}$, i.e., the inverse participation ration attains its minimal value.

On the other hand, if for an arbitrary vertex $k_0 \in V$, we have

$$(w_j)_k = \begin{cases} 1 & \text{if } k = k_0 \\ 0 & \text{otherwise} \end{cases},$$

then $I_j = 1$, i.e., the inverse participation ration attains its maximum value.

Offset of Largest Eigenvalue. In certain classes of graphs, the largest eigenvalue tends to 'escape' from the rest of the spectrum. For example, this is the case in certain models of random graphs. It therefore is interesting to study the quantity

$$R(G) := \frac{\lambda_n - \lambda_{n-1}}{\lambda_{n-1} - \lambda_1}. \tag{14.30}$$

$R(G)$ captures the offset of λ_n from the second largest eigenvalue λ_{n-1} normalized with respect to the range of the rest of the spectrum.

There is a correlation between $R(G)$ and the chromatic number $\chi(G)$, as was noticed in [198]. Define ε by the equation

$$-\lambda_1 = \lambda_{n-1} + \varepsilon.$$

For $|\varepsilon|$ small, the smallest interval containing all eigenvalues except λ_n is almost centered around 0. (For certain random graphs, $|\varepsilon|$ is in fact small.) Recall from 14.4 that there are bounds on the chromatic number in terms of extremal eigenvalues. In particular, we have by Theorem 14.4.12,

$$\begin{aligned} \frac{\chi(G)}{2} - 1 &\geq \frac{-\lambda_n}{2\lambda_1} - \frac{1}{2} = \frac{-\lambda_n - \lambda_1}{2\lambda_1} \\ &= \frac{-\lambda_n + \lambda_{n-1} + \varepsilon}{\lambda_1 - \lambda_{n-1} - \varepsilon} = \frac{\lambda_n - \lambda_{n-1} - \varepsilon}{\lambda_{n-1} - \lambda_1 + \varepsilon}. \end{aligned}$$

So, for graphs with $\varepsilon = 0$ the chromatic number is lower bounded in terms of $R(G)$ as

$$\chi(G) \geq 2R(G) + 2.$$

For small $|\varepsilon|$, this equation obviously still holds in an approximate sense.

14.5.2 Spectral Properties of Random Graphs

Can random graphs from different models be distinguished by looking at spectral properties? One way of approaching this problem is to study the outcome of a large number of random experiments. We will present some results of some such experiments and discuss possible interpretations. The three random models under consideration are the model by Erdős and Rényi, $\mathcal{G}(n, p)$, the scale-free graphs by Barabási and Albert — see 13.1.4 — and the small-world graphs by Watts and Strogatz — see 13.1.2.

First, we investigate how these models differ in their spectra by looking at histogram plots of the eigenvalues of a number of randomly generated graphs. Then, we compare the inverse participation ratios, defined in (14.29). Finally we also look at the offsets of the largest eigenvalues, defined in (14.30). Our focus will be on $\mathcal{G}(n, p)$ and Barabási-Albert-like graphs. For details on small-world graphs, see [198].

For our numerical experiments, we wrote a small C program (about 600 lines of code). To compute the eigenvalues and later (for the inverse participation ratios) also the eigenvectors, we use the function `ssyev` from the Sun Performance Library [537]. The actual plots were made using `gnuplot` [588].

Spectra. Let us start with $\mathcal{G}(n, p)$. We generated 100 graphs randomly according to $\mathcal{G}(2000, \frac{1}{2})$ and computed their spectra. A first observation is that the largest eigenvalue is significantly set off from the rest of the spectrum in all of these experiments. Because this offset will be explicitly regarded later, we for now exclude the largest eigenvalue from our considerations. So, when talking of 'spectrum', for the rest of this section, we mean 'spectrum without the largest eigenvalue'.

To get a visualization of all the spectra, we computed a histogram of the eigenvalues of all 100 random graphs. This technique will be used for the other random graph models as well. The quantity approximated by those histograms is also known as the *spectral density*. Although we do not introduce this notion formally [198], we will in the following occasionally use that term when referring to the way eigenvalues are distributed.

All histograms, after being normalized to comprise an area of 1, were scaled in the following way. Let $\lambda_1, \ldots, \lambda_N$ be the eigenvalues. (In our case $N = 100 \cdot (2000 - 1)$, for we have 100 graphs with 2000 eigenvalues each, and we exclude the largest of them for each graph). Define $\bar{\lambda}$ as the mean of all these values

$$\bar{\lambda} = \frac{1}{N} \sum_{i=1}^{N} \lambda_i.$$

Then, we compute the standard deviation

$$\sigma = \sqrt{\sum_{i=1}^{N} (\lambda_i - \bar{\lambda})^2}.$$

The x-axis of our plots is scaled by $\frac{1}{\sigma}$ and the y-axis is scaled by σ. This makes it easy to compare spectra of graphs of different sizes.

Figure 14.10 shows the scaled histogram. The semicircle form actually is no surprise. It follows from a classical result from random matrix theory known as the *semicircle law*. It originally is due to Wigner [584, 585] and has later been refined by a number of researchers [34, 233, 337].

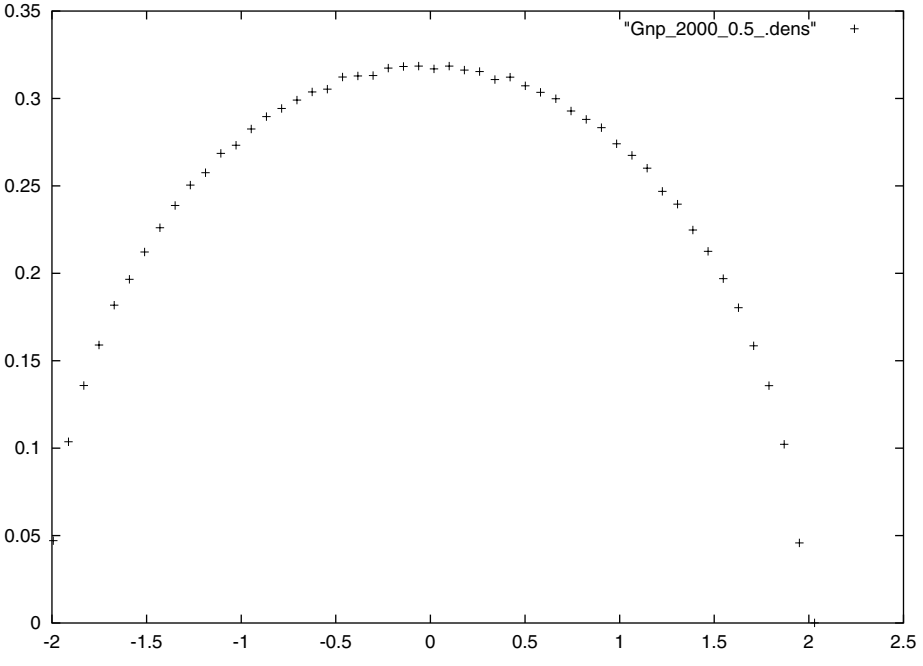


Fig. 14.10. A histogram of the union of the spectra of 100 random graphs from $\mathcal{G}(2000, \frac{1}{2})$

Now we look at graphs that originate from an evolutionary process with preferential attachment, like the Barabási-Albert graphs. We implemented a very simple algorithm for creating graphs with preferential attachment. There is only one parameter m (apart from the number of vertices n). The process starts with m unconnected vertices. Whenever a new vertex arrives, it is connected with m edges to older vertices. To this end, the algorithm m times chooses a vertex out of the set of old vertices at random. The probability of an old vertex being

chosen is proportional to its degree; at the very first step, when all vertices have degree 0, each of them is equally likely to be chosen.

This way of generating preferential attachment graphs is slightly different from what usually is considered in that multiple edges are allowed. However, the resulting histograms of the spectra look very similar to those of [198], where multiple edges do not occur. See Figure 14.11 for our results. For comparison, Figure 14.12 shows plots for our preferential attachment graphs and for $\mathcal{G}(n,p)$ graphs in one figure.

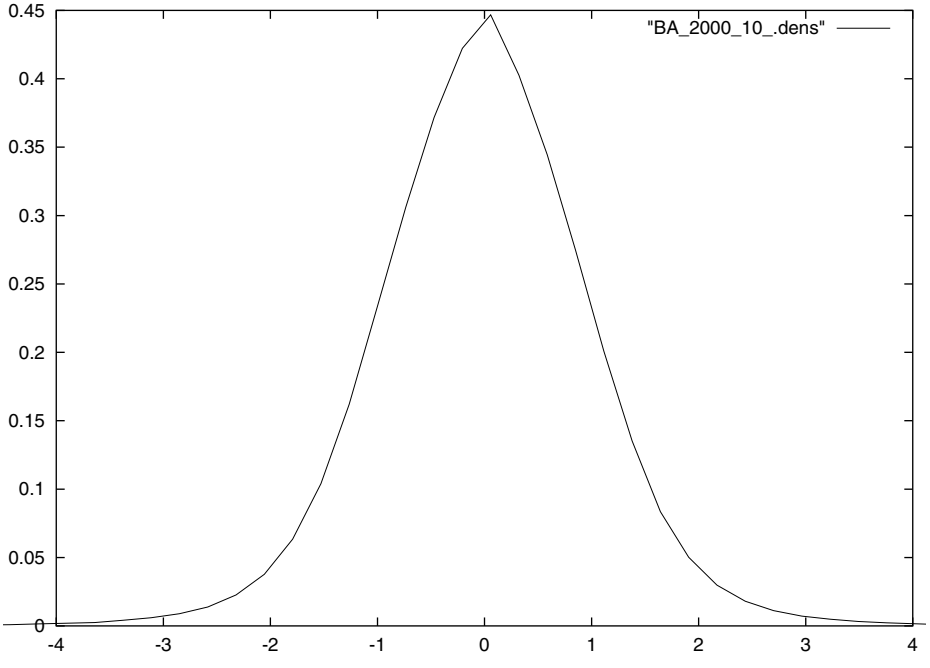


Fig. 14.11. A smoothed histogram of the union of the spectra of 100 random graphs with preferential attachment on 2000 vertices and with $m = 10$

The preferential attachment graph obviously has significantly more small eigenvalues than the $\mathcal{G}(n,p)$ graph. Since it essentially is connected[2] these small eigenvalues cannot originate from small connected components. In [198] it is suggested that these eigenvalues belong to eigenvectors that are highly localized. This is supported by high inverse participation ratios, which we will observe later.

An interesting case for our studies of $\mathcal{G}(n,p)$ are *sparse random graphs*. We used to look at large values of n, for which according to the semicircle law, our histograms should more and more (with increasing n) resemble a semicircle. In

[2] There might be a number of less than $m = 10$ isolated vertices.

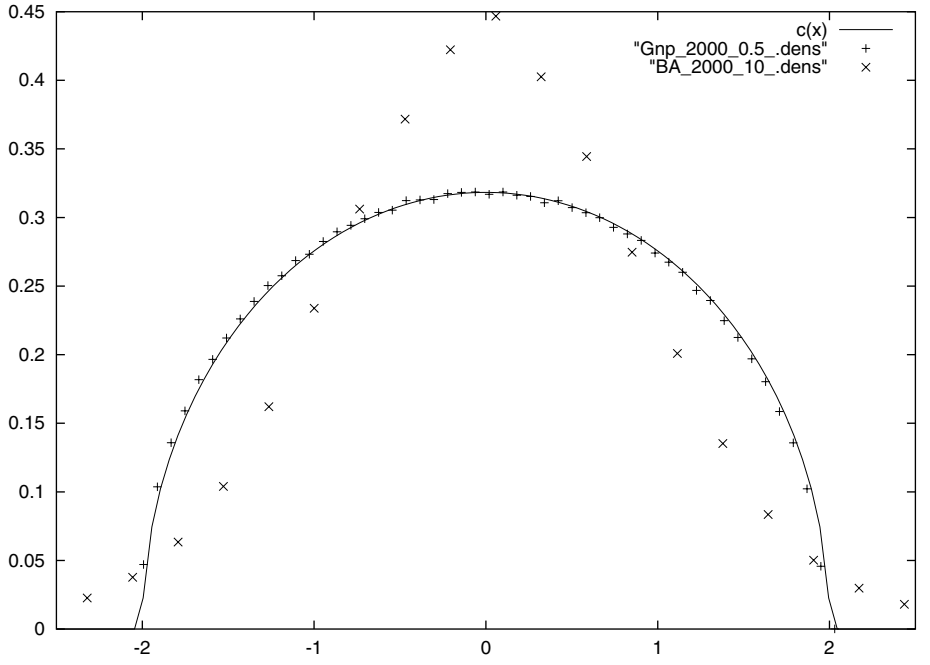


Fig. 14.12. Histograms of spectra of 100 random graphs with preferential attachment ($n = 2000$, $m = 10$) and from $\mathcal{G}(2000, \frac{1}{2})$ each. The solid line marks an ideal semicircle

the case displayed in Figure 14.10 we have an expected degree of approximately[3] $pn = \frac{1}{2}2000 = 1000$. This quantity pn is also referred to as the *connectivity* of the graph, although we will avoid this term, because it has already been extensively used in another context (see Chapter 7).

What if we look at graphs with fewer edges than in Figure 14.10, say, graphs in $\mathcal{G}(n, p)$ where $pn = 5$? Figure 14.13 shows that the spectral densities of such graphs rise above the semicircle in the vicinity of 0. Reasons for this have been discussed in [198].

One can also notice small peaks at larger eigenvalues. They become more obvious in plots of graphs with even lower expected degree. To study them in more detail, it is helpful to look at the *cumulative distribution* of eigenvalues, i.e., at the function

$$x \mapsto |\{i;\, \lambda_i \leq x\}|$$

Figure 14.14 shows an examplary plot.

[3] The expected degree is in fact $p(n-1)$. To see this, fix a vertex $i \in V$. This vertex has $n-1$ potential neighbors. Let $X_1, \ldots, X_{n-1}$ be 0/1 random variables, where X_j indicates whether or not an edge is drawn from i to j. If we put $X := \sum_{j=1}^{n-1} X_i$, then $\mathbb{E}[X]$ is the expected degree of i. The claim follows from linearity of expectation.

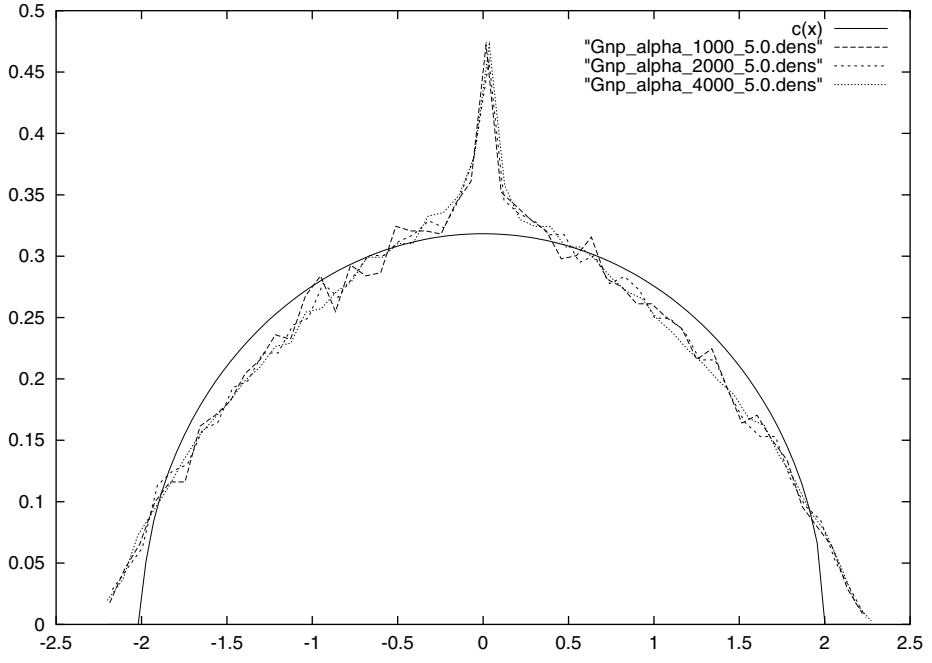


Fig. 14.13. Histograms of spectra of sparse random graphs. For $n = 1000$, 2000 and 4000 each we created 10 random graphs from $\mathcal{G}(n, p)$ with p set to satisfy $pn = 5$. The solid line marks an ideal semicircle

In [49], the reasons for the peaks are investigated. It is argued that they originate from small connected components and, for $pn > 1$, also from small trees grafted on the giant component.

Inverse Participation Ratios. Looking at Figure 14.12 has already lead us to conjecture that our graphs with preferential attachment have highly localized eigenvectors. To investigate this further, we created random graphs in all three models and plotted the inverse participation ratios of their eigenvectors. Figure 14.15 shows all three plots. Each circle represents an eigenvector. The x position of the circle corresponds to the eigenvalue and the y position to the inverse participation ratio. Note that in the second plot (which shows the results for the Barabási-Albert-like graph), there are even eigenvectors with inverse participation ratio near to 1.

It is also interesting that we obtain very distinguishing plots even for small numbers of vertices; all considered graphs only had 100 vertices each. We randomly created more such graphs and always could observe the same characteristics. Obviously one can recognize the $\mathcal{G}(n, p)$ by the fact that all eigenvectors have their inverse participation ratios rather evenly distributed in a small band at the bottom of the diagram. The Barabási-Albert-like graph exhibits as a salient

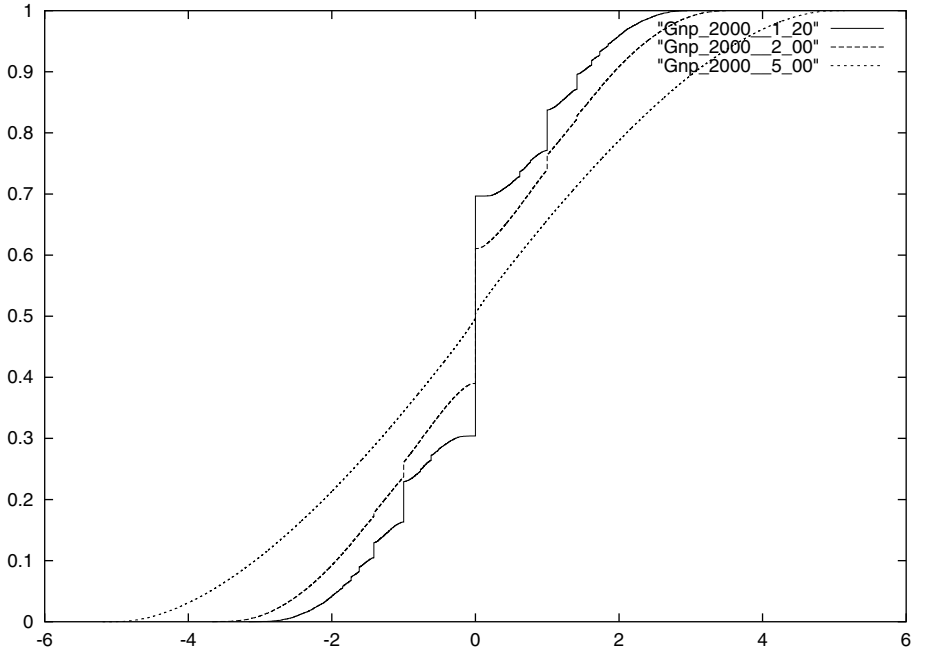


Fig. 14.14. The cumulative distribution of eigenvalues for sparse random graphs. For $n = 2000$ and $pn = 1.2$, 2.00 and 5.00 each we created 10 random graphs from $\mathcal{G}(n, p)$

feature eigenvectors with high inverse participation ratio. The small-world graph shows a very asymmetric structure.

We were not able to produce likewise distinguishing plots of the spectral density for such small graphs.

Offset of Largest Eigenvalue. We already mentioned that in the $\mathcal{G}(n, p)$ model as well as in the graphs with preferential attachment, the largest eigenvalue is significantly set off from the rest of the spectrum. The offset R, see (14.30), in these two models differs from that in the small-world graphs by several orders of magnitude. But there is also a difference between the R values of sparse $\mathcal{G}(n, p)$ graphs and graphs with preferential attachment. For the former, with increasing number of vertices and constant average degree, the R values seem to stay constant, while for the latter they decrease. See [198] for numerical results.

14.5.3 Random Power Law Graphs

In [127, 128], first the adjacency spectrum of a very general class of random graphs is examined. Given a sequence $\boldsymbol{w} = (w_1, w_2, \ldots, w_n)$ of non-negative reals satisfying

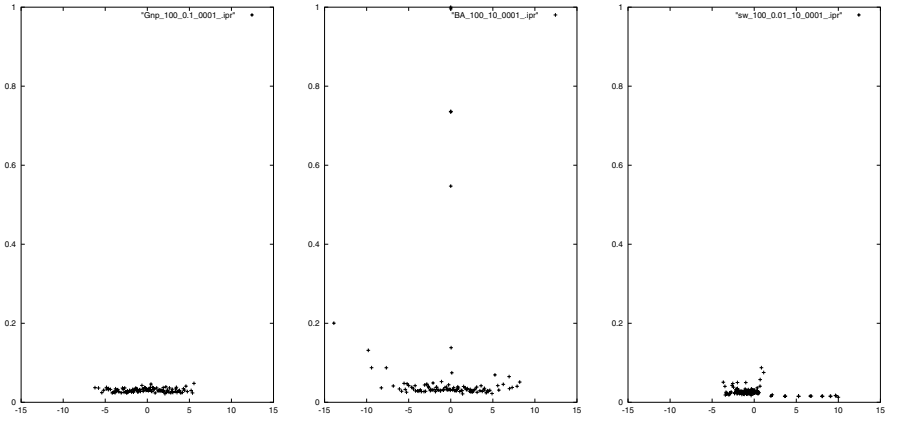


Fig. 14.15. Inverse participation ratios of three random graphs. The models are: $\mathcal{G}(n,p)$ (`Gnp_100_0.1_0001_ipr`), preferential attachment (`BA_100_10_0001_ipr`), small-world (`sw_100_0.01_10_0001_ipr`). All graphs have an expected degree of 10

$$\max_{i\in\{1,\dots,n\}} w_i^2 < \sum_{i=1}^{n} w_i,$$

a random graph $G(\boldsymbol{w})$ is constructed by inserting an edge between vertices i and j with probability

$$\frac{w_i w_j}{\sum_{k=1}^{n} w_k}.$$

It is easy to verify that in such a graph, vertex i has expected degree w_i.

A useful notation is the *second order average degree*, defined by

$$\tilde{d} := \frac{\sum_{i=1}^{n} w_i^2}{\sum_{i=1}^{n} w_i}.$$

Furthermore, we denote the largest expected degree by m and the average expected degree by d.

We can prove results on the largest eigenvalue of the adjacency spectrum of a random graph from $G(\boldsymbol{w})$, which hold almost surely[4] and under certain conditions on $\tilde{d}$ and m. We can also make such statements on the k largest eigenvalues, provided that $\tilde{d}$, m, and the k largest expected degrees behave appropriately.

An interesting application of these results concerns random power law graphs: we can choose the sequence $\boldsymbol{w}$ suitably, so that the expected number of vertices of degree k is proportional to $k^{-\beta}$, for some given β. Under consideration were values of $\beta > 2$.

Theorem 14.5.1 ([127, 128]). *Let G be a random power law graph with exponent β and adjacency spectrum $\lambda_1, \dots, \lambda_n$.*

[4] I.e., with probability tending to 1 as n tends to ∞.

1. *For* $\beta \geq 3$ *and*
$$m > d^2 \log^3 n, \tag{14.31}$$
we have almost surely
$$\lambda_n = (1 + o(1))\sqrt{m}.$$
2. *For* $2.5 < \beta < 3$ *and*
$$m > d^{\frac{\beta-2}{\beta-2.5}} \log^{\frac{3}{\beta-2.5}} n, \tag{14.32}$$
we have almost surely
$$\lambda_n = (1 + o(1))\sqrt{m}.$$
3. *For* $2 < \beta < 2.5$ *and*
$$m > \log^{\frac{3}{2.5-\beta}} n,$$
we have almost surely
$$\lambda_n = (1 + o(1))\tilde{d}.$$
4. *For* $2.5 < \beta$ *and* $k < n \left(\frac{d}{m \log n} \right)^{\beta-1}$, *almost surely the* k *largest eigenvalues of* G *have power law distribution with exponent* $2\beta - 1$, *provided* m *is large enough (satisfying* (14.31) *and* (14.32)*).*

We remark that the second order average degree $\tilde{d}$ can actually be computed in these cases. For details see [127, 128].

14.6 Chapter Notes

Fundamental Properties

The adjacency spectrum is discussed in a vast amount of papers and textbooks. The results presented in this chapter are taken from [135, 247, 576]. More on the Laplacian can be found in [135] (under the term 'admittance matrix') and in [427]. The normalized Laplacian is extensively studied in [125]. While the eigenvalues alone do not generally determine the structure of a graph (as shown by cospectral graphs), eigenvalues *plus* eigenvectors do: if $u_1, u_2, \ldots, u_n$ are linearly independent eigenvectors of A corresponding to $\lambda_1, \lambda_2, \ldots, \lambda_n$ respectively, then $A = UDU^{-1}$, where $U := \text{Mat}(u_1, \ldots, u_n)$ is the matrix with u_i as column vectors and $D := \text{diag}(\lambda_1, \ldots, \lambda_n)$ is the diagonal matrix with entries λ_i. Already the knowledge of some eigenvectors can be very useful to recognize important properties of a graph. This is elaborated on in [136]. The cited references contain also many results on the spectrum of regular graphs which we treated rather stepmotherly since in network analysis we are typically dealing with highly non-regular graphs.

Numerical Methods

The diagonalization strategy for small dense matrices is comprehensively treated in [482, 535]. For a discussion of QR-like algorithms including parallelizable versions see [571]. More on the Lanczos method can be found in [467, 591]. An Arnoldi code for real asymmetric matrices is discussed in [509].

Subgraphs and Operations on Graphs

The Interlacing Theorem plays an important role in many publications on spectral graph theory. In addition to the already mentioned literature, we point the reader to [561]. More on graph operations and resulting spectra can be found in [135, Chapter 2] and [427]. As already mentioned, symmetric grafting also plays a role in [49].

Bounds on Global Statistics

For more results on the connection between eigenvalues and graph parameters see [427, 428] and the references therein, such as [426, 425]. More on the role of the eigenvalues of the normalized Laplacian for graph parameters can be found in [125]. More on the connection between $\lambda_2(L)$ and expansion properties can be found in [19]. Better spectral lower bounds on the bisection width have been given by Donath, Hoffman [159], Boppana [78], and Rendl, Wolkowicz [491]. Boppana's technique also yields an efficient algorithm with good average case behavior. For a discussion of spectral methods for the multiway partition problem of finding a k-partition with prescribed part sizes see [27, 389].

Heuristics for Graph Identification

For further reading, see [198, 49] as well as the already mentioned [127, 128]. The behavior of certain extremal eigenvalues is also considered in [337].