4

First Properties of the Spectrum

This chapter discusses the elementary properties of Laplace operators on graphs and hypergraphs. Many interesting examples will illustrate how special eigenvalues emerge. We also introduce discrete Pólya–Cheeger constants and their dual versions and provide the initial steps relating spectral clustering, spectra of neighborhood graphs, signed Laplacians, and spectra of simplicial complexes and hypergraphs.

4.1 The Laplacian and Its Spectrum on Graphs

In this section, we shall analyze Laplacians on *graphs*. From the general perspective, this means that we consider the case $q = 0$, because then simplices of dimension > 1 play no role, and only the vertices and the edges enter. But when vertices are connected by edges, we have a graph. This section can also serve to explicate the general theory in the simplest situation, and therefore, we try to make the reasoning here self-contained, instead of drawing upon that general theory.

The case of main interest will be the normalized combinatorial Laplacian, but we shall also discuss the algebraic Laplacian that is commonly used in graph theory.

4.1.1 General Aspects

We assume in this section, unless explicitly stated otherwise, that **the graph Γ is finite and connected**. Let it have N *vertices*, sometimes also called *nodes* for the sake of variety, and let V be the vertex set. For a subset W of V, we let $\overline{W}$ be its complement $V \setminus W$ in V.

$[v, v']$ denotes an oriented edge with vertices $v, v' \in V$. In this section, the orientation will play no role, and so, we write (v, v') or (vv') for the underlying unoriented edge.

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Definition 4.1.1. We say that two vertices v, v' in a graph are *neighbors*, in symbols

$$v \sim v',$$

if they are connected by an edge. We shall also denote that edge by (v, v') or (vv'), according to the conventions just established.

We also say that the graph has a *self-loop* at v if $v \sim v$.

The *degree* $\deg v$ of a vertex v is the number of its neighbors (including itself when v has a self-loop).

Remark 4.1.1. For simplicial complexes, we do not allow self-loops. Therefore, when we make general statements that also apply to simplicial complexes of dimension > 1, we require that there are no self-loops. Hence, in this section, if not explicitly stated otherwise, **the graph Γ has no self-loops**.

We consider the space $L^2(\Gamma)$ of functions $f : V \to \mathbb{R}$ on the vertex set V of a graph equipped with a scalar product

$$(f, g) = \sum_v b(v)\, f(v)g(v) \tag{4.1.1}$$

for some positive function b on the vertex set. We may consider $b(v)$ as the weight of the vertex v. We also let the edges carry weights. We write the weight of the unoriented edge $e = (vv')$ in a weighted graph as $b(e) = w_{vv'}$. And since weights are assigned to unoriented simplices, we have $w_{v'v} = w_{vv'}$. If we wish that the vertex and the edge weights are consistent, we should assume $b(v) = \sum_{v' \sim v} w_{vv'}$, but for the moment, we do not require that. But as for the vertex weights, we require the edge weights $b(e)$ to be positive. This then is the setting of this section.

We have from (2.5.7) and (2.5.17)

Definition 4.1.2. The Laplace operator associated with the scalar product b of (4.1.1) is given by

$$L^0(f)(v) = \frac{1}{b(v)} \sum_{e=(vv')} b(e)(f(v) - f(v')). \tag{4.1.2}$$

The Laplacian (4.1.2) thus is the weighted sum of the weighted differences between the value of a function at a vertex v and at its neighbors. This is also in accordance with the general scheme developed in Section 2.5.

Lemma 4.1.1. *Let Γ be a connected graph.*

1. L^0 is self-adjoint with respect to the scalar product (4.1.1), that is,

$$(f, L^0 g) = (L^0 f, g) \tag{4.1.3}$$

for all $f, g \in L^2(\Gamma)$.

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2. L^0 *is non-negative:*

$$(L^0 f, f) \geq 0 \tag{4.1.4}$$

for all f.

3. $L^0 f = 0$ *precisely when* f *is constant*.

Proof (4.1.3) follows from the definitions of the scalar product and the Laplacian. To see this in detail, we compute

$$\begin{aligned}(f, L^0 g) &= \sum_{v,v',v\sim v'} b(e)(f(v) - f(v'))g(v) \\ &= -\sum_{v,v',v\sim v'} b(e)(f(v) - f(v'))g(v') \\ &= \frac{1}{2} b(e) \sum_{v,v',v\sim v'} (f(v) - f(v'))(g(v) - g(v') \\ &= b(e) \sum_{e} (f(v) - f(v'))(g(v) - g(v'), \end{aligned} \tag{4.1.5}$$

and by symmetry, this then also equals $(L^0 f, g)$. And (4.1.5) also implies (4.1.4).

When $L^0 f = 0$, there can neither be a vertex v with $f(v) \geq f(v')$ for all $v' \sim v$ with strict inequality for at least one such v', that is, a nontrivial local maximum, nor a nontrivial local minimum, as this would contradict the fact that, by (4.1.2), $L^0 f(v) = 0$ means that the value $f(v)$ is the weighted average of the values at the neighbors of v. Since Γ is connected, f then has to be a constant (when Γ is not connected, a solution of $L^0 f = 0$ is constant on every connected component of Γ). □

Remark 4.1.2. The argument in the preceding proof is a special case of the maximum principle.

The preceding properties have consequences for the eigenvalues of L^0. We write them as λ_k so that the eigenvalue equation becomes

$$L^0 u_k = \lambda_k u_k, \tag{4.1.6}$$

with u_k being a corresponding *eigenfunction*. We order the eigenvalues as

$$\lambda_1 = 0 < \lambda_2 \leq \ldots \leq \lambda_N.$$

That $\lambda_2 > 0$ follows from the last item of Corollary 4.1.1, which is a consequence of Lemma 4.1.1.

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Corollary 4.1.1. *1. By 1, the eigenvalues are real.*

2. By 2, they are non-negative.

3. By 3, the smallest eigenvalue is $\lambda_1 = 0$. *Since we assume that* Γ *is connected, this eigenvalue is simple, that is,*

$$\lambda_k > 0 \tag{4.1.7}$$

for $k > 1$.

□

Formula (4.1.5) suggests to consider the difference operator 2.3.1. For neighbors $v \sim v'$,

$$\delta f(v,v') := f(v') - f(v). \tag{4.1.8}$$

The operator δ can be considered as a map from functions on the vertices of Γ to functions on the edges of Γ. In order to make the latter space also an L^2-space, we introduce the product

$$(\delta f, \delta g) := \sum_{e=(vv')} b(e)(f(v') - f(v))(g(v') - g(v)), \tag{4.1.9}$$

where we sum over edges and not over vertices. If we did the latter, we would need to put in a factor of $1/2$ because each edge would then be counted twice, as in the derivation of (4.1.5).

We now recall the Rayleigh quotients from Section 2.6.1. We may find an orthonormal basis of $L^2(\Gamma)$ consisting of eigenfunctions of L^0,

$$u_k,\ k = 1,\dots,N$$

for the eigenvalues $\lambda_k,\ k = 1,\dots,N$.

We may expand any function f on Γ as

$$f(v) = \sum_k (f,u_k)u_k(v) \tag{4.1.10}$$

and

$$(f,f) = \sum_k (f,u_k)^2 \tag{4.1.11}$$

and

$$(\delta f, \delta f) = \sum_k \lambda_k (f,u_k)^2. \tag{4.1.12}$$

We now recall Theorem 2.6.1.

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Lemma 4.1.2. *Let $\mathcal{H}^k$ be the collection of all k-dimensional linear subspaces of H. We have*

$$\lambda_k = \max_{H_{k-1}\in\mathcal{H}^{k-1}} \min\left\{\frac{(\delta u,\delta u)}{(u,u)} : u \neq 0,\ (u,f) = 0 \text{ for all } f \in H_{k-1}\right\} \quad (4.1.13)$$

and dually

$$\lambda_k = \min_{H_k\in\mathcal{H}^k} \max\left\{\frac{(\delta u,\delta u)}{(u,u)} : u \in H_k\backslash\{0\}\right\}. \quad (4.1.14)$$

In (4.1.13), we consider the minimal Rayleigh quotient under $k-1$ constraints, and we maximize that with respect to the constraints. In (4.1.14), we consider the maximal Rayleigh quotient for k degrees of freedom, and we minimize that with respect to those degrees of freedom.

An obvious consequence is

Corollary 4.1.2. *1. An eigenfunction u for an eigenvalue λ satisfies*

$$\lambda = \frac{(\delta u,\delta u)}{(u,u)}. \quad (4.1.15)$$

2. The second smallest eigenvalue of L^0 is given by

$$\lambda_2 = \min\left\{\frac{(\delta u,\delta u)}{(u,u)} :\ \sum_v b(v)u(v) = 0\right\} \quad (4.1.16)$$

(because

$$\sum_v b(v)u(v) = 0 \quad (4.1.17)$$

is equivalent to $(u,u_1) = 0$ where u_1 is a constant, that is, an eigenfunction for λ_1).

3. The largest eigenvalue of L^0 is given by

$$\lambda_N = \max\left\{\frac{(\delta u,\delta u)}{(u,u)} : u \in L^2(\Gamma)\backslash\{0\}\right\}. \quad (4.1.18)$$

□

4.1.2 The Algebraic Graph Laplacian

In this section, we consider the algebraic graph Laplacian. This is the Laplace operator that is usually treated in texts on graph theory, for instance, in [38, 113]. The role of the eigenvalue λ_2 of this Laplacian for connectivity properties was recognized by Fiedler [95, 96]. Here, we do not go deeply into

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this subject but only record some elementary properties of the algebraic graph Laplacian.

Definition 4.1.3. The *algebraic graph Laplacian*, also called the *Kirchhoff Laplacian*, is the Laplace operator (4.1.2) for the weights $b(v) = 1 = b(e)$ for all vertices and edges. Thus, the underlying scalar product is

$$(f,g) = \sum_v f(v)g(v), \tag{4.1.19}$$

and the operator is

$$\Lambda(f)(v) = \sum_{v'\sim v}(f(v) - f(v')) = \deg v\, f(v) - \sum_{v'\sim v} f(v'). \tag{4.1.20}$$

In order to formulate this in slightly more abstract terms, we define the *adjacency matrix* A on $V \times V$ by

$$A(v,v') := \begin{cases} 1 & \text{if } v' \sim v \\ 0 & \text{else} \end{cases} \tag{4.1.21}$$

and the diagonal *degree matrix* D by

$$D(v,v') := \begin{cases} \deg v & \text{if } v = v' \\ 0 & \text{else,} \end{cases} \tag{4.1.22}$$

we can write

$$\Lambda = D - A. \tag{4.1.23}$$

The adjacency matrix has some useful properties. We interpret $A(v,v')$ as the number of paths of length 1 between v and v'. There is such a path precisely if $A(v,v') = 1$, and none if it is 0. Therefore, if we take the power A^k of the adjacency matrix, then

Lemma 4.1.3. *$A^k(v,v')$ is the number of paths of length k between v and v'. So, $A^k(v,v)$ is the number of paths of length k that start and end at v. In particular, $A^2(v,v)$ is the degree of v.*

□

Lemma 4.1.4. *Let Γ be a graph without self-loops. The eigenvalues of Λ satisfy*

$$\sum_k \lambda_k = \sum_v \deg v. \tag{4.1.24}$$

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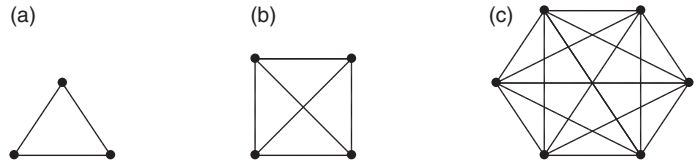


Figure 4.1 The complete graphs K_3 (a), K_4 (b) and K_6 (c).

If Γ *is – as always – connected, eigenfunctions* u_k *for eigenvalues* λ_k *for* $k \geq 2$ *satisfy*

$$\sum_v u_k(v) = 0. \tag{4.1.25}$$

Proof The sum of the eigenvalues of a matrix equals its trace. The adjacency matrix A is trace-free, and so, in (4.1.24), we only have the trace of D.

(4.1.25) is (4.1.17) for the algebraic Laplacian, since here all $b(v) = 1$.

□

Naturally, we should consider some examples.

Definition 4.1.4. The *complete graph* K_N is the graph on N vertices with $v \sim v'$ for any two different vertices. We also let K_N^0 be the graph on N vertices with $v \sim v'$ for any two not necessarily different vertices.

Thus, every vertex of K_N^0 has a self-loop. The vertices of K_N all have degree $N-1$, while those of K_N^0 have degree N.

Figure 4.1 shows some complete graphs.

We can easily determine the spectra of K_N and K_N^0.

Lemma 4.1.5. *The spectra of* K_N *and* K_N^0 *both consist of the eigenvalue* $\lambda_1 = 0$ *and the eigenvalue* $\lambda_2 = \ldots = \lambda_N = N$.

Proof For a complete graph K_N, all the degrees $\deg v$ have the value $N-1$ and are therefore equal. Hence, also all the nontrivial eigenvalues are equal. They are

$$\lambda_2 = \ldots = \lambda_N = N, \tag{4.1.26}$$

since

$$\Lambda u(v) = (N-1)u(v) - \sum_{v' \neq v} u(v') = Nu(v) \tag{4.1.27}$$

for any u with values $u(v_1) = 1, u(v_2) = -1$ for two distinct vertices and $u(v) = -0$ on all other vertices.

$$\lambda_2 = \ldots = \lambda_N = N + 1 \tag{4.1.28}$$

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For K_N^0, we have the same eigenfunctions and eigenvalues, that is, the non-trivial one is N. In fact, the algebraic Laplacian is the same. If J is the $N \times N$-matrix with all entries $= 1$, then this is the adjacency matrix $A(K_N^0)$, while the adjacency matrix $A(K_N)$ is $J - \mathrm{Id}$. And since the degree matrix $D(K_N^0)$ of K_N^0 is $N\mathrm{Id}$, while $D(K_N) = (N-1)\mathrm{Id}$, the two Laplacians agree, $D(K_N^0) - A(K_N^0) = D(K_N) - A(K_N)$.

□

Thus, the spectrum of the algebraic graph Laplacian does not distinguish these two graphs.

Of course, the spectrum of K_N checks with (4.1.24), since for K_N, both sides are equal to $(N-1)N$.

From the preceding, we record

$$\Lambda(K_N) = N\mathrm{Id} - J. \tag{4.1.29}$$

This has a corollary.

Corollary 4.1.3. *For a graph Γ with N vertices, let $\overline{\Gamma}$ be the complementary graph, that is, the graph with the same vertex set in which two vertices are connected by an edge precisely if they are not connected in Γ. Then, its eigenvalues are given by*

$$\lambda_k(\overline{\Gamma}) = N - \lambda_{N-k+2}(\Gamma) \quad \text{for } k = 2, \dots, N. \tag{4.1.30}$$

Proof The Laplacians satisfy

$$\Lambda(\overline{\Gamma}) + \Lambda(\Gamma) = \Lambda(K_N) = N\mathrm{Id} - J \tag{4.1.31}$$

by (4.1.29). Let u_k be an eigenfunction of Γ for λ_k, $k \geq 2$. Since we may assume (4.1.25), we have $Ju_k = 0$. Hence,

$$Nu_k = (N\mathrm{Id} - J)u_k = \Lambda(\overline{\Gamma})u_k + \Lambda(\Gamma)u_k = \Lambda(\overline{\Gamma})u_k + \lambda_k u_k$$

from which the result follows.

□

The next example is the *complete bipartite* graph $K_{m,n}$, which will be treated in more detail in Section 4.1.3. It consists of two classes of vertices, V_1 with m and V_2 with n members. Every vertex in V_1 is connected with every vertex in V_2, but no vertices in the same class are connected.

Figure 4.2 shows $K_{3,5}$ and $K_{1,6}$. The latter is an example of a *star graph*.

Like all graphs, $K_{m,n}$ has the eigenvalue 0 with a constant eigenfunction. The function that is equal to n on all vertices in V_1 and equal to $-m$ on all vertices of V_2 satisfies (4.1.25) and is an eigenfunction for the eigenvalue $m+n$.

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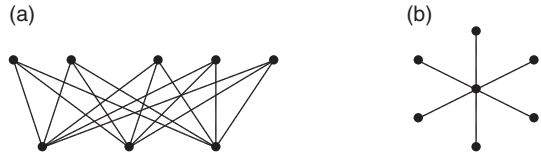


Figure 4.2 The complete bipartite graphs $K_{3,5}$ (a) and $K_{1,6}$ (b).



Figure 4.3 Two graphs ((a) and (b)) that are isospectral for the algebraic graph Laplacian.

Let $v, v' \in V_1$. We put $f(v) = 1, f(v') = -1$, and $f(w) = 0$ for all other vertices. Then, f is an eigenfunction with eigenvalue n, and there are $m - 1$ linearly independent such functions, and hence, we get the eigenvalue n with multiplicity $m-1$. Analogously, we get the eigenvalue m with multiplicity $n-1$. Thus, we have altogether found all the $m + n$ eigenvalues of the graph $K_{m,n}$ with its $m + n$ vertices. In fact, the functions f will also be eigenfunctions for the normalized graph Laplacian; see Corollary 4.1.11, but the corresponding eigenvalue will be 1.

The complement graph of $K_{m,n}$ is the disjoint union $K_m + K_n$ of the complete graphs K_m and K_n. The eigenvalues of $K_{m,n}$ could therefore also have been derived from those of K_m and K_n by Corollary 4.1.3.

Figure 4.3 shows another example of two graphs, taken from [269], with the same spectrum of the algebraic Laplacian. These graphs both have the spectrum $0, 3 - \sqrt{5}, 2, 3, 3, 3 + \sqrt{5}$. In fact, the second graph is bipartite, that is, the vertices can be grouped into two classes without connections inside either class (see Definition 4.1.5). The first one is not bipartite, however, and so the spectrum of the algebraic graph Laplacian cannot determine bipartiteness. This is different for the spectrum of the normalized graph Laplacian, as we shall see in Lemma 4.1.12.

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4.1.3 The Normalized Graph Laplacian

We now move to the *normalized graph Laplacian*, the Laplace operator on graphs that is of most interest to us.

Let us put this operator into the general perspective developed in Section 2.5.1. In general, the simplices of a simplicial complex have weights. But since the dimension of a graph as a simplicial complex is 1, the edges are the highest-dimensional simplices, and therefore, according to our convention, as formalized in Definition 2.5.6, their weights are 1. And the weight of a vertex then is its degree. This defines an *unweighted graph*, and in this section, if not explicitly stated otherwise, **the graph Γ is unweighted**.

We now equip the space $L^2(\Gamma)$ of functions $f : V \to \mathbb{R}$ on the vertex set V of a graph with the scalar product

$$(f,g) = \sum_v \deg v \, f(v)g(v). \tag{4.1.32}$$

This then is the setting of this section.

Remark 4.1.3. The constructions of this section naturally extend to *weighted graphs*. We write the weight of the unoriented edge (vv') in a weighted graph as $w_{vv'}$. And since weights are assigned to unoriented simplices, we have $w_{v'v} = w_{vv'}$. The degree of a vertex v in a weighted graph then is $\deg v = \sum_{v' \sim v} w_{vv'}$. And we can then use this in the scalar product (4.1.32) and also in the subsequent formula for the Laplacian $\Delta = L^0$, see (4.1.35).

We have from (2.5.7) and (2.5.17)

Lemma 4.1.6. *The normalized combinatorial Laplace operator is given by*

$$L^0(f)(v) = f(v) - \frac{1}{\deg v} \sum_{v' \sim v} f(v') \tag{4.1.33}$$

We shall simply speak of L^0 of (4.1.33) as the *Laplacian* of the graph in question, and we shall usually write

$$\Delta \coloneqq L^0. \tag{4.1.34}$$

As explained in Section 2.5.3, the Laplacian (4.1.33) evaluates the difference between the value of a function at a vertex v and the average of the values at its neighbors.

Proof According to the general scheme developed in Section 2.5, we have

$$L^0(f)(v) = f(v) - \frac{1}{\deg v} \sum_{v' \sim v} w_{vv'} f(v') = \frac{1}{\deg v} \sum_{v' \sim v} w_{vv'}(f(v) - f(v')), \tag{4.1.35}$$

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a special case of (4.1.2). And, as explained, since the dimension of a graph as a simplicial complex is 1, the edges are the highest-dimensional simplices, and therefore, according to Definition 2.5.6, their weights are 1, and this then leads to (4.1.35). □

Our eventual aim will be to analyze the spectrum of the operator L^0, that is, the collection of its eigenvalues. When we speak of the eigenvalues of a graph in the sequel, we shall always mean those of L^0. Let us formulate the problem in slightly more abstract terms. With the *adjacency matrix* A (4.1.21) and the diagonal *degree matrix* D (4.1.22), we can write

$$\Delta = \mathrm{Id} - D^{-1}A. \tag{4.1.36}$$

Remark 4.1.4. This should be compared with (4.1.23).

The scheme also works in the weighted case, putting $A(v, v') := w_{vv'}$.

Remark 4.1.5. Concerning our notation and conventions, we point out:

- While some of the subsequent material is taken from [146], we should alert the reader that our conventions here are different from those of [146]. In fact, our Δ is the negative of that in that reference. The reason lies in the systematic development of Section 2.5 of which Δ is a special case. There is some analogous notational discrepancy for the Laplace operator used in analysis and geometry, also usually denoted by Δ. Analysts usually define the Laplacian of a function f on $\mathbb{R}^n$ as $\Delta f = \sum_{i=1}^n \frac{\partial^2 f}{\partial x_i^2}$. That operator is a negative operator because integration by parts yields (for compactly supported functions, say) $\int f\Delta f = -\int |df|^2$. The geometers therefore prefer to introduce a minus sign into the preceding definition in order to turn the Laplacian into a positive operator, actually for reasons that are completely analogous to those of Section 2.5. And in fact, Eckmann's Theorem 4.8.1 is analogous to the Hodge Theorem in Riemannian geometry that represents de Rham cohomology classes by harmonic differential forms (see [150]).

  Another notational difference between the present text and [146] is that here we denote the smallest eigenvalue by λ_1 (and, therefore, the largest one is λ_N, with N being the number of vertices), whereas there, it had been denoted by λ_0. The reason was that the smallest eigenvalue is always 0, and so, there is also some advantage in that notation.

  Most of the conventions, however, agree with those of [217], from which some of the material in this chapter is taken.
- In graph theory, often a different Laplacian is considered, the algebraic graph Laplacian (4.1.20) that we have briefly discussed in Section 4.1.2. While that operator is also quite useful in graph theory, we prefer the operator

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(4.1.33) because it is derived from systematic constructions on simplicial complexes, and also, because it is naturally related to random walks and diffusion processes on graphs.

We now list the important properties of Δ. The first three have already been stated in Lemma 4.1.1 and Corollary 4.1.1. As before, we denote the eigenvalues by λ_k so that the eigenvalue equation becomes

$$\Delta u_k = \lambda_k u_k, \tag{4.1.37}$$

with u_k being a corresponding *eigenfunction*, and we order the eigenvalues as

$$\lambda_1 = 0 < \lambda_2 \leq \ldots \leq \lambda_N.$$

Lemma 4.1.7. *Let Γ be a connected graph.*

1. *Δ is self-adjoint with respect to the scalar product $(\cdot,\cdot)$, that is,*

$$(f, \Delta g) = (\Delta f, g) \tag{4.1.38}$$

   for all $f, g \in L^2(\Gamma)$. Hence, all eigenvalues are real
2. *Δ is non-negative:*

$$(\Delta f, f) \geq 0 \tag{4.1.39}$$

   for all f. Hence, all eigenvalues are non-negative.
3. *$\Delta f = 0$ precisely when f is constant. Hence, the smallest eigenvalue is $\lambda_1 = 0$. Since we assume that Γ is connected, this eigenvalue is simple, that is,*

$$\lambda_k > 0 \tag{4.1.40}$$

   for $k > 1$.
4. *When Γ has no self-loops, then the trace of Δ is N. Hence*

$$\sum_{k=1}^{N} \lambda_k = N. \tag{4.1.41}$$

Proof The first three have already been derived in Lemma 4.1.1 and Corollary 4.1.1. Concerning the last one, since for loopless graphs, the adjacency matrix A has only 0s on the diagonal, the last claim follows from (4.1.36). □

By (4.1.33), λ is an eigenvalue with eigenfunction f if

$$f(v) - \frac{1}{\deg v} \sum_{v' \sim v} f(v') = \lambda f(v), \tag{4.1.42}$$

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or equivalently

$$(1-\lambda)f(v) = \frac{1}{\deg v}\sum_{v'\sim v} f(v'). \tag{4.1.43}$$

We next consider the difference operator (2.3.1) that was also displayed in (4.1.8). For neighbors $v \sim v'$,

$$\delta f(v,v') := f(v') - f(v). \tag{4.1.44}$$

The operator δ can be considered as a map from functions on the vertices of Γ to functions on the edges of Γ. In order to make the latter space also an L^2-space, we consider the product

$$(\delta f, \delta g) := \sum_{e=(vv')} (f(v') - f(v))(g(v') - g(v))), \tag{4.1.45}$$

which is of course the special case of (4.1.9) for edge weights $b(e) = 1$. Note that we are summing here over edges and not over vertices. If we did the latter, we would need to put in a factor of $1/2$ because each edge would then be counted twice. We also point out that in contrast to the product of (4.1.32), $(f,g) = \sum_v \deg v\, f(v)g(v)$, we do not include weights here. The reason is that, here, the sum should be considered as a sum of edges and not one over vertices, and since we are considering unweighted graphs at this point, the edges do not carry any natural weights. This is in accordance with the general principle of Definition 2.5.6.

We also note that (4.1.45) does not depend on the orientations of the edges (and therefore, our convention to count edges only once in the undirected case is appropriate).

The product (4.1.45) encodes more information about the graph than the product (4.1.32). The latter only depends on the weights (as given by the vertex degrees) but not on the connection structure of the graph. There exist many structurally quite diverse graphs with the same degree sequence, and given a graph, one can rewire it by a cross exchange of edges without changing the degrees of the nodes. Namely, given vertices $v_1 \sim v_1'$ and $v_2 \sim v_2'$, but without edges between v_1 and v_2, or between v_1' and v_2', we create a new graph by deleting the edges between v_1 and v_1' and between v_2 and v_2' and inserting new edges between v_1 and v_2 and between v_1' and v_2'. That operation preserves the degrees of all vertices and therefore also the product (4.1.32) for any functions f, g on the graph. (4.1.45), in contrast, is affected because the edge set is changed.

From (4.1.5), we recall

$$(\delta f, \delta g) = (f, \Delta g). \tag{4.1.46}$$

Thus, our product (4.1.45) is naturally related to the Laplacian Δ.

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As in Section 4.1.1, we can use the Rayleigh quotients from Section 2.6.1 and Theorem 2.6.1 and Lemma 4.1.2 to characterize the eigenvalues.

Corollary 4.1.4. *1. Any eigenfunction u for some eigenvalue λ satisfies*

$$\lambda = \frac{(\Delta u, u)}{(u,u)} = \frac{(\delta u, \delta u)}{(u,u)}. \tag{4.1.47}$$

2. Since the eigenfunctions can be taken orthogonal to each other and since $(u, u_1) = 0$ (where u_1 is a constant, that is, an eigenfunction for λ_1) means

$$\sum_v \deg v \, u(v) = 0, \tag{4.1.48}$$

the second smallest eigenvalue of Δ is

$$\lambda_2 = \min \left\{ \frac{(\delta u, \delta u)}{(u,u)} : \sum_v \deg v \, u(v) = 0 \right\}. \tag{4.1.49}$$

3. The largest eigenvalue of Δ is

$$\lambda_N = \max \left\{ \frac{(\delta u, \delta u)}{(u,u)} : u \in L^2(\Gamma) \backslash \{0\} \right\}. \tag{4.1.50}$$

4. The eigenvalues satisfy

$$0 \le \lambda \le 2. \tag{4.1.51}$$

Proof The first three items have already been stated in Corollary 4.1.2, and the lower bound in (4.1.51) is also obvious, for instance, from (4.1.47). It remains to show the upper bound.
By the 3rd statement of Corollary 4.1.4, the largest eigenvalue is

$$\lambda_N = \max_{u \neq 0} \frac{\sum_{e=(v_0,v_1)} (u(v_0) - u(v_1))(u(v_0) - u(v_1))}{\sum_v \deg v \, u(v)^2}. \tag{4.1.52}$$

The largest possible value of this quantity is 2, and this value is realized when

$$u(v_1) = -u(v_0) \tag{4.1.53}$$

for every edge. □

Recalling (4.1.45), we can rewrite (4.1.47) to obtain

Corollary 4.1.5. *Any eigenfunction u for some eigenvalue $\lambda \neq 0$ satisfies*

$$\lambda = \frac{\sum_{e=(v_0,v_1)} (u(v_0) - u(v_1))^2}{\sum_v \deg v \, u(v)^2}. \tag{4.1.54}$$

□

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Let us also derive another characterization.

Corollary 4.1.6. *Any eigenfunction u for some eigenvalue $\lambda \neq 0$ satisfies*

$$2-\lambda = \frac{\sum_v \frac{1}{\deg v} \sum_{v',v'':\, v'\sim v, v''\sim v} (u(v')-u(v''))^2}{\sum_{v,v':\, v\sim v'} (u(v)-u(v'))^2} \tag{4.1.55}$$

Proof We first derive some general identities for a function u on the vertex set of Γ.

$$\begin{aligned}
&\sum_v \frac{1}{\deg v} \sum_{v',v'':\, v'\sim v, v''\sim v} (u(v')-u(v''))^2 \\
&= \sum_v \left(\sum_{v'':\, v\sim v''} \frac{1}{\deg v} \sum_{v':\, v'\sim v} (u(v'')-u(v'))^2 \right) \\
&= \sum_v \left(\sum_{v'':\, v\sim v''} \frac{1}{\deg v} \sum_{v':\, v'\sim v} u(v')^2 - \frac{2}{\deg v} \sum_{v':\, v'\sim v} u(v'')u(v') + u(v'')^2 \right) \\
&= \sum_v \left(2 \sum_{v':\, v'\sim v} u(v')^2 - \frac{2}{\deg v} \left(\sum_{v':\, v'\sim v} u(v') \right)^2 \right) \\
&= 2 \sum_v \sum_{v':\, v'\sim v} u(v')^2 - \sum_v 2 \deg v \left(\frac{1}{\deg v} \sum_{v':\, v'\sim v} u(v') \right)^2 .
\end{aligned}$$

We now observe that we can replace u by $u-u(v)$ in the first and hence also in all subsequent lines. This yields

$$\begin{aligned}
&\sum_v \frac{1}{\deg v} \sum_{v',v'':\, v'\sim v, v''\sim v} (u(v')-u(v''))^2 \\
&= 2 \sum_v \sum_{v':\, v'\sim v} (u(v')-u(v))^2 - \sum_v 2 \deg v \left(\frac{1}{\deg v} \sum_{v':\, v'\sim v} (u(v')-u(v)) \right)^2 \\
&= 2 \sum_v \sum_{v':\, v'\sim v} (u(v')-u(v))^2 - \sum_v 2 \deg v (\Delta u(v))^2 .
\end{aligned}$$

When u now is an eigenfunction, $\Delta u = \lambda u$ for some eigenvalue λ, then, by (4.1.47), $\sum_v \sum_{v':\, v'\sim v} (u(v')-u(v))^2 = 2\lambda \sum_v \deg v\, u(v)^2$, and we obtain

$$\sum_v \frac{1}{\deg v} \sum_{v',v'':\, v'\sim v, v''\sim v} (u(v')-u(v''))^2 = 2\lambda(2-\lambda) \sum_v \deg v\, u(v)^2 . \tag{4.1.56}$$

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Using (4.1.47) again, we can also reformulate this as

$$2-\lambda=\frac{\sum_v \frac{1}{\deg v}\sum_{v',v''\colon v'\sim v, v''\sim v}(u(v')-u(v''))^2}{\sum_v\sum_{v'\colon v'\sim v}(u(v')-u(v))^2}. \tag{4.1.57}$$

□

Let us also go into the details of the computation of the normalized combinatorial Laplacian L^1 on a graph. We consider an oriented edge $e=[v_0,v_1]$. Let $f\colon V\to\mathbb{R}$ be a function on the vertex set V of our graph. Then (4.1.44) becomes

$$\delta f(e)=f(v_1)-f(v_0), \tag{4.1.58}$$

and so, for a function $\omega\colon E\to\mathbb{R}$ on the edges of our graph, which, according to (2.5.1), satisfies $\omega[v_1,v_0]=-\omega[v_0,v_1]$,

$$\begin{aligned}\sum_v \deg v\ f(v)\delta^*\omega(v) &= (f,\delta^*\omega)\\ &= (\delta f,\omega)\\ &= \sum_e \delta f(e)\omega(e)\\ &= \sum_{e=[v_0,v_1]}(f(v_1)-f(v_0))\omega(e)\\ &= \sum_{v_0,v_1}\deg v_1\ f(v_1)\omega(v_0,v_1)-\sum_{v_0,v_1}\deg v_0\ f(v_0)\omega(v_0,v_1)\end{aligned}$$

and hence

$$\delta^*\omega(v)=\frac{1}{\deg v}\sum_{v\in e}(-1)^{i(e)}\omega(e) \tag{4.1.59}$$

with

$$i(e)=\begin{cases}1 & \text{if } e=(v,v')\\ 0 & \text{if } e=(v',v).\end{cases}$$

Moreover, for $e=[v_0,v_1]$ as before,

$$\begin{aligned}L^1\omega(e)=\delta\delta^*\omega(e)=\delta f(e),\ \text{with } f(v)&=\frac{1}{\deg v}\sum_{v\in e}(-1)^{i(e)}\omega(e),\\ &=\frac{1}{\deg v_0}\sum_{v_0\in g=[v_0,v']}\omega(g)-\frac{1}{\deg v_1}\sum_{v_1\in f=[v_1,v']}\omega(f).\end{aligned} \tag{4.1.60}$$

From (4.8.6), we obtain

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Corollary 4.1.7. *The operators Δ in (4.1.33) and L^1 in (4.1.60) on a graph have the same nonzero eigenvalues.* □

Moreover, by Theorem 4.8.1, the multiplicities of the eigenvalue 0 of Δ and L^1 on a graph Γ with vertex set V and edge set E equal the Betti numbers b_0 and b_1. Thus, also

$$\chi(\Gamma) = |V| - |E| = b_0 - b_1 = \dim\ker\Delta - \dim\ker L^1. \tag{4.1.61}$$

In particular, when the graph is connected, $b_0 = 1$, that is, the eigenvalue 0 of Δ is simple, and by (4.1.61), the multiplicity of the eigenvalue 0 of L^1 then is $|E| - |V| + 1$. A connected graph with $|E| = |V| - 1$ is called a *tree*, and we conclude

Corollary 4.1.8. *A connected graph $\Gamma = (V, E)$ is a tree if and only if the kernel of L^1 is trivial.* □

More generally, we can express the vanishing of the Laplacian of a function ω at an edge in terms of diffusion through that edge as governed by ω. In fact, from (4.1.60), we have that for an edge $e = [v_0, v_1]$, $L^1\omega(e) = \delta\delta^*\omega(e) = 0$ precisely if what comes into the initial vertex v_0 and leaves at the terminal vertex v_1 is balanced by what exits at v_0 and enters at v_1. We note that in particular, the edge $e = [v_0, v_1]$ enters into (4.1.60) with the contribution $\left(\frac{1}{\deg v_0} + \frac{1}{\deg v_1}\right)\omega(e)$, and from this subtraction, it is subtracted what enters into v_0 from other edges and what leaves at v_1 into other edges, while the opposite contributions, leaving at v_0 or entering at v_1, have a positive sign.

In particular, on a *chain*, that is, a set of different vertices $\{v_0, \ldots, v_m\}$ with edges $e_1 = [v_0, v_1], \ldots, e_m = [v_{m-1}, v_m]$, the only solution of $L^1\omega = 0$ is $\omega \equiv 0$, but on a *cycle*, that is, when we close the chain by an edge $e_0 = [v_m, v_0]$, $\omega \equiv constant$ is also a solution.

We now apply these principles to study the eigenvalue problem for some other simple examples. We first consider the complete graphs K_N and K_N^0, see Definition 4.1.4.

As in Lemma 4.1.5, we can easily determine the spectra of K_N and K_N^0.

Lemma 4.1.8. *The spectrum of K_N consists of the eigenvalue $\lambda_1 = 0$ and the eigenvalue $\lambda_2 = \ldots = \lambda_N = \frac{N}{N-1}$.*

K_N^0 has $\lambda_1 = 0$ and $\lambda_2 = \ldots = \lambda_N = 1$.

Proof For a complete graph K_N, all the degrees $\deg v$ have the value $N - 1$ and are therefore equal. Hence, also all the nontrivial eigenvalues are equal. We have

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$$\lambda_2 = \ldots = \lambda_N = \frac{N}{N-1} \tag{4.1.62}$$

since

$$\Delta u(v) = u(v) - \frac{1}{N-1}\sum_{v' \neq v} u(v') = \frac{N}{N-1}u(v) \tag{4.1.63}$$

for any u that is orthogonal to the constants, that is,

$$\frac{1}{N}\sum_{v' \in V} \deg v'\, u(v') = \frac{N-1}{N}\sum_{v' \in V} u(v') = 0. \tag{4.1.64}$$

Similarly, on K_N^0, we have

$$\lambda_2 = \ldots = \lambda_N = 1 \tag{4.1.65}$$

since $\Delta u = u$ whenever u is orthogonal to the constants.

□

In fact, we could have deduced this result directly from Lemma 4.1.5 because of the following:

Lemma 4.1.9. *Let Γ be a graph with constant degree, that is,* $\deg v = k$ *for some k and all vertices v. Then, the eigenvalues of the algebraic Laplacian Λ are k times those of the normalized Laplacian Δ.*

Proof In that case, the two Laplacians are related by

$$\Lambda = k\Delta. \tag{4.1.66}$$

and therefore also the eigenvalues differ by that factor. □

The example of complete graphs shows that neither the smallest nonzero nor the largest eigenvalue of a graph needs to be simple.

In fact, the spectral properties found in Lemma 4.1.8 characterize the complete graphs.

Lemma 4.1.10. *A graph with N vertices without self-loops is complete if and only if its spectrum consists of* 0 *as a simple eigenvalue and $\frac{N}{N-1}$ with multiplicity $N-1$.*

More precisely, for a graph with N vertices without self-loops that is not complete, we have

$$\lambda_2 \leq 1 \text{ and } \lambda_N > \frac{N}{N-1}. \tag{4.1.67}$$

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Proof We have already verified that the spectrum of K_N has those values. For the converse direction, by Corollary 4.1.4,

$$\lambda_2 = \min_{g:\ \sum_v \deg v\ g(v)=0} \frac{(\Delta g, g)}{(g,g)}. \tag{4.1.68}$$

When Γ is not complete, we can find two vertices v_1, v_2 that are not connected by an edge and take g with $g(v_1), g(v_2) \neq 0$, but

$$\deg v_1\ g(v_1) + \deg v_2\ g(v_2) = 0 \text{ and } g(v) = 0 \text{ for all other } v. \tag{4.1.69}$$

Inserting this into the Rayleigh quotient (4.1.68) makes that expression 1, and the minimum therefore is ≤ 1. The second inequality of (4.1.67) follows by taking two connected vertices v_1 and v_2 and g as before and verifying that the Rayleigh quotient then becomes $> \frac{N}{N-1}$. □

From Lemma 4.1.10, we see that there are graphs, such as the complete graphs K_N, that are completely determined by their spectrum. Thus, there are no other graphs that are isospectral with K_N. And in fact, there do not even exist graphs whose spectrum is very close to that of K_N. This follows from Theorem 4.1.1, which was found in [73].

Theorem 4.1.1. *For a noncomplete graph with N vertices,*

$$\lambda_N \geq \frac{N+1}{N-1}. \tag{4.1.70}$$

Proof The proof is taken from [155]. We may assume that the graph is connected. In fact, for a nonconnected graph, the smallest connected component has at most $N/2$ vertices. Thus, its largest eigenvalue, and hence also the largest eigenvalue λ_N of the entire graph, satisfies

$$\lambda_N \geq \frac{N/2}{N/2-1} = \frac{N}{N-2} > \frac{N+1}{N-1},$$

which proves the theorem for nonconnected graphs.

Thus, we may indeed assume that the graph is connected. Since it is not complete, there exists a vertex v with $\deg v \leq N-2$. As the graph is connected, we can find some other vertex w that is a neighbor of some neighbor of v but not a neighbor of v itself. Then, $\deg v' \leq N-2$ as well, since v is not a neighbor of w. For any collection $v_1, v_2, \ldots, v_m$ of vertices, let $S(v_1, \ldots, v_m)$ be the set of their joint neighbors, and let $s(v_1, \ldots, v_m)$ be its cardinality. Let $S = S(v, v')$ be the nonempty set of vertices that are neighbors of both v and v', and let s be the cardinality of S, that is, the number of joint neighbors of v and w. We shall construct a function f with $(f, \Delta f) \geq \frac{N+1}{N-1}(f, f)$. Then, the result follows from (4.1.50).

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We put

$$f(u) \coloneqq \begin{cases} -1 & : u \in S, \\ \frac{N-1}{2}\frac{s}{\deg v} & : u = v, \\ \frac{N-1}{2}\frac{s}{\deg v'} & : u = v', \\ 0 & : \text{else.} \end{cases}$$

f satisfies

$$\deg v\, \Delta f(v) = \deg v f(v) + s = \frac{N+1}{2} s$$

and thus, $\Delta f(v) = \frac{N+1}{N-1} f(v)$. Likewise, $\Delta f(v') = \frac{N+1}{N-1} f(v')$. We now claim that $-\Delta f(u) \geq \frac{N+1}{N-1}$ for all $u \in S$. We observe $s \geq \max(1, \deg v + \deg v' + 2 - N)$ and calculate

$$-\Delta f(u) = \frac{\deg u - s(u,v,v') + f(v) + f(v')}{\deg u} \geq 1 + \frac{1 - s + f(v) + f(v')}{\deg u}. \tag{4.1.71}$$

As $f(v) + f(v') \geq s$, we can use $\deg u \leq N - 1$ and continue

$$\begin{aligned} \frac{1 - s + f(v) + f(v')}{\deg u} &\geq \frac{1-s}{N-1} + \frac{s}{2\deg v} + \frac{s}{2\deg v'} \\ &= \frac{1}{N-1} + s\left(\frac{1}{2\deg v} + \frac{1}{2\deg v'} - \frac{1}{N-1}\right). \end{aligned} \tag{4.1.72}$$

Since $\deg v \leq N - 2$ and $\deg v' \leq N - 2$, the term in brackets is positive, and thus,

$$\begin{aligned} &s\left(\frac{1}{2\deg v} + \frac{1}{2\deg v'} - \frac{1}{N-1}\right) \\ &\quad \geq \max(1, \deg v + \deg v' + 2 - N)\left(\frac{1}{2\deg v} + \frac{1}{2\deg v'} - \frac{1}{N-1}\right). \end{aligned} \tag{4.1.73}$$

We write $D \coloneqq (\deg v + \deg v')/2$, then the harmonic–arithmetic mean gives

$$\frac{1}{2\deg v} + \frac{1}{2\deg v'} \geq \frac{1}{D}.$$

Thus,

$$s\left(\frac{1}{2\deg v} + \frac{1}{2\deg v'} - \frac{1}{N-1}\right) \geq \max(1, 2D + 2 - N)\left(\frac{1}{D} - \frac{1}{N-1}\right). \tag{4.1.74}$$

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We aim to show that the latter term is at least $1/(N-1)$, which, by multiplying with $D(N-1)$ and subtracting D is equivalent to

$$\max(1, 2D+2-N)(N-1-D) - D \geq 0. \tag{4.1.75}$$

If $D \leq (N-1)/2$, then the maximum equals 1 and the inequality follows immediately. If $D \geq (N-1)/2$, then $\max(1, 2D+2-N) = 2D+2-N$, and so the left-hand side becomes a concave quadratic polynomial in D with its zero points at $D = N-2$ and $D = (N-1)/2$. Thus, the inequality (4.1.75) holds for all D between those zeroes. But by assumption, D lies between the zero points, which proves the claim that $-\Delta f(u) \geq \frac{N+1}{N-1}$ for all $u \in S$. In particular, this shows that $f\Delta f \geq \frac{N+1}{N-1} f^2$. Summation over the vertex set proves the claim of the theorem for all connected graphs.

□

Remark 4.1.6. Reference [73] could also determine the graphs for which (4.1.70) becomes an equality; see also [155] for a simpler proof. These graphs are the complete graphs with a single edge removed, or when N is odd, two complete graphs of size $(N+1)/2$ joined at a single vertex. The simplest nontrivial example for the latter case, two copies of K_3 joined at a single vertex, will be examined in Figure 4.5. For all other graphs, the inequality (4.1.70) is strict, and one may derive more precise lower bounds for them; see [155].

We now come to another class of graphs where in contrast to complete graphs, connections between vertices are restricted. This will in particular lead to a behavior of the largest eigenvalue λ_N that is opposite to what we see on complete graphs.

Definition 4.1.5. A graph Γ is *bipartite* if its vertex set V can be decomposed as $V = V_+ \cup V_-$ with disjoint V_+, V_- such that there are no edges connecting vertices in the same components. That is, every edge has one of its endpoints in V_+ and the other in V_-.

For instance, every tree is bipartite. Starting with any vertex v_0 of a tree, one puts v_0 into V_+, all neighbors of v_0 into V_-, the neighbors of those neighbors into V_+ again, and so on. Likewise, cycles, that is, graphs with vertices $v_1, \dots, v_N$ and edges $(v_1, v_2), \dots (v_{N-1}, v_N), (v_N, v_1)$ for even N, are bipartite, with V_+ containing the vertices with an even index. Cycles with an odd N are not bipartite, however. In fact, we have

Lemma 4.1.11. *A graph is bipartite if and only if it does not contain cycles of odd length.*

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Proof Without loss of generality, we may assume that our graph Γ is connected, that is, any two vertices can be joined by a path. (Otherwise, we would apply the subsequent reasoning to every connected component of Γ.) Take any vertex v_0 in Γ. Let V_+ be the class of all vertices v that have an even distance from v_0, that is, a shortest path connecting v_0 has an even number of edges. Likewise, let V_- consist of those vertices that have an odd distance to v_0. If there is no edge connecting any two vertices in V_+, or any two vertices in V_-, the graph is bipartite. Assume now that there is an e edge connecting $v_1, v_2 \in V_+$, for instance. We then create a cycle of odd length by taking the path from V_0 to v_1, which has an even length, the edge from v_1 to v_2, which has length 1, and then the path of even length from v_2 to v_0. □

The cycle constructed in the preceding proof may traverse some edges back and forth, that is, it need not consist of disjoint edges. Any such cycle, however, has a subcycle with disjoint edges. We simply take away all edges traversed back and forth and take a component of the rest. The parity of the length, that is, whether it is even or odd, is not affected by this procedure.

Lemma 4.1.12. *A graph Γ is bipartite if and only if its largest eigenvalue is 2. And a corresponding eigenfunction is a multiple of the function that is $+1$ on one class and -1 on the other.*

Proof In (4.1.53) in the proof of Corollary 4.1.4, we have seen that the largest possible value of the Rayleigh quotient giving λ_N is realized for a function u that satisfies $u(v_1) = -u(v_0)$ whenever $v_1 \sim v_0$, that is, a function of the type claimed in the Lemma. In that case, $\lambda_N = 2$. And that is possible if and only if the graph is bipartite. □

From Lemma 4.1.12, we see that a single eigenvalue can already encode a distinctive characteristic feature of a graph, in the case at hand being bipartite. More generally,

Lemma 4.1.13. *A graph Γ is bipartite if and only if whenever λ is an eigenvalue, then $2 - \lambda$ is an eigenvalue as well.*

Proof Let λ be an eigenvalue with eigenfunction f on a bipartite graph with vertex set $V = V_+ \cup V_-$. Then,

$$\tilde{f} := \begin{cases} f(v) & \text{for } v \in V_+ \\ -f(v) & \text{for } v \in V_- \end{cases} \tag{4.1.76}$$

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is an eigenfunction for the eigenvalue $2-\lambda$. In fact, for the eigenfunction f, we have by (4.1.43)

$$(1-\lambda)f(v) = \frac{1}{\deg v}\sum_{v'\sim v} f(v'), \tag{4.1.77}$$

and hence

$$(1-(2-\lambda))f(v) = (\lambda-1)f(v) = -\frac{1}{\deg v}\sum_{v'\sim v} f(v'), \tag{4.1.78}$$

and on a bipartite graph; therefore, $\tilde{f}$ from (4.1.76) is an eigenfunction for the eigenvalue $2-\lambda$.

Conversely, if whenever λ is an eigenvalue, then so is $2-\lambda$, then since 0 is always an eigenvalue (with the constants as eigenfunctions), 2 has to be an eigenvalue. By Lemma 4.1.12, this implies that the graph is bipartite. □

The proof also yields

Corollary 4.1.9. *When λ is an eigenvalue of a bipartite graph with eigenfunction f, then according to* (4.1.76)*, we obtain an eigenfunction for $2-\lambda$ by changing the sign of f on one of the components. Unless f vanishes identically on one component, this function $\tilde{f}$ is linearly independent of f. Thus, only eigenfunctions for the eigenvalue 1 can vanish identically on one of the components.*

More generally, on a bipartite graph, we only need to know half of the eigenvalues and eigenfunctions to reconstruct the entire spectrum. □

This Corollary will be quite useful later when we compute the spectra of certain classes of bipartite graphs.

Corollary 4.1.10. *Let Γ be a connected graph. If 2 is an eigenvalue of Γ, then it is simple.*

Proof By Lemma 4.1.13, when 2 is an eigenvalue, the graph is bipartite, and furthermore, its multiplicity equals that of the eigenvalue 0. By Lemma 4.1.7, that eigenvalue is simple since Γ is connected. □

We have now seen that the eigenvalues 0 and 2, the minimal and maximal possible values by Lemma 4.1.12, play special roles. The eigenvalue 1 is also very interesting. According to (4.1.43), f is an eigenfunction for the eigenvalue 1 if and only if

$$\sum_{v'\sim v} f(v') = 0 \text{ for every vertex } v. \tag{4.1.79}$$

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This can, for instance, be achieved as follows. Suppose the graph contains two vertices v_1 and v_2 that are not connected by an edge but have the same neighbors, that is,

$$v \sim v_1 \text{ if and only if } v \sim v_2. \tag{4.1.80}$$

In such a situation, we can define

$$f(v) = \begin{cases} +1 & \text{for } v = v_1 \\ -1 & \text{for } v = v_2 \\ 0 & \text{else.} \end{cases} \tag{4.1.81}$$

This function f then satisfies (4.1.79) because $f(v') = 0$ for all neighbors of v_1 and for all neighbors of v_2, and for any v that has both v_1 and v_2 as its neighbors, the sum also vanishes, since $f(v_2) = -f(v_1)$. And since v_1 and v_2 have the same neighbors, any v is either a neighbor of both or of neither of them. Since we know that $\Delta = L^0$ and L^1 have the same nonzero eigenvalues, in the preceding situation, we should also generate an eigenvalue 1 of L^1. This is simply achieved by putting

$$\omega(e) = \begin{cases} +1 & \text{for } e = (v, v_1) \\ -1 & \text{for } e = (v, v_2) \text{ (or equivalently 1 for } e = (v_2, v)) \\ 0 & \text{else.} \end{cases} \tag{4.1.82}$$

Then, at any $v \neq v_1, v_2$, there is no contribution to $L^1\omega$ as given in (4.1.60) because what comes in equals what flows out. At v_1, for an edge $e = (v, v_1)$, we get the contribution $\deg v_1 \left(\frac{1}{\deg v_1}\omega(e)\right) = 1$, and analogously at v_2, and hence the ω of (4.1.82) is an eigenvector for the eigenvalue 1. Geometrically, v_2 is a source, and v_1 is a sink for that ω.

We also observe the remarkable fact that eigenfunctions can be very local, that is, be nonzero only on a small set of vertices in the present case of the eigenfunction f from (4.1.81) for Δ, only on two vertices, which, in fact, is the minimal possible number for the support of an eigenfunction.

The preceding can be turned into a constructive process the *duplication of vertices*. We start with some vertex v_1 in a graph Γ and construct a graph Γ' that has one additional vertex v_2 that is not connected with v_1 but has the same neighbors as it. Such a graph Γ' has the eigenvalue 1. Also, when Γ already possesses the eigenvalue 1 from a previous vertex duplication process, then this eigenvalue with its eigenfunction carries over to Γ'. To see this, consider an eigenfunction f_1 for the eigenvalue 1. It satisfies (4.1.79), and if we extend it to Γ' by putting $f_1(v_2) = 0$, this still holds for all vertices v of Γ. (4.1.79) also holds for v_2 because it holds for v_1, and v_1 and v_2 have the same neighbors.

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Thus, let us start with the simplest nontrivial graph, consisting of two vertices v_+, v_-, connected by an edge $e = (v_+, v_-)$. This graph is denoted by $K_{1,1}$, for a reason that will become apparent in a moment. When we now iteratively duplicate v_+ $m-1$ times and v_- $n-1$ times, we obtain a bipartite graph with vertex set V_+ having m and V_- having n vertices. Also, every vertex in V_+ is connected with every vertex in V_-. This is the *complete bipartite* graph $K_{m,n}$. And, we already know its spectrum. As a bipartite graph, it has the eigenvalues 0 and 2 (which are simple by Lemma 4.1.13 as the graph is connected), and since $K_{m,n}$ is the result of $m+n-2$ vertex duplications, it possesses the eigenvalue 1 with multiplicity $m+n-2$. Since $K_{m,n}$ has $m+n$ vertices, we therefore have found all its eigenvalues. This shows

Corollary 4.1.11. *The spectrum of the complete bipartite graph $K_{m,n}$ consists of the eigenvalues 0 and 2 with multiplicity 1 and the eigenvalue 1 with multiplicity $m+n-2$.*

This also leads to the following observation. Any two graphs $K_{m,n}$ and $K_{m',n'}$ with $m'+n' = m+n$ have the same spectrum, or as one says, they are *isospectral*. (For systematic constructions of isospectral graphs, see for instance, [112, 258].) Thus, graphs cannot always be distinguished by their spectra. The different complete bipartite graphs with the same number of vertices can, however, be distinguished by the multiplicity of the eigenvalue 0 of L^1 because they have different first Betti numbers; see (4.1.61). In fact, $K_{m,n}$ has mn edges, and since by (4.1.61), $m+n-mn = 1-b_1$, the multiplicity of that eigenvalue is $b_1 = mn-m-n+1$. (Note that of course $K_{m,n}$ and $K_{n,m}$ are isomorphic graphs, that is, there exists a bijection between the vertex sets that maps edges to edges; in fact, we simply have to interchange V_+ and V_- to effect that isomorphism.)

Of course, (4.1.79) has a simple algebraic explanation.

Lemma 4.1.14. *The multiplicity of the eigenvalue 1 equals the dimension of the kernel of the adjacency matrix (4.1.21).*

Proof Obvious, since by (4.1.21),

$$0 = \sum_{v'} a_{vv'} f(v') = \sum_{v' \sim v} f(v') \quad \text{for every } v$$

precisely if f is in the kernel of the adjacency matrix $(a_{vv'})$. □

Thus, it is easy to construct further examples of graphs with the eigenvalue $\lambda = 1$, for example:

1. A *cycle graph* C_N consists of nodes $v_1, \dots, v_N$ such that the node v_i is connected to the nodes v_{i-1} and v_{i+1} mod N (i.e., there is a connection

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between v_1 and v_N). When $N = 4m$, we put $u(v_j) = 0$ when j is odd and $u(v_j) = (-1)^{j/2}$ for even j. Then, (4.1.79) holds, and this function is an eigenfunction for the eigenvalue 1. (For $m = 1$, we have in fact a node duplication but no longer for $m > 1$.)

2. The same construction works for the *wheel graph* W_N where we add to C_N a single central vertex v_0 that is connected to all other vertices. For $N = 4m$, we use the function u from the previous example, extended by $u(v_0) = 0$.

   (In fact, all eigenfunctions of W_N vanish at the central vertex v_0, except for the multiples of the function with $u(v_0) = -3$ and $u(v) = 1$ at all other vertices. This function belongs to the eigenvalue $4/3$. For even N, we also have the eigenvalue $5/3$, with an eigenfunction that vanishes again at v_0 and alternatingly assumes the values ± 1 at the other vertices.)
3. We connect C_3 and C_5 at a single node v_0. We put $u(v_0) = 1$, $u(v) = -1$ at the two other nodes from C_3, $u(v) = 1$ at the two neighbors of v_0 in C_5, and $u(v) = -1$ at the remaining two nodes in C_5. This u again satisfies (4.1.79).
4. A bipartite graph with an odd number of vertices must possess the eigenvalue 1 because by Lemma 4.1.13 or Corollary 4.1.9, all other eigenvalues occur in pairs, and so, 1 is needed to produce an odd number of eigenvalues.

Corollary 4.1.12. *Let Γ with N vertices have an induced subgraph Γ_0 with M vertices, that is, a graph containing M of the vertices of Γ and all edges between those vertices that are present in Γ, and assume that Γ_0 does not have the eigenvalue 1. Then, the multiplicity of the eigenvalue 1 of Γ is at most $N - M$.*

The *proof* follows directly from Lemma 4.1.14.

For instance, when Γ contains K_M as an induced subgraph (such an induced subgraph K_M is also called an *M-clique*), then the multiplicity of 1 is at most $N - M$, see [57].

Remark 4.1.7. We observe that a complete graph K_N^0 with self-loops and a complete bipartite graph $K_{m,n}$ with $m + n = N$ have almost the same spectrum. While K_N^0 has the eigenvalue 1 with multiplicity $N - 1$, $K_{m,n}$ has this eigenvalue with multiplicity $N - 2$. But as we shall understand in Section 4.5, the appropriate comparison is that between $K_{m,n}$ and the disjoint union of K_m^0 and K_n^0. Both have the eigenvalue 1 with multiplicity $N - 2$, and instead of the eigenvalue 2 of $K_{m,n}$, the latter graph has an additional eigenvalue 0 because it has two components.

One of the complete bipartite graphs deserves a special name.

Definition 4.1.6. The graph $K_{1,n}$ is called a *star graph*.

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Thus, a star graph consists of one central vertex, a hub, that is connected to all other vertices, but none of those are connected with each other. A star graph is a tree. In fact, conversely, any tree is bipartite, as we have observed earlier.

The preceding can also be understood in terms of symmetries (see Section 2.7 for the abstract setting). When we have two vertices v_1, v_2 as in (4.1.80), that is, $v \sim v_1$ if and only if $v \sim v_2$ for all vertices (and so, in particular, $v_1 \not\sim v_2$, as we are currently not allowing for self-loops), then we have a graph automorphism $\tau\colon V \to V$ (meaning that $v \sim v'$ if and only if $\tau(v) \sim \tau(v')$ given by

$$\tau(v_1) = v_2, \quad \tau(v_2) = v_1, \quad \tau(v) = v \text{ for all } v \neq v_1, v_2. \tag{4.1.83}$$

The Laplacian commutes with τ, that is, with $\tau_* f(v) \coloneqq f(\tau v)$,

$$\Delta(\tau_* f)(v) = \tau_*(\Delta f)(v). \tag{4.1.84}$$

In particular, it leaves the eigenspaces of τ invariant. The eigenvalues of τ are 1 and -1, and the latter is spanned by the function f of (4.1.81). Therefore, this space is one-dimensional and mapped to itself by Δ, and from (4.1.84) we then see that its eigenvalue for Δ is 1. The eigenspace of τ for the eigenvalue 1 consists of functions with $f(v_1) = f(v_2) = 0$, and that space then is spanned by the other eigenfunctions of Δ.

For another example, let τ again be as in (4.1.83), but assume now that v_1 and $v_2 = \tau(v_1)$ are connected by an edge. Then, the eigenvalue equation for f as in (4.1.81) at v_1 becomes

$$f(v_1) - \frac{1}{\deg v_1} f(v_2) = \lambda f(v_1),$$

that is, since $f(v_2) = -f(v_1)$,

$$\lambda = 1 + \frac{1}{\deg v_1}. \tag{4.1.85}$$

Let $e = (v_1, v_2)$ and $e' = (v_1', v_2')$ be duplicate edges, that is, $v \sim v_j$ if and only if $v \sim v_j'$ for $j = 1,2$ and $v \neq v_1, v_2, v_1', v_2'$ and $v_j \not\sim v_k'$ for $j,k = 1,2$. Then, we can determine two eigenvalues and eigenfunctions of Δ by solving

$$\begin{aligned} f(v_1) - \frac{1}{\deg v_1} f(v_2) &= \lambda f(v_1) \\ f(v_2) - \frac{1}{\deg v_2} f(v_1) &= \lambda f(v_2) \\ \text{analogously for } v_1', v_2' & \\ f(v) &= 0 \quad \text{for all other } v. \end{aligned}$$

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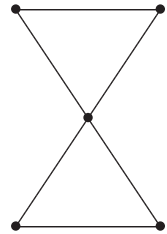


Figure 4.4 An example of edge duplication.

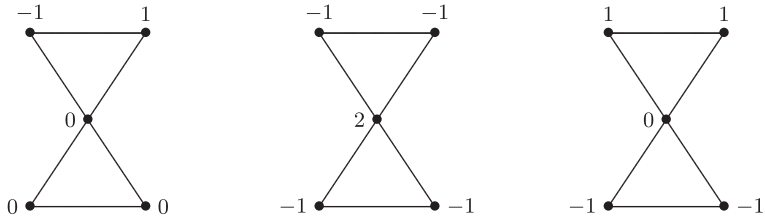


Figure 4.5 Eigenfunctions of the graph of Figure 4.4.

This yields

$$\lambda = 1 \pm \frac{1}{\sqrt{\deg v_1 \deg v_2}}, \tag{4.1.86}$$

see [19].

Let us determine the spectra of some further classes of graphs. We first look at the graph in Figure 4.4, which is obtained by duplicating an edge of a triangle. According to (4.1.86), this generates the eigenvalues $1/2$ and $3/2$. And according to (4.1.85), two eigenvalues $3/2$ are generated by the symmetries of switching the two vertices inside a petal, but the two classes are not disjoint, and so, this construction only yields two eigenvalues $3/2$ altogether. In fact, all eigenfunctions arising from these constructions vanish at the central vertex. But, a further eigenvalue $3/2$ arises from the symmetry exchanging the two triangles, with the central vertex being a fixed point, and this yields an eigenfunction that is nonzero at the center. Thus, we have determined all the eigenvalues of this graph. Let us indicate the corresponding eigenfunctions in Figure 4.5.

The first produces the eigenvalue $3/2$ with multiplicity 2, the second again yields the eigenvalue $3/2$, so that it has multiplicity 3 altogether, while the last one yields the eigenvalue $1/2$. And of course, we have the eigenvalue 0 with multiplicity 1. In passing, we observe that for this graph, the inequality (4.1.70) for the largest eigenvalue becomes an inequality. We can view this graph as two copies of K_3 joined at a single vertex.

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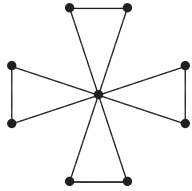


Figure 4.6 The petal graph P_4.

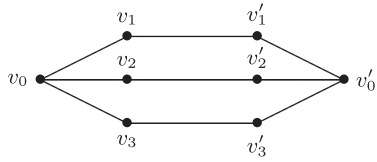


Figure 4.7 A book graph.

We can then construct the family of graphs P_ℓ, called the *petal graphs*, where ℓ triangles are joined at a single central vertex v_0. In Figure 4.4, we see the case $\ell = 2$, and in Figure 4.6, $\ell = 4$.

Iterating the above construction, or alternatively, applying (4.1.85) and (4.1.86) repeatedly, we obtain the eigenvalue $3/2$ with multiplicity $\ell + 1$, $1/2$ with multiplicity $\ell - 1$, and 0 with multiplicity 1. Since P_ℓ has $2\ell + 1$ vertices, this is the entire spectrum.

In particular, for petal graphs with more than two petals, like for complete graphs with more than two vertices, neither the smallest nonzero nor the largest eigenvalue is simple.

Petal graphs have an odd number of vertices. There also is a family with the same spectral properties but an even number of vertices. These are the *book graphs*. They are obtained by joining two star graphs. One star graph has a central vertex v_0 connected to m peripheral vertices $v_1, \dots, v_m$, which are not connected to each other. The other star similarly has a central vertex v_0' connected to m peripheral vertices $v_1', \dots, v_m'$. We then join them by connecting v_i to v_i' for $i = 1, \dots, m$, as shown in Figure 4.7.

For the book graph on $N = 2m + 2$ nodes, 0 and 2 are eigenvalues with multiplicity 1, since Γ is connected and bipartite. Moreover, since the book graph is obtained by the m-fold duplication of the edge (v_1, v_1') in the line graph with vertices v_0, v_1, v_1', and v_0', by (4.1.86), and again, we have a symmetry, this time without a fixed point, obtained by exchanging the two stars, and so, similar to the petal graph, $\lambda = 1/2$ and $\lambda = 3/2$ are eigenvalues with multiplicity m each. In fact, the corresponding eigenfunctions can be constructed as follows:

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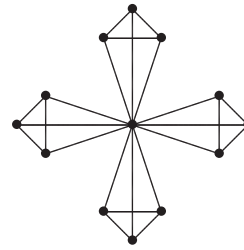


Figure 4.8 A windmill graph.

1. By letting $\sum_{i=1}^{m} f(v_i) = 0$, $f(v_0) = f(v_0') = 0$, $f(v_i') = \mp f(v_i)$, we obtain $m-1$ linearly independent eigenfunctions;
2. By letting $f(v_i) = -f(v_i') = 1$ for $i = 1,\dots,m$ and $f(v_0) = -f(v_0') = 2$, we obtain one more eigenfunction for $1/2$ and similarly by letting $g(v_i) = g(v_i') = -1$ for $i = 1,\dots,m$ and $g(v_0) = g(v_0') = 2$, we obtain one more eigenfunction for $3/2$.

Hence, also in this case, we have a spectral gap of size 1 about 1.

In fact, the spectral gap at 1 here is the largest possible; we have

Theorem 4.1.2 ([158])**.** *For any connected graph* Γ *on* $N \geq 3$ *nodes,*

$$\min_i |1 - \lambda_i| \leq \frac{1}{2}. \tag{4.1.87}$$

Moreover, equality is achieved if and only if Γ *is either a petal graph (for N odd) or a book graph (for N even).*

Remark 4.1.8. Petal graphs are also known as *friendship graphs*. The famous Friendship Theorem [90] states that the only finite graphs with the property that every two vertices have exactly one neighbor in common are precisely the petal graphs. In [62], it has been proved that, among connected graphs, the petal graphs are uniquely determined by the eigenvalues of the adjacency matrix. And, Theorem 4.1.2 implies that both petal graphs and book graphs are characterized by their normalized Laplacian spectra.

In fact, the star and the petal graphs belong to a larger family, that of the *windmill graphs* $Wd(n,\ell)$ obtained by taking ℓ copies of the complete graph K_{n-1} and then adding a single central vertex connected to all others. Equivalently, we take ℓ copies of K_n and join all of them at a single vertex. Thus, $Wd(n,\ell)$ has $\ell(n-1)+1$ vertices. The star graphs S_ℓ then are $Wd(2,\ell)$ and the petals P_ℓ are $Wd(3,\ell)$. Figure 4.8 shows $Wd(4,4)$: Again, the spectra of the windmill graphs are easily determined. We have the eigenvalue 0, as always.

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Figure 4.9 An eigenfunction on the bistar $S_{3,3}$.

The eigenvalue $\frac{n}{n-1}$ occurs with multiplicity $\ell(n-2)+1$ and $\frac{1}{n-1}$ with multiplicity $\ell-1$. We get $\ell(n-2)$ for $\frac{n}{n-1}$ by taking an eigenfunction for that eigenvalue on one of the K_n that vanishes at the central vertex. The remaining eigenfunction for that eigenvalue is obtained by taking the same eigenfunction on all the K_n that has the same value b on all noncentral vertices. And if it then has the value a at the remaining vertex, we assign the value ℓa to the central vertex. And for the eigenvalue $\frac{1}{n-1}$, we take a function with the value $+1$ on all noncentral vertices of one wing, -1 on those of another wing, and 0 everywhere else, including the central vertex. While we have just constructed the eigenvalues and eigenfunctions explicitly, of course they can be derived from general symmetry principles.

We observe that all windmill graphs have only two nonvanishing eigenvalues, and the gap between them is 1.

We next consider the *symmetric bistar* $S_{q,q}$ where to each vertex of a central edge, q other vertices are connected. Figure 4.9 shows $S_{3,3}$ and indicates an eigenfunction.

The corresponding eigenfunction and eigenvalue λ need to satisfy

$$\begin{aligned} a-1 &= \lambda a,\\ 1+\frac{1}{q+1}-\frac{q}{q+1}a &= \lambda, \end{aligned}$$

whence

$$\begin{aligned} a_\pm &= \frac{q}{2} \pm \sqrt{\frac{1}{4q^2}+\frac{q+1}{q}},\\ \lambda_\pm &= \frac{a_\pm - 1}{a_\pm}. \end{aligned}$$

Thus, $a_- = -1$, leading to the eigenvalue $\lambda = 2$, reflecting the bipartiteness of $S_{q,q}$, whereas $a_+ = \frac{q+1}{q}$, leading to $\lambda = \frac{1}{q+1}$, which for $q = 1$ is $= 1/2$, but which goes to 0 for $q \to \infty$.

In Figure 4.10, we seek an eigenfunction of the form

which leads to

$$\begin{aligned} -b-1 &= \lambda(-b),\\ 1-\frac{1}{q+1}+\frac{q}{q+1}b &= \lambda. \end{aligned}$$

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Figure 4.10 Another eigenfunction on $S_{3,3}$.

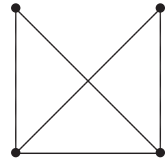


Figure 4.11 Duplicating a vertex of K_3.

The solution $b = -1$ leads to a constant eigenfunction for the eigenvalue 0, but $b = \frac{q+1}{q}$ gives the eigenvalue $\frac{2q+1}{q+1}$, which tends to 2 for $q \to \infty$. Since $S_{q,q}$ is obtained from $S_{1,1}$ by repeated node duplication, the remaining eigenvalue is 1 with multiplicity $2q-2$, with eigenfunctions as above. Thus, we have obtained all eigenvalues and a basis of the eigenfunctions for $S_{q,q}$. Note that all the eigenfunctions are either symmetric or antisymmetric for some automorphism of $S_{q,q}$. This, in fact, can be turned into a general principle.

Duplicating a node produces the eigenvalue 1 but may change some of the other eigenvalues of the graph we started with. Thus, let us duplicate one of the nodes of K_3 to obtain the graph of Figure 4.11.

This has the eigenvalue 0, the eigenvalue 1 because the two upper nodes are duplicates, the eigenvalue 4/3 with an eigenfunction that is ± 1 on the two lower and 0 on the two upper nodes, and finally the eigenvalue 5/3, as the sum of the eigenvalues is 4 by (4.1.41). Another reason is that this graph is K_4 minus one edge (between the two upper vertices), which is a case for which Theorem 4.1.1 is sharp. The graph K_3 that we started with had the eigenvalue 3/2 with multiplicity 2.

When, however, as in Figure 4.12, we duplicate all three vertices of K_3 to obtain the graph we have the eigenvalue 1 with multiplicity 3 because of the three vertex duplications, and the eigenvalue 3/2 of K_3 with multiplicity 2, with one eigenfunction indicated in Figure 4.12, obtained from the corresponding eigenfunction on K_3. The same mechanism works to show more generally

Corollary 4.1.13. *Let Γ be obtained by duplicating all the vertices of some graph Γ_0. Then Γ retains all the eigenvalues of Γ_0 and in addition has the eigenvalue 1 with multiplicity given by the number of vertices of Γ_0.* □

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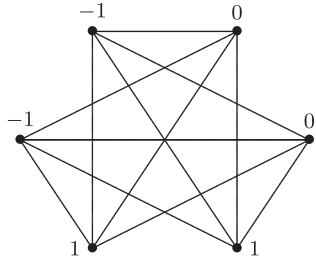


Figure 4.12 Duplicating all three vertices of K_3, and an eigenfunction.

The graph we have just constructed is the complete *tripartite graph* $K_{2,2,2}$. In a general tripartite graph, the vertex set V consists of three disjoint vertex sets V_1, V_2, and V_3 without any connections between members of the same V_i, for $i = 1,2,3$. The complete tripartite graph K_{n_1,n_2,n_3} has three such vertex sets with V_i containing n_i vertices, and for which any vertex in some V_i is connected to all vertices in the other two vertex sets $V_j, j \neq i$. It is obtained by repeated vertex duplications from $K_3 = K_{1,1,1}$, and the above argument shows that K_{n_1,n_2,n_3} has the eigenvalue 1 with multiplicity $N - 3$, where $N = n_1 + n_2 + n_3$. (By Lemma 4.1.14, this also follows from [57].) And it also follows from our considerations, recalling (4.1.41), that the sum of the other two nontrivial eigenvalues is 3, and hence, since none of them is 2, as the graph is not bipartite, they both are larger than 1. When $n_1 = n_2 = n_3$, they are both $3/2$, but for other values, they may be different, as our examples show. And again, complete tripartite graphs are characterized by their spectrum.

Of course, these notions and results permit an obvious generalization when we duplicate the vertices of K_k.

Corollary 4.1.14. *A complete k-partite graph $K_{n_1,\ldots,n_k}$ has the eigenvalue 1 with multiplicity $N - k$ (where $N = \sum n_j$). The sum of the remaining $k - 1$ nonvanishing eigenvalues is k, and when $n_1 = \ldots = n_k$, they are all equal to $\frac{k}{k-1}$.* □

The preceding considerations are of course special cases of the general scheme established in Section 2.7.

We also recall that since Γ is connected, the trivial eigenvalue $\lambda_1 = 0$ is simple. If Γ had two components, then the next eigenvalue λ_2 would also become 0. A corresponding eigenfunction would be equal to a constant on each component, the two values chosen such (4.1.64) is satisfied; in particular, one of the two would be positive, the other one, negative. We therefore expect that for graphs with a pronounced community structure, that is, for ones that can be

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broken up into two large components by deleting only a few edges as discussed above, the eigenvalue λ_2 should be close to 0. Formally, this is easily seen from the variational characterization

$$\lambda_2 = \min\left\{ \frac{\sum_{e=(v,v')\in E}(u(v')-u(v))^2}{\sum_v \deg v\, u(v)^2} : \sum_v \deg v\, u(v) = 0 \right\} \tag{4.1.88}$$

(see (2.6.8) and observe that $\sum_v \deg v\, u(v) = 0$ is equivalent to $(u,u_1) = 0$ as the eigenfunction u_1 is constant). Namely, if two large components of Γ are only connected by few edges, then one can make u constant on either side, with opposite signs so as to respect the normalization (4.1.64) with only a small contribution from the numerator.

More generally, when Γ consists of several clusters with only very few connections between them, one should find several eigenvalues close to 0.

The strategy for obtaining an eigenfunction for the second eigenvalue λ_2 is, according to (4.1.88), to do the same as one's neighbors. Because of the constraint $\sum_v \deg v\, u(v) = 0$, this is not globally possible, however. The second eigenfunction thus exhibits oscillations with the lowest possible frequency. Thus, if we take such a second eigenfunction u_2 and consider the connected components that remain after deleting all edges at whose endpoints u_2 has different signs, then there are precisely two such components, one on which u_2 is positive and one on which it is negative.

This issue will be taken up very systematically in Chapter 8, but in Section 4.3, we shall offer a preliminary elementary treatment.

4.2 Some Elementary Estimates

In Lemma 4.1.12, we had seen that the largest eigenvalue λ_N is 2 when the graph is bipartite and smaller when it is not. Therefore, we may naturally ask in which sense $2-\lambda_N$ quantifies how different the graph is from being bipartite. In order to develop some intuition about this question, let us consider the following example. Let Γ_0 be a bipartite graph with N vertices. We consider a highest eigenfunction $\bar{u}$ that is $+1$ on one class and -1 on the other class of vertices, as described in Lemma 4.1.12. In particular by (4.1.47),

$$\frac{\frac{1}{2}\sum_{v_1,v_2:\, v_1\sim v_2}(\bar{u}(v_1)-\bar{u}(v_2))^2}{\sum_v \deg v\, \bar{u}(v)^2} = 2. \tag{4.2.1}$$

By adding another vertex v_0 and connecting it to one of the vertices v_1 of Γ_0, we obtain a new bipartite graph Γ_1. We extend $\bar{u}$ by $\bar{u}(v_0) = 0$ to Γ_1. Thus, the numerator and the denominator of (4.2.1) are both increased by 1.

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Let the volume $\sum_v \deg v$ of Γ_0 be sufficiently large. Then, on Γ_1 for any small $\varepsilon > 0$,

$$\frac{\frac{1}{2}\sum_{v_1,v_2:\, v_1\sim v_2}(\bar{u}(v_1)-\bar{u}(v_2))^2}{\sum_v \deg v\, \bar{u}(v)^2} > 2-\varepsilon. \tag{4.2.2}$$

This is not affected when we construct a graph Γ by attaching another graph Γ_2 at v_0 and extend $\bar{u}$ by 0 to all of Γ_2. For instance, Γ_2 could be a complete graph K_M with M vertices, for any M. In particular, the difference $2-\lambda_N$, which by our construction is smaller than ε, is not very sensitive to the global shape of Γ_2. This implies, for instance, that $2-\lambda_N$ cannot control a global quantity like the *clustering coefficient* C, defined as

$$C := \frac{3\times \text{ number of triangles}}{\text{number of connected triples of vertices}}, \tag{4.2.3}$$

where a *triangle* is a triple of mutually connected vertices. The clustering coefficient measures how many connections there exist between the neighbors of a node. C becomes maximal if Γ is a fully connected graph. In contrast, C vanishes when Γ is a bipartite graph. In that sense, the clustering coefficient expresses an averaged difference from a graph being bipartite.

Our construction of attaching a complete graph K_M to a bipartite graph Γ_0 through a connecting node produces a graph with C arbitrarily close to its maximal value 1 when M is sufficiently large. But since, by our construction, $2-\lambda_N < \varepsilon$ is arbitrarily small, the largest eigenvalue does not control the clustering coefficient.

But we can use Corollary 4.1.6 to control $2-\lambda_N$ by a local clustering measure. We let $\triangle$ be the collection of triangles in Γ, that is, triples (v_1,v_2,v_3) of vertices for which $v_i \sim v_j$ for $i \neq j = 1,2,3$. For an edge $e = (v,v')$, we then define

$$c(e) = c(v,v') = \sum_{v'':\,(v,v',v'')\in\triangle} \frac{1}{\deg v''} \tag{4.2.4}$$

and put

$$c(\Gamma) := \min_{e\in E} c(e). \tag{4.2.5}$$

We then have

Theorem 4.2.1. *The largest eigenvalue λ_N of the graph Γ satisfies*

$$2-\lambda_N \geq c(\Gamma). \tag{4.2.6}$$

Proof We use (4.1.55), that is,

$$2-\lambda_N = \frac{\sum_z \frac{1}{\deg z}\sum_{z',z'':\,(z,z')\in E,(z,z'')\in E}(u(z')-u(z''))^2}{\sum_{v,v':\,(v,v')\in E}(u(v)-u(v'))^2}$$

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where u is an eigenfunction for the eigenvalue λ_N. For every edge $(v, v') \in E$, the term $(u(v) - u(v'))^2$ in the denominator also appears in the numerator for every triangle $(v, v', z) \in \triangle$, with $z' = v$, $z'' = v'$. This yields the estimate (4.2.6). □

For the graph K_3, that is, a single triangle, we have $c(e) = 1/2$ for every edge, and the highest eigenvalue is $3/2$, and so, (4.2.6) is sharp in this case.

A more refined estimate can be found in [24].

With the scheme developed in this section, the control in the other direction, that is, estimating the largest eigenvalue from below, does not quite work because of the following example. Consider a graph with many cycles of odd length, but all of length at least 5. Here, $c(e) = 0$ for every edge as there are no triangles, but $2 - \lambda_{N-1} \neq 0$ because the graph is not bipartite as bipartite graphs can only have cycles of even length.

However, we can control the largest eigenvalue from below in a different way, as we will see in Section 4.4.

In contrast to the largest eigenvalue λ_N, the smallest nonvanishing eigenvalue λ_2 cannot be controlled by the minimum of such a purely local constant. We also need to invoke some global quantities. We recall that the *volume* of Γ is defined as

$$\operatorname{vol}\Gamma = \sum_v \deg v. \tag{4.2.7}$$

Definition 4.2.1. The *diameter* $d(\Gamma)$ of Γ is the maximal distance between two vertices of Γ. Here, the *distance* between two vertices is the minimal number of edges needed to connect them.

For instance, a complete graph has diameter 1, whereas a chain with $m + 1$ vertices has diameter m.

For an edge $e = (v, v')$, let

$$b(e) := \text{number of triangles containing } e, \tag{4.2.8}$$

and

$$b(\Gamma) := \min_{e \in E} b(e). \tag{4.2.9}$$

Then we have refining Lemma 1.9 in [61]

Theorem 4.2.2.

$$\lambda_2 \geq \frac{1 + \frac{1}{2} b(\Gamma)}{d(\Gamma)\operatorname{vol}\Gamma}. \tag{4.2.10}$$

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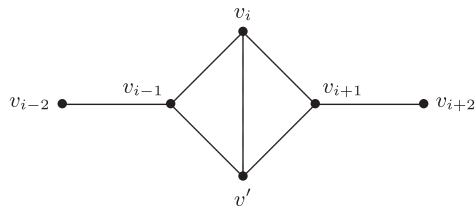


Figure 4.13 A graph used in the proof of Theorem 4.2.2.

Proof For $x_0, x_1, \ldots, x_m \in \mathbb{R}$, we have the inequality

$$\sum_{i=1}^{m} (x_{i-1} - x_i)^2 \geq \frac{1}{m}(x_0 - x_m)^2. \tag{4.2.11}$$

We let u be an eigenfunction for λ_2 and choose a vertex v_0 where $|u(v)|$ assumes its maximum. Since $\sum_v \deg v \; u(v) = 0$ for such an eigenfunction, there is some other vertex v_m with $u(v_0)u(v_m) < 0$, and let us assume that the distance between v_0 and v_m is m, with a path $v_0 \sim v_1 \ldots \sim v_m$ connecting them. We recall

$$\lambda_2 = \frac{\sum_{v \sim v'} (u(v) - u(v'))^2}{\sum_v \deg v \; u(v)^2}.$$

For an estimate from below, we only count some of the terms $(u(v) - u(v'))^2$ with $v \sim v'$. These include, first of all, the terms $(u(v_{i-1}) - u(v_i))^2$ for $i = 1, \ldots, m$. Next, we count the terms $(u(v_{i-1}) - u(v'))^2$ and $(u(v') - u(v_i))^2$ for triangles (v_{i-1}, v_i, v'). Here, we have to distinguish two cases.

1. v' is not contained in any triangle with another edge (v_{j-1}, v_j) from the path. We then use (4.2.11) to get

$$(u(v_{i-1}) - u(v'))^2 + ((u(v') - u(v_i))^2) \geq \frac{1}{2}(u(v_{i-1}) - u(v_i))^2.$$

2. v' is a vertex of a triangle for two adjacent edges, as indicated in Figure 4.13. We note that since $v_0, v_1, \ldots, v_m$ is a shortest path, it is not possible that more than two of its edges or two non-adjacent edges are contained in some triangles with the same third vertex. In the situation of Figure 4.13, we may assume

$$(u(v_{i-1}) - u(v'))^2 + (u(v') - u(v_{i+1}))^2) \geq (u(v_{i-1}) - u(v_i))^2 + (u(v_i) - u(v_{i+1}))^2),$$

since replacing v_i by v' also yields a shortest path.

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We therefore get

$$\begin{aligned}\lambda_2 &\geq \frac{(1+\frac{1}{2}b(\Gamma))\sum_{i=1,\dots,m}((u(v_{i-1})-u(v_i))^2}{\operatorname{vol}\Gamma\, u^2(v_0)}\\ &\geq \frac{\frac{1}{d(\Gamma)}(1+\frac{1}{2}b(\Gamma))(u(v_0)-u(v_m))^2}{\operatorname{vol}\Gamma\, u^2(v_0)}\\ &\geq \frac{1+\frac{1}{2}b(\Gamma)}{d(\Gamma)\operatorname{vol}\Gamma},\end{aligned}$$

where we have used (4.2.11) again in the second-to-last step. □

We note that, in contrast to (4.2.6), the estimate (4.2.10) is not sharp for K_3.

4.3 Cutting a Graph Optimally, or the Pólya–Cheeger Constant and Eigenvalue Estimates

We shall now take up the discussion at the end of Section 4.2 and introduce a quantity h that will control the first nontrivial eigenvalue λ_2 of a graph. This quantity was introduced by Pólya and Szego in graph theory in 1951, see [230]. An analogous quantity was defined in Riemannian geometry by Cheeger in 1970 [56], and his important insight was that this quantity could be used to estimate the first non-vanishing eigenvalue of the Laplace–Beltrami operator of the underlying Riemannian manifold. Dodziuk [82] and Alon-Milman [4] then derived an analogous estimate for the algebraic graph Laplacian, and Chung [61] carried this over to the normalized Laplacian that we are using here. The relevant constant on a graph therefore is usually also called the Cheeger constant.

Let us first recall the general setting from Section 3.2. We want to look at isoperimetric problems. In Euclidean space, for some (sufficiently regular) set S, one compares the volume $|S|$ of S with that of its boundary, $|\partial S|$. For instance, for some fixed volume $|S|$, one may want to minimize $|\partial S|$, or conversely, for fixed $|\partial S|$, one wants to maximize $|S|$. The solution in either case is given by a ball, and the boundary is a sphere. One can pose the same problem in a Riemannian manifold and show the existence of a solution. One can also try to divide a compact Riemannian manifold M into two large pieces S and $M \setminus S$ with small $|\partial S|(= |\partial(M \setminus S)|)$, that is, try to minimize

$$\frac{|\partial S|}{\min(|S|, |M \setminus S|)}. \tag{4.3.1}$$

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Here, we want to examine analogous problems on graphs. For a subset $A \subset V$ of the vertex set of a graph Γ, we want to control the measure of its boundary $|\partial A|$. For any $B \subset V$, its measure or volume is, as we recall, $\operatorname{vol} B = \sum_{v \in B} \deg v$. But a question that arises here is how to define that boundary. In fact, there are two options, a vertex boundary and an edge boundary. For the vertex boundary, we consider pairs v, v' with $v \sim v'$, $v \in A, v' \notin A$, and we may then define the *vertex boundary* as either the set of all those v or as the set of all those v'. Thus, there are two possible choices, an external and an internal vertex boundary, and in general, their volumes may be quite different from each other. We shall encounter them at the end of Section 6.3. When we, instead, define the *edge boundary*, there is a canonical choice. The edge boundary ∂A simply consists of the set $E(A, V \setminus A)$ of all edges $e = (v, v')$ with $v \in A$, $v' \notin A$, and the measure of any subset $E_0 \subset E$ of the edge set of Γ is simply the number of edges it contains. (We are discussing here unweighted graphs; in the weighted case, one would take the sum of the weights of the edges in E_0.) The problem analogous to (4.3.1) then is to minimize

$$\frac{|\partial A|}{\min(|A|, |M \setminus A|)}. \tag{4.3.2}$$

This is called the *Cheeger problem*, in analogy with the problem (4.3.1), which is the problem that Cheeger himself [56] actually studied by relating it to the first nonzero Laplacian eigenvalue. (For the minimization problem (4.3.1) itself and its history, see for instance [110]. And the problem of minimizing (4.3.2) can already be found in [230].)

In this section, we shall treat the relation between (4.3.2) and the eigenvalue λ_2. Let us first prepare the setting.

Let $\phi \colon V \to \mathbb{R}_{\geq 0}$ be a function, with $M := \max \phi(v)^2$. We put, for $t \geq 0$,

$$\Phi_v(t) := \begin{cases} 1 & \text{if } \phi(v) \geq t \\ 0 & \text{else.} \end{cases} \tag{4.3.3}$$

Let $V_\phi^+(\tau) := \{v \in V \colon \phi(v) \geq \tau\}$. Then, for every $t \geq 0$,

$$\sum_{u \sim v} |\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})| = |E(V_\phi^+(\sqrt{t}), \overline{V_\phi^+(\sqrt{t})})|, \tag{4.3.4}$$

where $\overline{S} = V \setminus S$ is the complement of a subset $S \subset V$ and where $|E(V_1, V_2)|$ denotes the number of edges with one endpoint in V_1 and the other in V_2, for $V_1, V_2 \subset V$. Thus,

$$\int_0^M \sum_{u \sim v} |\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})| dt = \int_0^M \left| E\left(V_\phi^+(\sqrt{t}), \overline{V_\phi^+(\sqrt{t})}\right) \right| dt$$

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$$\geq \inf_t \frac{|E(V_\phi^+(\sqrt{t})), \overline{V_\phi^+(\sqrt{t})})|}{\sum_{v:\, \phi(v)\geq\sqrt{t}} \deg(v)} \int_0^M \sum_{v:\, \phi(v)\geq\sqrt{\tau}} \deg(v) d\tau$$

$$= \inf_t \frac{|E(V_\phi^+(\sqrt{t})), \overline{V_\phi^+(\sqrt{t})})|}{\sum_{v:\, \phi(v)\geq\sqrt{t}} \deg(v)} \sum_v \deg(v)\phi(v)^2, \tag{4.3.5}$$

where the last equality follows from the fact that

$$\int \sum_{v:\, \phi(v)\geq\sqrt{\tau}} \deg(v) d\tau = \sum_v \deg(v) \int_{\tau:\, 0\leq\tau\leq\phi(v)^2} 1 d\tau = \sum_v \deg(v)\phi(v)^2.$$

We put, for $\emptyset \neq S \subsetneq V$,

$$\eta_1(S) := \frac{|E(S, \overline{S})|}{\mathrm{vol}(S)}. \tag{4.3.6}$$

For purposes that will become clear in Section 4.6, we shall first derive a trivial toy version of the estimate that we are after. We introduce the constant

$$h_1(\Gamma) := \min_S \eta_1(S). \tag{4.3.7}$$

Of course, $h_1 = 0$, but what will be relevant will be the structure of the argument to follow. From (4.3.5), we then obtain

$$\int_0^M \sum_{u\sim v} |\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})| dt \geq h_1 \sum_v \deg(v)\phi(v)^2. \tag{4.3.8}$$

Now, fix $v \sim u$ and assume that $\phi(v) \leq \phi(u)$. Then, $\left|\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})\right| = 1$ if and only if $\phi(v) < \sqrt{t} \leq \phi(u)$, while $\left|\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})\right| = 0$ otherwise. Hence,

$$\begin{aligned}\int_0^M \left|\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})\right| dt &= \int_{t\in[0,M]:\, \phi(v)<\sqrt{t}\leq\phi(u)} 1 dt \\ &= \phi(u)^2 - \phi(v)^2 \\ &= (|\phi(u) - \phi(v)|)\,(|\phi(u) + \phi(v)|).\end{aligned} \tag{4.3.9}$$

From (4.3.8) and (4.3.9), we obtain

$$\begin{aligned} h_1 &\leq \frac{\sum_{u\sim v} |\phi(u) - \phi(v)|(|\phi(u)| + |\phi(v)|)}{\sum_v \deg(v)\phi(v)^2} \\ &\leq \frac{\sqrt{\sum_{u\sim v} |\phi(u) - \phi(v)|^2}\, \sqrt{\sum_{u\sim v}(|\phi(u)| + |\phi(v)|)^2}}{\sum_v \deg(v)\phi(v)^2} \\ &\leq \frac{\sqrt{\sum_{u\sim v} |\phi(u) - \phi(v)|^2}\, \sqrt{2\sum_u \deg(u)|\phi(u)|^2}}{\sum_v \deg(v)\phi(v)^2}. \end{aligned}$$

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Hence,

$$h_1 \leq \sqrt{\frac{2\sum_{u\sim v}|\phi(u)-\phi(v)|^2}{\sum_v \deg(v)\phi(v)^2}},$$

for all $\phi\colon V \to \mathbb{R}_{\geq 0}$. It follows that, for all (not necessarily non-negative) functions $\phi\colon V \to \mathbb{R}$,

$$h_1 \leq \sqrt{\frac{2\sum_{u\sim v}(|\phi(u)|-|\phi(v)|)^2}{\sum_v \deg(v)\phi(v)^2}} \leq \sqrt{\frac{2\sum_{u\sim v}|\phi(u)-\phi(v)|^2}{\sum_v \deg(v)\phi(v)^2}}. \tag{4.3.10}$$

Of course, we can take here a constant function ϕ and get $h_1 = 0$, which in fact can also be readily seen from its definition (4.3.7). The important thing, however, is that inside the root on the right-hand side, we have the Rayleigh quotient of the function ϕ, and subsequently, we shall insert eigenfunctions of Δ into such inequalities to control eigenvalues in terms of such global quantities as h_1, or conversely, estimate those quantities by eigenvalues.

With this argument in place, we now go for the real thing. We consider a subset S of the vertex set V and its complement $\overline{S} = V \setminus S$. For any subsets $V_1, V_2 \subset V$, $|E(V_1, V_2)|$ denotes the number of edges with one endpoint in V_1 and the other in V_2. Since the conventions here can be confusing, let us point out explicitly that each edge with $v_1 \in V_1$ and $v_2 \in V_2$ is counted only once. (This is different from the convention in [11].) In particular, $|E(V_1, V_1)|$ is the number of edges with both endpoints in V_1. Thus, for $S \subset V$, we have

$$\operatorname{vol} S = 2|E(S,S)| + |E(S,\overline{S})|. \tag{4.3.11}$$

(We consider here again the unweighted case, but everything naturally extends to weighted graphs. On a weighted graph, of course, the edges carry their weights, and $|E(V_1, V_2)|$ then becomes the sum of the weights of the edges between V_1 and V_2.)

We then put

$$\eta(S) := \frac{|E(S,\overline{S})|}{\min(\operatorname{vol}(S), \operatorname{vol}(\overline{S}))} = \max(\eta_1(S), \eta_1(\overline{S})), \tag{4.3.12}$$

with $\eta_1(S) = \frac{|E(S,\overline{S})|}{\operatorname{vol}(S)}$, and introduce the *(Pólya)–Cheeger constant*

$$h := \min_S \eta(S). \tag{4.3.13}$$

Thus, we have the minimization problem of cutting V into two parts $S, \overline{S}$ by removing as few edges as possible, but such that both parts have a large volume, since the numerator in (4.3.12) is symmetric in $S, \overline{S}$. In particular, when Γ is not connected, then $h = 0$, because we can let S be one component, and then, there

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Figure 4.14 The bistar of Figure 4.9.

are no edges to its complement $\overline{S}$, that is, $|E(S,\overline{S})| = 0$. When Γ is connected, however, this is not possible, and we have $h > 0$ in that case.

In the example of the bistar $S_{q,q}$ of Figure 4.14, it is obvious that it is best to cut the central edge. This disconnects the graph into two pieces $S, \overline{S}$ of equal volume $2q + 1$ (in each piece, there are q vertices with a single neighbor, a central vertex, and that central vertex has $q + 1$ neighbors). Thus,

$$h = \frac{1}{2q+1}. \tag{4.3.14}$$

Thus, the larger q, the smaller the Pólya–Cheeger constant.

The star graph $K_{1,n}$ becomes disconnected by cutting any edge, thereby cutting off a single peripheral vertex. Then, $h = 1$. This does not depend on n. In fact, the star graph cannot be cut into two large connected components at all. Whichever way we cut it, there is at most one large component. The rest will just be a collection of isolated vertices. Similarly for the petal graph where again the second largest component after a cut contains at most two vertices.

We next consider the complete graph K_N and cut it into two components. The smaller then has $n \leq N/2$ vertices and volume $n(N-1)$. We need to cut $n(N-n)$ edges, and the ratio $\frac{n(N-n)}{n(N-1)} = \frac{N-n}{N-1}$ becomes smallest for $n = N/2$ when N is even, and $n = (N-1)/2$ for odd N. This then is the value of h in this case.

The fundamental inequality obtained in [4, 61, 82] then says that the constant h controls the eigenvalue λ_2 from above and below, or conversely and better, that this eigenvalue can be used to estimate h, as λ_2 in practice is much easier to compute than h. The essential idea is that the eigenfunction for λ_2 divides V into two parts where it is positive or negative, and that this yields a decomposition that realizes a value for η, which is not too much larger than the minimal value required in the definition of h.

Theorem 4.3.1.

$$1 - \sqrt{1-h^2} \leq \lambda_2 \leq 2h. \tag{4.3.15}$$

We note that (4.3.15) implies the slightly weaker lower bound

$$\frac{1}{2}h^2 \leq \lambda_2, \tag{4.3.16}$$

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which is the bound often quoted in the literature and which is also the type of bound the argument leading to (4.3.10) gives.

In fact, the upper estimate in (4.3.15) holds under rather general conditions, and an appropriate version is also true for the algebraic (non-normalized) graph Laplacian. In contrast, the lower bound crucially needs the normalization.

The *proof* that we shall provide is taken from [24].

We first prove the easier part, the upper bound. We use the variational characterization (4.1.88). Let the vertex set be divided into the two disjoint sets $U, \overline{U}$ of nodes, and let U be the one with the smaller volume. We consider a function u that is =1 on all the nodes in U and $= -\alpha$ for some positive α on $\overline{U}$ so that the normalization $\sum_{v\in V} u(v) \deg v = 0$ holds, that is, $\sum_{v\in U} \deg v - \sum_{v\in\overline{U}} \deg v\ \alpha = 0$. Since $\overline{U}$ is the subset with the larger volume $\sum_{v\in\overline{U}} \deg v$, we have $\alpha \leq 1$. Thus, for our choice of u, the quotient in (4.1.88) becomes

$$\begin{aligned}
\lambda_2 &= \min\left\{\frac{\sum_{e=(v,v')\in E}(u(v')-u(v))^2}{\sum_v \deg v\, u(v)^2} :\ \sum_v \deg v\, u(v) = 0\right\}\\
&\leq \frac{(1+\alpha)^2|E(U,\overline{U})|}{\sum_{v\in U}\deg v\ + \sum_{v\in\overline{U}}\deg v\,\alpha^2}\\
&= \frac{(1+\alpha)|E(U,\overline{U})|}{\sum_{v\in U}\deg v}\\
&\leq 2\frac{|E(U,\overline{U})|}{\sum_{v\in U}\deg v}\\
&= 2\frac{|E(U,\overline{U})|}{\mathrm{vol}(U)}.
\end{aligned}$$

Since this holds for all such splittings of our graph Γ, we obtain from (4.3.12) and (4.1.88) the upper bound

$$\lambda_2 \leq 2h. \tag{4.3.17}$$

For the lower bound, we shall use arguments that mainly come from [79] and also contain some generalizations from [61].

Remark 4.3.1. Given $g : V \to \mathbb{R}$, let

$$g_+(v) := \begin{cases} g(v), & \text{if } g(v) \geq 0\\ 0, & \text{if } g(v) < 0 \end{cases}$$

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be the *positive part of g,* and let

$$g_-(v) := \begin{cases} |g(v)|, & \text{if } g(v) \le 0 \\ 0, & \text{if } g(v) > 0 \end{cases}$$

be the *negative part of g*. Then, $g(v) = g_+(v) - g_-(v)$, $g(v)^2 = g_+(v)^2 + g_-(v)^2$, and

$$\sum_{v\sim w} \Big(g(v) - g(w)\Big)^2 \ge \sum_{v\sim w} \left[\Big(g_+(v) - g_+(w)\Big)^2 + \Big(g_-(v) - g_-(w)\Big)^2\right].$$

Therefore, the Rayleigh quotient $\mathcal{R}(g)$ of g is such that

$$\begin{aligned} \mathcal{R}(g) &= \frac{\sum_{v\sim w}\Big(g(v) - g(w)\Big)^2}{\sum_{v\in V} \deg v \cdot g(v)^2} \\ &\ge \frac{\sum_{v\sim w}\left[\Big(g_+(v) - g_+(w)\Big)^2 + \Big(g_-(v) - g_-(w)\Big)^2\right]}{\sum_{v\in V} \deg v \cdot (g_+(v)^2 + g_-(v)^2)} \\ &\ge \min\{\mathcal{R}(g_+), \mathcal{R}(g_-)\}, \end{aligned}$$

since $\frac{a+b}{c+d} \ge \min\{\frac{a}{c}, \frac{b}{d}\}$.

Lemma 4.3.1. *Let $g \in L^2(\Gamma)$ with $S(g) := \{v \in V : g(v) > 0\} \ne \emptyset$, let*

$$h(g) := \min_{\emptyset \ne S \subseteq S(g)} \frac{|E(S, \overline{S})|}{\operatorname{vol}(S)}$$

and let g_+ be the positive part of g. Then,

$$1 + \sqrt{1 - h^2(g)} \ge \frac{\sum_{e=(v,v')}(g_+(v) - g_+(v'))^2}{\sum_v \deg v \; g_+(v)^2} \ge 1 - \sqrt{1 - h^2(g)}.$$

The same holds if we consider g_- instead of g_+.

Proof First, we write

$$\begin{aligned} W &:= \frac{\sum_{e=(v,v')}(g_+(v) - g_+(v'))^2}{\sum_v \deg v \; g_+(v)^2} \\ &= \frac{\sum_{e=(v,v')}(g_+(v) - g_+(v'))^2 \sum_{e=(v,v')}(g_+(v) + g_+(v'))^2}{\sum_v \deg v \; g_+(v)^2 \sum_{e=(v,v')}(g_+(v) + g_+(v'))^2} \\ &=: \frac{I}{II}. \end{aligned}$$

With the Cauchy–Schwarz inequality,

$$I^{\frac{1}{2}} \ge \sum_{e=(v,v')} |g_+(v)^2 - g_+(v')^2|$$

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$$
\begin{aligned}
&= \sum_{e=(v,v')\colon g_+(v)\geq g_+(v')} (g_+(v)^2 - g_+(v')^2) \\
&= 2 \sum_{e=(v,v')\colon g_+(v)\geq g_+(v')} \int_{g_+(v')}^{g_+(v)} t\,dt \\
&= 2 \int_0^\infty \sum_{e=(v,v')\colon g_+(v')\leq t\leq g_+(v)} t\,dt.
\end{aligned}
$$

Now,

$$
\sum_{\substack{e=(v,v')\colon \\ g_+(v')\leq t\leq g_+(v)}} 1 = E(S_t, \overline{S_t}),
$$

where $S_t := \{v\colon g_+(v) > t\}$. Thus,

$$
\begin{aligned}
I^{\frac{1}{2}} &\geq 2h(g) \int_0^\infty \mathrm{vol}(S_t)\,t\,dt \\
&= 2h(g) \int_0^\infty \sum_{v\colon g_+(v)>t} \deg v\; t\,dt \\
&= 2h(g) \sum_{v\in V} \deg v \int_0^{g_+(v)} t\,dt \\
&= h(g) \sum_v \deg v\; g_+(v)^2
\end{aligned}
$$

and therefore we obtain

$$
I \geq h^2(g)\Big(\sum_v \deg v\; g_+(v)^2\Big)^2. \tag{4.3.18}
$$

Next,

$$
\begin{aligned}
II &= \sum_v \deg v\; g_+(v)^2 \sum_{e=(v,v')} (g_+(v) + g_+(v'))^2 \\
&= \sum_v \deg v\; g_+(v)^2 \left(\sum_v \deg v\; g_+(v)^2 + 2 \sum_{e=(v,v')} g_+(v) g_+(v') \right) \\
&= \sum_v \deg v\; g_+(v)^2 \left(2 \sum_v \deg v\; g_+(v)^2 - \sum_{e=(v,v')} (g_+(v) - g_+(v'))^2 \right) \\
&= (2 - W) \left(\sum_v \deg v\; g_+(v)^2 \right)^2.
\end{aligned} \tag{4.3.19}
$$

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From (4.3.18) and (4.3.19), we obtain

$$W \geq \frac{h^2(g)}{(2-W)},$$

and therefore,

$$1 + \sqrt{1-h^2(g)} \geq W \geq 1 - \sqrt{1-h^2(g)}.$$

The proof for g_- is analogous. □

We can now conclude the *proof* of Theorem 4.3.1 as follows. Let f be an eigenfunction for λ_2. Then, $\sum_v \deg(v) f(v) = 0$. Thus, f attains both positive and negative values, and the function

$$\begin{aligned} p(t) :&= \sum_{v\in V} \deg v \, (f(v)-t)^2 \\ &= \sum_{v\in V} \deg v \left(f(v)^2 + t^2 - 2tf(v)\right) \\ &= \sum_{v\in V} \deg v f(v)^2 + t^2 \sum_{v\in V} \deg v - 2t \sum_{v\in V} \deg v f(v) \\ &= \sum_{v\in V} \deg v f(v)^2 + t^2 \sum_{v\in V} \deg v \end{aligned}$$

attains its minimum at $t = 0$.

Now, reorder the vertices so that

$$f(v_1) \leq \ldots \leq f(v_N).$$

Let k be the largest integer such that $\sum_{i=1}^{k} \deg(v_i) \leq \operatorname{vol}(V)/2$, and let $c := f(v_{k+1})$. Then,

$$\operatorname{vol}(\{v \in V : f(v) < c\}) \leq \sum_{i=1}^{k} \deg(v_i) \leq \frac{\operatorname{vol}(V)}{2}$$

and, since k is the largest integer such that $\sum_{i=1}^{k} \deg(v_i) \leq \operatorname{vol}(V)/2$, we have that $\sum_{i=1}^{k+1} \deg(v_i) > \operatorname{vol}(V)/2$, therefore $\sum_{i=k+2}^{N} \deg(v_i) \leq \operatorname{vol}(V)/2$, implying that

$$\operatorname{vol}(\{v \in V : f(v) > c\}) \leq \sum_{i=k+2}^{N} \deg(v_i) \leq \frac{\operatorname{vol}(V)}{2}.$$

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Therefore,

$$\max\{\mathrm{vol}(\{v \in V\colon f(v) > c\}), \mathrm{vol}(\{v \in V\colon f(v) < c\})\} \leq \frac{\mathrm{vol}(V)}{2}.$$

Hence, by letting

$$g(v) := f(v) - c \quad \text{for } v \in V,$$

we get that

$$\max\{\mathrm{vol}(\{v \in V\colon g(v) > 0\}), \mathrm{vol}(\{v \in V\colon g(v) < 0\})\} \leq \frac{\mathrm{vol}(V)}{2}. \quad (4.3.20)$$

Now, since we observed that the function $p(t) = \sum_{v\in V} \deg v\,(f(v) - t)^2$ attains its minimum at $t = 0$, we have that

$$\sum_{v\in V} \deg v f(v)^2 \leq \sum_{v\in V} \deg v g(v)^2.$$

Moreover, it follows from the definition of g that

$$\sum_{u\sim v} |f(u) - f(v)|^2 = \sum_{u\sim v} |g(u) - g(v)|^2.$$

This implies that

$$\mathcal{R}(f) = \frac{\sum_{u\sim v} |f(u) - f(v)|^2}{\sum_v \deg(v) f(v)^2} \geq \frac{\sum_{u\sim v} |g(u) - g(v)|^2}{\sum_v \deg(v) g(v)^2} = \mathcal{R}(g).$$

Now, let ϕ be either g_+ or g_-, such that (by Remark 4.3.1)

$$\mathcal{R}(g) \geq \min\{\mathcal{R}(g_+), \mathcal{R}(g_-)\} = \mathcal{R}(\phi).$$

Then, $\mathcal{R}(f) \geq \mathcal{R}(\phi)$. Moreover, let $S(g) := \{v \in V\colon g(v) > 0\}$ and note that, by (4.3.20), $\mathrm{vol}\, S(g) \leq \mathrm{vol}\, \overline{S(g)}$. Therefore, $h \leq h(g)$. Together with Lemma 4.3.1, this implies that

$$1 - \sqrt{1 - h^2} \leq 1 - \sqrt{1 - h^2(g)} \leq \mathcal{R}(\phi) \leq \mathcal{R}(f) = \lambda_2.$$

□

Of course, $\lambda_2 = 0$ if and only if $h = 0$, if and only if the graph Γ is not connected, that is, if its vertex set can be decomposed into two nonempty subsets V_1, V_2 such that there are no edges between vertices in different components. More generally, the number of connected components equals the multiplicity of the eigenvalue $\lambda = 0$.

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We had seen that for the bistar $S_{q,q}$ Figure 4.9, (Figure 4.14), the smallest positive eigenvalue behaves like $1/q$, and we had determined h as $1/(2q+1)$ in (4.3.14). Thus, here λ_2 behaves like the upper bound in (4.3.12). For the star graph $K_{1,n}$, we know that the smallest positive eigenvalue is 1, as for every complete bipartite graph, and we had seen that also $h = 1$ in that case.

For the complete graph K_N with even N, we had computed $h = \frac{N}{2(N-1)}$, and since $\lambda_2 = \frac{N}{N-1}$, the upper bound in (4.3.15) is sharp in this case. For odd N, $h = \frac{N+1}{2(N-1)}$, and so, the upper bound here is only asymptotically sharp for $N \to \infty$.

4.4 Dividing a Graph Optimally into Opposite Classes, or the Dual Cheeger Constant and Estimates for the Largest Eigenvalue

In qualitative terms, the Cheeger inequalities (4.3.15) say that λ_2 becomes small when the graph can be easily (that is, by cutting only a few edges) decomposed into two large parts. Thus, λ_2 is small, that is, close to its minimal value of 0, when Γ is similar to a disconnected graph, with equality if and only if Γ is disconnected itself. Similarly, the largest eigenvalue is large, that is, close to its maximal value of 2, when Γ is close to a bipartite graph, with equality precisely if Γ is bipartite itself, by Lemma 4.1.12.

The characteristic property of a bipartite graph is that it can be decomposed into two opposite classes, with connections only between members of different classes. For a general graph, such a perfect division is not possible, but we can ask for a division that comes as close as possible to such a one. Such a division should yield two classes that are almost opposite, in the sense that there are only few, if any, connections inside each of them, plus perhaps a third class that may contain many internal connections. We shall define a constant quantifying this in (4.4.1). We shall interpret that constant as a dual version of the (Pólya–)Cheeger constant (4.3.13), and we shall justify this dual interpretation in this section.

The main purpose of this section, which follows [24], then is a dual version of (4.3.15) for the largest eigenvalue λ_N. More precisely, we shall obtain an estimate for λ_N in terms of a dual version of the Cheeger constant, which we now introduce.

Definition 4.4.1. Let V_1, V_2 and $\overline{V_1 \cup V_2} =: V_3$ be a partition of the vertex set V of the graph Γ into three disjoint sets for which V_1 and V_2 are nonempty. For such a partition V_1, V_2, V_3 of the vertex set V, we define the *dual Cheeger constant* as

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$$\overline{h}(\Gamma) := \max_{V_1,V_2} \frac{2|E(V_1,V_2)|}{\mathrm{vol}(V_1)+\mathrm{vol}(V_2)}. \tag{4.4.1}$$

We recall from (4.2.7) that the volume of a vertex set W is defined as $\mathrm{vol}(W) = \sum_{v\in W} \deg v$. $|E(V_1,V_2)|$ as before counts the number of edges between V_1 and V_2. On the other hand, $\mathrm{vol}(V_1)$ also has contributions from edges from V_1 to the remainder set V_3, and so does $\mathrm{vol}(V_2)$.
We should think of $V_1 \cup V_2$ as the (almost) bipartite part of Γ and V_3 as the part of Γ that contains many cycles of odd length, that is, a part of Γ that is different from being bipartite.

Remark 4.4.1. Independently of [24], Trevisan [263] introduced the *bipartiteness ratio*

$$\beta(\Gamma) := \min_{V_1,V_2} \frac{2|E(V_1,V_1)| + 2|E(V_2,V_2)| + |E(V_1\cup V_2, \overline{V_1\cup V_2})|)}{\mathrm{vol}(V_1)+\mathrm{vol}(V_2)}, \tag{4.4.2}$$

which by (4.3.11) is equivalent to our $\overline{h}(\Gamma)$, in the sense that

$$\beta(\Gamma) = 1 - \overline{h}(\Gamma), \tag{4.4.3}$$

and with this quantity, he obtained estimates equivalent to (4.4.7).

We first observe that $\overline{h}$ characterizes bipartite graphs.

Lemma 4.4.1. *$\overline{h} \le 1$, and $\overline{h} = 1$ if and only if Γ is bipartite.*

Proof With (4.3.11), $\overline{h}$ becomes

$$\overline{h} = \max_{V_1,V_2} \frac{2|E(V_1,V_2)|}{2|E(V_1,V_1)| + 2|E(V_2,V_2)| + 2|E(V_1,V_2)| + |E(V_1,V_3)| + |E(V_2,V_3)|}. \tag{4.4.4}$$

Thus,

$$\overline{h} \le 1. \tag{4.4.5}$$

If Γ is bipartite, there exists a partition V_1, V_2, V_3 of V with $V_3 = \emptyset$ and without edges within the subsets V_1 and V_2. Thus, $|E(V_1,V_3)| = |E(V_2,V_3)| = |E(V_1,V_1)| = |E(V_2,V_2)| = 0$. By (4.4.4), we have $\overline{h} \ge 1$. Together with (4.4.5), it follows that $\overline{h} = 1$.

Now assume that $\overline{h} = 1$. Equation (4.4.4) implies that there exists a partition V_1, V_2, V_3 of V such that $|E(V_1,V_3)| = |E(V_2,V_3)| = |E(V_1,V_1)| = |E(V_2,V_2)| = 0$. Since Γ is connected, $V_3 = \emptyset$. Thus, Γ is bipartite. □

Lemma 4.4.2.

$$\frac{1}{2} \le \overline{h}.$$

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Proof If there exists a partition V_1, V_2, and $V_3 = \emptyset$ of the vertex set V with

$$|E(V_1, V_2)| \geq \max_{i=1,2} |E(V_i, V_i)|, \tag{4.4.6}$$

then

$$\begin{aligned} \overline{h} &\geq \max_{V_1,V_2,V_3=\emptyset} \frac{2|E(V_1,V_2)|}{2|E(V_1,V_2)| + |E(V_1,V_1)| + |E(V_2,V_2)|} \\ &\geq \max_{V_1,V_2,V_3=\emptyset} \frac{|E(V_1,V_2)|}{|E(V_1,V_2)| + \max_{i=1,2} |E(V_i,V_i)|} \\ &\geq \frac{1}{2}. \end{aligned}$$

It is easy to find a partition that satisfies (4.4.6). For instance, we can start with an arbitrary partition V_1, V_2. If (4.4.6) is not satisfied, we assume, without loss of generality, that $|E(V_1, V_1)| > |E(V_1, V_2)|$. Then, there has to exist some vertex $v \in V_1$ that has more neighbors in V_1 than in V_2. If we remove the vertex v from V_1 and put it into V_2, then $|E(V_1, V_2)|$ and $|E(V_2, V_2)|$ are increased, while $|E(V_1, V_1)|$ is decreased. Repeating this procedure, if necessary, eventually (4.4.6) has to hold. □

Remark 4.4.2. Lemma 4.4.2 need not hold for graphs with self-loops.

The dual Cheeger constant $\overline{h}$ controls, or is controlled by, the largest eigenvalue λ_N in the same way that the Cheeger inequalities (4.3.15) estimate h and λ_2 in terms of each other. This is the content of

Theorem 4.4.1.

$$2\overline{h} \leq \lambda_N \leq 1 + \sqrt{1 - (1 - \overline{h})^2}. \tag{4.4.7}$$

For a better comparison with (4.3.15), we can reformulate (4.4.7) as

$$1 - \sqrt{1 - (1 - \overline{h})^2} \leq 2 - \lambda_N \leq 2 - 2\overline{h}. \tag{4.4.8}$$

This implies, in analogy to (4.3.16), the weaker bound

$$\lambda_N \leq 2 - \frac{1}{2}(1 - \overline{h})^2. \tag{4.4.9}$$

This, in particular, implies Lemma 4.1.12 again. Of course, this bound, and the stronger upper bound in (4.4.7), constitutes a quantitative version of that Lemma.

Starting with the *proof* of Theorem 4.4.1, we first prove the easier lower bound. We recall (4.1.50),

$$\lambda_N = \max_{u \neq 0} \frac{(\delta u, \delta u)}{(u, u)}. \tag{4.4.10}$$

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Let V_1, V_2, and V_3 be a partition that achieves $\overline{h}$. We construct a function f for which (4.4.10) is not smaller than $2\overline{h}$ as

$$f(v) = \begin{cases} \frac{1}{\mathrm{vol}(V_1)} & \text{if} \quad v \in V_1 \\ \frac{-1}{\mathrm{vol}(V_2)} & \text{if} \quad v \in V_2 \\ 0 & \text{else.} \end{cases}$$

This yields

$$\begin{aligned}
\lambda_N &= \sup_{u \neq 0} \frac{(\delta u, \delta u)}{(u.u)} = \sup_{u \neq 0} \frac{\sum_{e=(v,v')} (u(v) - u(v'))^2}{\sum_v \deg v \, u(v)^2} \\
&\geq \frac{\left(\frac{1}{\mathrm{vol}(V_1)} + \frac{1}{\mathrm{vol}(V_2)}\right)^2 E(V_1, V_2) + \left(\frac{1}{\mathrm{vol}(V_1)}\right)^2 E(V_1, V_3) + \left(\frac{1}{\mathrm{vol}(V_2)}\right)^2 E(V_2, V_3)}{\left(\frac{1}{\mathrm{vol}(V_1)} + \frac{1}{\mathrm{vol}(V_2)}\right)} \\
&\geq \frac{(\mathrm{vol}(V_1) + \mathrm{vol}(V_2))^2}{2\mathrm{vol}(V_1)\mathrm{vol}(V_2)} \frac{2E(V_1, V_2)}{\mathrm{vol}(V_1) + \mathrm{vol}(V_2)} \\
&+ \frac{\min(\mathrm{vol}(V_1), \mathrm{vol}(V_2))}{\max(\mathrm{vol}(V_1), \mathrm{vol}(V_2))} \frac{E(V_1 \cup V_2, V_3)}{(\mathrm{vol}(V_1) + \mathrm{vol}(V_2))} \\
&\geq 2\overline{h} + \frac{\min(\mathrm{vol}(V_1), \mathrm{vol}(V_2))}{\max(\mathrm{vol}(V_1), \mathrm{vol}(V_2))} \frac{E(V_1 \cup V_2, V_3)}{(\mathrm{vol}(V_1) + \mathrm{vol}(V_2))} \\
&\geq 2\overline{h},
\end{aligned}$$

using $\frac{(a+b)^2}{2ab} \geq 2$ for $a, b \in \mathbb{R}$.

We now turn to the upper bound $\lambda_N \leq 1 + \sqrt{1 - (1 - \overline{h})^2}$. The graph Laplacian $\Delta = I - P$ and the operator $\Sigma = I + P$ have the same eigenfunctions, and if λ is an eigenvalue of Δ, the corresponding eigenvalue of Σ is $\mu = 2 - \lambda$. In particular,

$$\lambda_N = \mu_1. \tag{4.4.11}$$

Thus, controlling the largest eigenvalue λ_N of Δ from above is equivalent to controlling the smallest eigenvalue μ_1 of Σ from below. The smallest eigenvalue μ_1 of Σ is

$$\begin{aligned}
\mu_1 &= \inf_{u \neq 0} \frac{(\Sigma u, u)}{(u, u)} \\
&= \inf_{u \neq 0} \frac{\frac{1}{2} \sum_{(v,v') \in E} (u(v) + u(v'))^2}{\sum_{v \in V} \deg v \, u(v)^2}
\end{aligned}$$

In order to prove the lower bound for μ_1, we will use the idea of [78] to construct a bipartite graph Γ' out of Γ for which the quantity $h'(g)$ in Lemma 4.3.1 for Γ' can be controlled by the quantity $1 - \overline{h}$ of Γ.

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Let u be an eigenfunction for the eigenvalue μ_1 and define

$$S(u) := \{v \in V : u(v) > 0\}, \quad T(u) := \{v \in V : u(v) < 0\}.$$

Since u is also an eigenfunction for λ_N of Δ, we know that $(u,1) = 0$ and thus $S(u), T(u) \neq \emptyset$. For constructing the new graph $\Gamma' = (V', E')$ from Γ, we duplicate all vertices in $S(u) \cup T(u)$ and denote the copies by a prime, for example, if $v \in S(u)$, then its copy is $v' \in S'(u)$. The vertex set V' of Γ' is $V' = V \cup S'(u) \cup T'(u)$. Every edge $(v, \hat{v}) \in E(S(u), S(u))$ in Γ is replaced by two edges $(v, \hat{v}')$ and $(\hat{v}, v')$ in Γ' and analogously for the edges in $E(T(u), T(u))$. The edges between $S(u)$ and $T(u)$ remain and are not replaced or duplicated. Thus, $S'(u)$ has no edges to $T(u)$ or $T'(u)$ and analogously for $T'(u)$. In particular, when u has no zeroes, that is, $S(u) \cup T(u) = V$, then Γ' is bipartite, with the two classes $V_1 = S(u) \cup T'(u)$ and $V_2 = T(u) \cup S'(u)$.

We consider the function $g : V' \to \mathbb{R}$,

$$g(v) = \begin{cases} |u(v)| & \text{if} \quad v \in S(u) \cup T(u) \\ 0 & else. \end{cases}$$

Then, since $u(v)$ and $u(\hat{v})$ have opposite signs when $v \in S(u)$ and $\hat{v} \in T(u)$, but the same sign when both of them are either in $S(u)$ or in $T(u)$,

$$\begin{aligned} \mu_1 &= \frac{\sum_{e=(v,\hat{v})\in E} (u(v) + u(\hat{v}))^2}{\sum_{v\in V} \deg v \, u(v)^2} \\ &\geq \frac{\sum_{e'=(v,\hat{v})\in E'} (g(v) - g(\hat{v}))^2}{\sum_{v\in V'} \deg v \, g(v)^2} \\ &\geq 1 - \sqrt{1 - (h'(g))^2} \end{aligned} \tag{4.4.12}$$

where the last inequality follows from Lemma 4.3.1. For a nonempty subset $W \subseteq S(g) = S(u) \cup T(u)$, we define $S_W = W \cap S(u)$ and $T_W = W \cap T(u)$. Let $\emptyset \neq U \subseteq S(g)$ realize the infimum, that is,

$$\begin{aligned} h'(g) &= \inf_{\emptyset \neq W \subseteq S(g)} \frac{|E'(W, \overline{W})|}{\mathrm{vol}(W)} = \frac{|E'(U, \overline{U})|}{\mathrm{vol}(U)} \\ &= \frac{2|E(S_W, S_W)| + 2|E(T_W, T_W)| + |E(S_W \cup T_W, \overline{S_W \cup T_W})|}{\mathrm{vol}(S_W) + \mathrm{vol}(T_W)} \\ &\geq \frac{|E(S_W, S_W)| + |E(T_W, T_W)| + |E(S_W \cup T_W, \overline{S_W \cup T_W})|}{\mathrm{vol}(S_W) + \mathrm{vol}(T_W)} \\ &= 1 - \frac{2|E(S_W, T_W)|}{\mathrm{vol}(S_W) + \mathrm{vol}(T_W)} \\ &\geq 1 - \overline{h}. \end{aligned} \tag{4.4.13}$$

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(4.4.11), (4.4.12), and (4.4.13) yield

$$2 - \lambda_N = \mu_1 \geq 1 - \sqrt{1 - (1 - \overline{h})^2},$$

and the upper bound in (4.4.7) follows. This completes the proof of Theorem 4.4.1. □

Corollary 4.4.1. *For complete graphs K_N,*

$$\overline{h}(K_N) \to \frac{1}{2} \quad \text{as } N \to \infty. \tag{4.4.14}$$

Proof This follows from Lemma 4.1.8 and the lower bound in (4.4.7). □

In fact, when N is even and we let V_1 and V_2 consist of $N/2$ vertices each, then each vertex has $N/2$ edges to vertices in the other component, while

$$\text{vol}\,(V_1) = \text{vol}\,(V_2) = \frac{N}{2}(N-1),$$

and so, for this partition

$$\frac{2|E(V_1, V_2)|}{\text{vol}\,(V_1) + \text{vol}\,(V_2)} = \frac{N}{2(N-1)} = \frac{1}{2}\lambda_N$$

by Lemma 4.1.13, and thus, by Theorem 4.4.1, $2\overline{h} = \lambda_N$, and the lower bound is sharp.

4.5 Neighborhood Graphs

In this section, which is mainly taken from [24], we consider a weighted graph that may also contain self-loops, that is, edges of the form (v, v) for $v \in V$, its vertex set. The weight of the edge (v, v') is denoted by $w_{vv'}$. We recall that the degree of vertex v in such a graph is given by

$$\deg v = \sum_{v'} w_{vv'}. \tag{4.5.1}$$

The neighborhood graph of order l of such a graph, to be defined in a moment, makes two vertices v, v' neighbors when there exists at least one path (with nonvanishing weights) of length l between them in the original graph. The weight of the edge between two such vertices is the sum over the weights of all such paths, and the weight of a path is the product of the weights of the edges contained in it, normalized by the degrees of its vertices. The idea behind this, to be explored in more detail later, is that this weight then equals

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the probability that a random walker starting at v reaches v' in l steps. And since a random walker may return to its starting position after some steps, these neighborhood graphs in general will possess self-loops.

The main point of this section is to relate the eigenvalues of a graph $\Gamma = (V, E)$ and those of its neighborhood graphs. The spectra are essentially equivalent to each other, and therefore, eigenvalue estimates for a neighborhood graph can be translated into eigenvalue estimates for the original graph, and vice versa. Since the neighborhood graphs encode properties of random walks on Γ, asymptotic ones if $l \to \infty$, we thereby gain a new source of geometric intuition for obtaining eigenvalue estimates.

Definition 4.5.1. The *neighborhood graph* $\Gamma^{[l]} = (V, E^{[l]})$ of order $l \geq 1$ of the weighted graph $\Gamma = (V, E)$ is the graph with the same vertex set V and the weighted edge set $E^{[l]}$ where the weight $w^{[l]}_{vv'}$ of the edge $e^{[l]} = (v, v')$ in $\Gamma^{[l]}$ is given by

$$w^{[l]}_{vv'} = \sum_{v_1,\dots,v_{l-1}} \frac{1}{\deg v_1} \cdots \frac{1}{\deg v_{l-1}} w_{vv_1} w_{v_1 v_2} \dots w_{v_{l-1}v'} \tag{4.5.2}$$

if $l > 1$, and we set $w^{[l]}_{vv'} = w_{vv'}$ if $l = 1$, that is, $\Gamma^{[1]} = \Gamma$.

Thus, v and v' are neighbors in $\Gamma^{[l]}$ if there exists at least one path of length l between v and v' in Γ.

The simplest example is the following:

Example 4.5.1. The graph Γ has two vertices v, v', an edge (vv') of weight 1 and self-loops at v and v' of weight $c \geq 0$. Thus, each vertex has degree $1 + c$, and the adjacency matrix W is

$$W = W^{[1]} = \begin{pmatrix} c & 1 \\ 1 & c \end{pmatrix}.$$

The neighborhood graphs $\Gamma^{[l]}$ of Γ in this example have the same edges, and the weighted adjacency matrices $W^{[l]}$, for $l = 2, 3, 4, 5$, are

$$W^{[2]} = \frac{1}{(1+c)} \begin{pmatrix} c^2+1 & 2c \\ 2c & c^2+1 \end{pmatrix},$$

$$W^{[3]} = \frac{1}{(1+c)^2} \begin{pmatrix} c^3+3c & 3c^2+1 \\ 3c^2+1 & c^3+3c \end{pmatrix},$$

$$W^{[4]} = \frac{1}{(1+c)^3} \begin{pmatrix} (c^2+1)^2+4c^2 & 4c^3+4c \\ 4c^3+4c & (c^2+1)^2+4c^2 \end{pmatrix},$$

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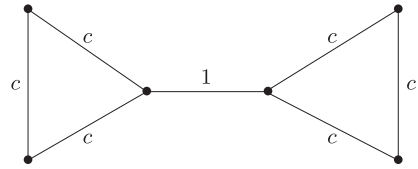


Figure 4.15 A graph for which we want to compute the neighborhood graphs.

$$W^{[5]} = \frac{1}{(1+c)^4}\begin{pmatrix} c(5+10c^2+c^4) & 1+10c^2+5c^4 \\ 1+10c^2+5c^4 & c(5+10c^2+c^4) \end{pmatrix},$$

and so on.

Example 4.5.2. For the family of graphs in Figure 4.15,
$W^{[1]}$ is given by

$$\begin{pmatrix} 0 & c & c & 0 & 0 & 0 \\ c & 0 & c & 0 & 0 & 0 \\ c & c & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & c & c \\ 0 & 0 & 0 & c & 0 & c \\ 0 & 0 & 0 & c & c & 0 \end{pmatrix},$$

and $W^{[2]}$ is

$$\begin{pmatrix} c/2+c^2/(1+2c) & c^2/(1+2c) & c/2 \\ c^2/(1+2c) & c/2+c^2/(1+2c) & c/2 \\ c/2 & c/2 & 1/(1+2c)+c \\ c/(1+2c) & c/(1+2c) & 0 \\ 0 & 0 & c/(1+2c) \\ 0 & 0 & c/(1+2c) \end{pmatrix}$$

$$\begin{pmatrix} c/(1+2c) & 0 & 0 \\ c/(1+2c) & 0 & 0 \\ 0 & c/(1+2c) & c/(1+2c) \\ 1/(1+2c)+c & c/2 & c/2 \\ c/2 & c/2+c^2/(1+2c) & c^2/(1+2c) \\ c/2 & c^2/(1+2c) & c/2+c^2/(1+2c) \end{pmatrix}.$$

We first record some simple properties of neighborhood graphs $\Gamma^{[l]}$.

Lemma 4.5.1. *(i) The vertex degrees do not depend on l, that is.*

$$\deg v = \deg v^{[l]} \tag{4.5.3}$$

for all $v \in V$ and $l \geq 1$. In particular, the scalar products are the same for all l, $(\cdot,\cdot)_\Gamma = (\cdot,\cdot)_{\Gamma^{[l]}}$.

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(ii) If l is even and Γ is connected, then $\Gamma^{[l]}$ consists of exactly two connected components if Γ is bipartite, and if it is not bipartite, then $\Gamma^{[l]}$ is connected.

(iii) If l is odd and Γ is connected, then $\Gamma^{[l]}$ is also connected, and $\Gamma^{[l]}$ is bipartite if and only if Γ is bipartite.

Proof (i).

$$\begin{aligned}
\deg v^{[l]} &= \sum_{v'} w_{vv'}^{[l]} \\
&= \sum_{v_1,\dots,v_{l-1}} \frac{1}{\deg v_1} \cdots \frac{1}{\deg v_{l-1}} w_{vv_1} w_{v_1v_2} \dots w_{v_{l-2}v_{l-1}} \sum_{v'} w_{v_{l-1}j} \\
&= \sum_{v_1,\dots,v_{l-2}} \frac{1}{\deg v_1} \cdots \frac{1}{\deg v_{l-2}} w_{vv_1} w_{v_1v_2} \cdots \sum_{v_{l-1}} w_{v_{l-2}v_{l-1}} \\
&\vdots \\
&= \sum_{v_1} w_{vv_1} = \deg v
\end{aligned}$$

(ii). When Γ is not bipartite, it contains at least one loop of odd length. When it is connected, therefore, from any vertex v, any other vertex can be reached by some path of even length. Since such a path can be decomposed into paths of length 2, Γ^2 is connected. And since Γ, not being bipartite, contains a path of odd length, so does $\Gamma^{[2]}$, and hence, it is not bipartite either, and we can iterate the argument. When Γ, however, is bipartite, then only other vertices in the same class as v can be reached from v by a path of even length, and since Γ is connected, this is possible for every other vertex in the same class. Therefore, that class yields one component of $\Gamma^{[2]}$, and the other class, the other. Again, the argument iterates.

(iii). When v and v' are connected by an edge in Γ, then one can go from v to v' in any odd number l of steps by going forth and back between v and v' $\frac{l-1}{2}$ times and then again from v to v'. This implies that for odd l, $\Gamma^{[l]}$ is connected if and only if Γ is. And if Γ is bipartite, from a vertex v, one can reach a vertex in the same class only in an even number of steps. Therefore, $\Gamma^{[l]}$ then remains bipartite. □

Remark 4.5.1. We can now understand the observation made in the remark before Definition 4.1.6. For the complete bipartite graph $\Gamma^{[1]} = K_{m,n}$, its neighborhood graph $\Gamma^{[2]}$ is simple the disjoint union of the two complete graphs K_m^0 and K_n^0 with self-loops, and this is the reason why their spectra are so similar. We shall now investigate the spectra of neighborhood graphs systematically.

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We shall first express the Laplacian of $\Gamma^{[l]}$ in terms of the Laplacian Δ of Γ.

Lemma 4.5.2. *The graph Laplacian $\Delta^{[l]}$ on $\Gamma^{[l]}$ satisfies*

$$\Delta^{[l]}u = (\mathrm{Id} - (\mathrm{Id} - \Delta)^l)u \tag{4.5.4}$$

for $u \in L^2(\Gamma)$. In particular, the eigenvalues of $\Delta^{[l]}$ are of the form

$$\lambda^{[l]} = 1 - (1-\lambda)^l, \tag{4.5.5}$$

where λ is an eigenvalue of Δ.

Proof For $u \in L^2(\Gamma)$,

$$\begin{aligned}(\mathrm{Id} - (\mathrm{Id} - \Delta)^l)u(i) &= u(i) - \sum_j \sum_{v_1,\dots,v_{l-1}} \frac{w_{vv_1}}{\deg v} \cdots \frac{w_{v_{l-1}j}}{\deg v_{l-1}} u(j) \\ &= \frac{1}{\deg v^{[l]}} \sum_j w^{[l]}_{vv'}(u(i) - u(j)) \\ &= \Delta^{[l]}u(i),\end{aligned}$$

by (4.5.2) and since $\deg v = \deg v^{[l]}$ by (4.5.3). □

Remark 4.5.2. For $l = 2$, Lemma 4.5.2 says $\lambda^{[2]} = \lambda(2-\lambda)$ for the eigenvalues, and this also implies Corollary 4.1.6.

Corollary 4.5.1. *Let Γ be a graph and $\Gamma^{[l]}$ its neighborhood graph of order l. The eigenvalues of $\Delta^{[l]}$ satisfy*

$$0 = \lambda_1^{[l]} \le \ldots \le \lambda_N^{[l]} \le 1 \qquad \textit{for even } l \tag{4.5.6}$$

and

$$0 = \lambda_1^{[l]} \le \ldots \le \lambda_N^{[l]} \le 2 \qquad \textit{for odd } l. \tag{4.5.7}$$

Proof All eigenvalues λ_k of Δ satisfy $\lambda_k \in [0,2]$ and thus $1-(1-\lambda_k)^l \in [0,1]$ if l is even and $1-(1-\lambda_k)^l \in [0,2]$ if l is odd. □

Remark 4.5.3. By Corollary 4.5.1, for l even, all eigenvalues are ≤ 1 and thus in particular $\lambda_N \le 1$. This is caused by the fact that for even l, $\Gamma^{[l]}$ contains a self-loop at every vertex, since a random walker can return to its starting vertex in two steps, or equivalently, in any graph without isolated vertices, there is a path of length 2 from each vertex to itself. In contrast, we recall that for loopless graphs, we have $1 < \frac{N}{N-1} \le \lambda_N$ by Lemma 4.1.10.

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Corollary 4.5.2. *1 is an eigenvalue of $\Delta^{[l]}$ precisely if it is an eigenvalue of Δ, and the multiplicity m_1 of the eigenvalue 1 is the same for all neighborhood graphs, that is, $m_1(\Delta) = m_1(\Delta^{[l]})$ for all $l \geq 1$.*

And if $\lambda \neq 0, 2$ then

$$\lambda^{[l]} = 1 - (1 - \lambda)^l \to 1 \qquad \text{as } l \to \infty. \tag{4.5.8}$$

Proof Γ and $\Gamma^{[l]}$ have the same vertex set; thus, both Δ and $\Delta^{[l]} = (\mathrm{Id} - (\mathrm{Id} - \Delta)^l)$ have $N = |V|$ eigenvalues. Every eigenfunction u_k for Δ and eigenvalue λ_k is also an eigenfunction for $\Delta^{[l]}$ and the eigenvalue $1 - (1 - \lambda_k)^l$.

We have $1 - (1 - \lambda_k)^l = 1$ if and only if $\lambda_k = 1$.
If $\lambda \neq 0, 2$ is an eigenvalue of Δ, then $|1 - \lambda| < 1$. Hence, $|1 - \lambda|^l \to 0$ as $l \to \infty$, and the result follows from (4.5.4). □

For some eigenvalues, we can make the convergence in (4.5.8) quantitative.

Theorem 4.5.1. *For every Γ with at least three vertices, there is some eigenvalue $\lambda^{[l]}$ of $\Delta^{[l]}$ with*

$$|1 - \lambda^{[l]}| \leq \frac{1}{2^l}. \tag{4.5.9}$$

When l is even, the largest eigenvalue of $\Gamma^{[l]}$ satisfies

$$1 - \frac{1}{2^l} \leq \lambda_N^{[l]} \leq 1, \tag{4.5.10}$$

and both bounds are sharp.

Proof The bound (4.5.9) follows from (4.5.5) and from Theorem 4.1.2, where we have shown that $\min_{\lambda_i} |1 - \lambda_i| \leq 1/2$ for all connected graphs with at least three nodes, and that this bound is realized for the petal and book graphs. By Corollary 4.5.2, when l is even, this concerns the largest eigenvalue. The upper bound in (4.5.10) is already contained in (4.5.6). It is realized whenever Γ possesses the eigenvalue 1, for instance, if it has duplicated nodes. □

Thus, we can control the eigenvalues of $\Delta^{[l]}$ in terms of those of Δ. We shall now derive controls in the opposite direction. That is, we can control eigenvalues of Γ by using geometric properties of its neighborhood graphs $\Gamma^{[l]}$.

Theorem 4.5.2. *If $a^{[l]} \leq \lambda_2^{[l]}$, then*

$$1 - \left(1 - a^{[l]}\right)^{\frac{1}{l}} \leq \lambda_2 \leq \ldots \leq \lambda_N \leq 1 + \left(1 - a^{[l]}\right)^{\frac{1}{l}} \text{ for even } l, \tag{4.5.11}$$

and

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$$1 - \left(1 - a^{[l]}\right)^{\frac{1}{l}} \leq \lambda_2 \text{ for odd } l. \tag{4.5.12}$$

Proof Since by Lemma 4.5.2, the eigenvalues of $\Delta^{[l]}$ are $1 - (1 - \lambda_k)^l$ where λ_k are the eigenvalues of Δ, we have

$$1 - (1 - \lambda_k)^l \geq \min_{k \neq 0} 1 - (1 - \lambda_k)^l = \lambda_2^{[l]} \geq a^{[l]}.$$

This implies that for all $k \neq 0$

$$|1 - \lambda_k| \leq (1 - a^{[l]})^{\frac{1}{l}}$$

if l is even, and

$$1 - \lambda_k \leq (1 - a^{[l]})^{\frac{1}{l}}$$

if l is odd. □

As a concrete example, we use the Cheeger inequality (4.3.12), that is,

$$a^{[l]} = 1 - \sqrt{1 - (h^{[l]})^2} \leq \lambda_2^{[l]}.$$

Corollary 4.5.3. *All eigenvalues of* $\Delta(\Gamma)$ *satisfy*

$$1 - \left(1 - (h^{[l]})^2\right)^{\frac{1}{2l}} \leq \lambda_2 \leq \ldots \leq \lambda_N \leq 1 + \left(1 - (h^{[l]})^2\right)^{\frac{1}{2l}} \text{ for even } l, \tag{4.5.13}$$

and

$$1 - \left(1 - (h^{[l]})^2\right)^{\frac{1}{2l}} \leq \lambda_2 \text{ for odd } l. \tag{4.5.14}$$

Remark 4.5.4. While Theorem 4.5.1 is concerned with $\min_k |1 - \lambda_k|$, Theorem 4.5.2 yields estimates for $\max_{k \neq 1} |1 - \lambda_k|$.

Remark 4.5.5. For bipartite graphs Γ, we have $\lambda_N = 2$. If l is even, then $h^{[l]} = 0$ since by Lemma 4.5.1, the neighborhood graph $\Gamma^{[l]}$ of a bipartite graph is disconnected. Thus, for bipartite graphs, the upper bound in (4.5.13) is sharp. On the other hand, if l is even and the graph is bipartite, then the lower bound in Corollary 4.5.3 yields only the trivial estimate $0 \leq \lambda_2$. In contrast, if l is even and Γ is not bipartite or if l is odd, then Corollary 4.5.3 yields a nontrivial lower bound

$$0 < 1 - \left(1 - (h^{[l]})^2\right)^{\frac{1}{2l}} \leq \lambda_2$$

for the second smallest eigenvalue. These new lower bounds for λ_2 can actually improve the Cheeger estimate (4.3.12).

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In Theorem 4.5.2, we have seen, in particular, that a lower bound for $\lambda_2^{[l]}$ for even l turns into an upper bound for λ_N. Conversely, an upper bound for $\lambda_2^{[l]}$ for even l yields a lower bound for λ_N, as a special case of Theorem 4.5.3.

Theorem 4.5.3. *If $\lambda_2^{[l]} \le b^{[l]}$, then*

$$\lambda_2 \le 1 - \left(1 - b^{[l]}\right)^{\frac{1}{l}} \tag{4.5.15}$$

or

$$\lambda_N \ge 1 + \left(1 - b^{[l]}\right)^{\frac{1}{l}} \text{ for even } l, \tag{4.5.16}$$

and

$$\lambda_2 \le 1 - \left(1 - b^{[l]}\right)^{\frac{1}{l}} \text{ for odd } l. \tag{4.5.17}$$

Proof By Lemma 4.5.1, if l is even, we can assume $b^{[l]} \le 1$, and hence (4.5.15) and (4.5.16) are well-defined. If $b^{[l]} \ge \lambda_2^{[l]} = \min_{k>1} 1 - (1 - \lambda_k)^l$ (by (4.5.5)), then for at least one eigenvalue λ_i, $i \ne 0$, we have

$$(1 - b^{[l]})^{\frac{1}{l}} \le |1 - \lambda_i|$$

if l is even and

$$(1 - b^{[l]})^{\frac{1}{l}} \le 1 - \lambda_i$$

if l is odd. □

Using the Cheeger inequality (4.3.19) for $\Gamma^{[l]}$, we obtain:

Corollary 4.5.4. *Assume that $2h^{[l]} \le 1$ and l is even; then we have*

$$\lambda_2 \le 1 - \left(1 - 2h^{[l]}\right)^{\frac{1}{l}}. \tag{4.5.18}$$

or

$$\lambda_N \ge 1 + \left(1 - 2h^{[l]}\right)^{\frac{1}{l}}. \tag{4.5.19}$$

If l is odd, then we have

$$\lambda_2 \le 1 - \left(1 - 2h^{[l]}\right)^{\frac{1}{l}}.$$

Remark 4.5.6. We now want to discuss under which conditions the estimate (4.5.18) for λ_2 can improve the Cheeger estimate. Comparing Corollary 4.5.3 with (4.3.12), the preceding estimates improve the Cheeger estimate (4.3.12) if

$$h^{[l]} \ge \sqrt{1 - (1 - h^2)^l}, \tag{4.5.20}$$

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for some $l \geq 2$. For discussing (4.5.20), let us first look at even l. It cannot hold when Γ is bipartite, since then, by Lemma 4.5.1, $\Gamma^{[l]}$ is disconnected and thus $h^{[l]} = 0$. For graphs that are not bipartite, however, the estimate in (4.5.13) always yields a nontrivial lower bound

$$0 < 1 - \left(1 - (h^{[l]})^2\right)^{\frac{1}{2l}} \leq \lambda_2$$

for the second smallest eigenvalue λ_2. We then need to understand under which conditions $h^{[l]} > h$. We distinguish two cases. If $\lambda_2 \geq 2 - \lambda_N$, then $\lambda_2^{[l]} = 1 - (1 - \lambda_N)^l$, and so it is possible that $\lambda_2^{[l]} < \lambda_2$. If this is the case, we cannot expect (4.5.20). But if $\lambda_2 < 2 - \lambda_N$, then $\lambda_2^{[l]} = 1 - (1 - \lambda_1)^l > \lambda_2$, and so we can expect $h^{[l]} > h$. Thus, if l is even, graphs that are closer to disconnected graphs than to bipartite graphs are good candidates for satisfying (4.5.20).

We now turn to the effect of bounds on the largest eigenvalue $\lambda_N^{[l]}$.

Theorem 4.5.4. *If $c^{[l]} \leq \lambda_N^{[l]}$, then there exists at least one eigenvalue λ_k in the interval*

$$\left[1 - \left(1 - c^{[l]}\right)^{\frac{1}{l}}, 1 + \left(1 - c^{[l]}\right)^{\frac{1}{l}}\right] \tag{4.5.21}$$

if l is even and

$$\lambda_N \geq 1 + \left(1 - c^{[l]}\right)^{\frac{1}{l}}$$

if l is odd.

Proof We recall from Corollary 4.5.1 that if l is even, $c^{[l]} \leq \lambda_N^{[l]} \leq 1$. Recalling (4.5.5) again, we have $c^{[l]} \leq \lambda_N^{[l]} = \max_k (1 - (1 - \lambda_k)^l)$. Thus,

$$\min_k |1 - \lambda_k| \leq \left(1 - c^{[l]}\right)^{\frac{1}{l}}$$

if l is even and

$$\min_k (1 - \lambda_k) = 1 - \max_k \lambda_k \leq \left(1 - c^{[l]}\right)^{\frac{1}{l}}$$

if l is odd. □

In particular, we have from Theorems 4.4.1 and 4.5.4:

Corollary 4.5.5. *Assume that $2\overline{h}^{[l]} \leq 1$ and l is even, then there exists at least one eigenvalue λ_k in the interval*

$$\left[1 - (1 - 2\overline{h}^{[l]})^{\frac{1}{l}}, 1 + (1 - 2\overline{h}^{[l]})^{\frac{1}{l}}\right]. \tag{4.5.22}$$

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If l is odd, then

$$\lambda_N \geq 1 + \left(1 - 2\overline{h}^{[l]}\right)^{\frac{1}{l}}.$$

We now turn to the gap phenomenon for eigenvalues, that is, finding some interval that does not contain any eigenvalue.

Theorem 4.5.5. *If $\lambda_N^{[l]} \leq d^{[l]}$, then all eigenvalues λ_k of Δ are contained in the union of intervals*

$$\left[0, 1 - \left(1 - d^{[l]}\right)^{\frac{1}{l}}\right] \bigcup \left[1 + \left(1 - d^{[l]}\right)^{\frac{1}{l}}, 2\right] \tag{4.5.23}$$

if l is even and

$$\lambda_N \leq 1 - \left(1 - d^{[l]}\right)^{\frac{1}{l}}$$

if l is odd.

The proof is similar to the preceding proofs and hence omitted. Theorem 4.5.5 says that if l is even, then an upper bound $d^{[l]} < 1$ for $\lambda_N^{[l]}$ of $\Delta^{[l]}$ on $\Gamma^{[l]}$ bounds all eigenvalues of Δ on Γ away from 1. In particular, in that case, Γ cannot contain duplicated nodes, as they would cause an eigenvalue 1.

Recalling Lemma 4.1.10 and Theorem 4.1.2, the preceding considerations also imply

Theorem 4.5.6. *Considering the extreme cases for the largest eigenvalue $\lambda_N^{[l]}$, if l is even,*

$$\min_{\text{connected graph } \Gamma} \lambda_N^{[l]}(\Gamma) = 1 - \frac{1}{2^l},$$

and this minimum is realized if and only if Γ is a petal or a book graph.

While if l is odd,

$$\min_{\text{connected graph } \Gamma} \lambda_N^{[l]}(\Gamma) = 1 - \frac{1}{(N-1)^l},$$

and this minimum is realized if and only if Γ is a complete graph.

Moreover, for any l,

$$\max_{\text{connected graph } \Gamma} \lambda_2^{[l]}(\Gamma) = 1 - \frac{1}{(N-1)^l},$$

and this maximum is again realized if and only if Γ is a complete graph.

□

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4.6 Signed Graphs

We now turn to graphs with an additional structure, a sign function. This class of graphs, the *signed graphs*, is not only important for several applications but will also naturally occur in our analysis of the Laplacians of simplicial complexes.

In this section, we shall describe the results of [11] (which turn the results of [10, 187] into a general perspective). See also [179, 188] and the references therein, which discuss more general signatures than we do here. We shall only discuss the case where the possible signatures are taken from $\{\pm 1\}$, but for instance in [251, 255] signatures with values in $U(1)$ were also introduced (leading to the notion of a *magnetic Laplacian*), and one can then naturally also allow for signatures with values in other groups like $O(n)$ or $U(n)$ (*connection Laplacian*). For us, however, the signatures ± 1 will become important in Section 8.3.

All graphs in this section are *undirected*.

Definition 4.6.1. A *signed graph* Γ consists of a vertex set V and a set E of undirected edges with a sign function

$$s\colon E \to \{+1, -1\} \tag{4.6.1}$$

and a weight function

$$w\colon E \to \mathbb{R}_+. \tag{4.6.2}$$

While in some applications, such as neural networks, negative weights would naturally occur, we here consider only positive edge weights, because in the framework developed here, which originally goes back to Harary [124], the signs are carried by the sign function and not by the weights. In social networks [123, 125], a positive sign $s(uv)$ would indicate a positive relation, like friendship, between the individuals represented by the vertices u and v, whereas a negative sign might indicate that they are enemies or opponents.

In the special case where $w(e) = 1$ for every edge, we speak of an unweighted signed graph.

Definition 4.6.2. The *opposite graph* of the signed graph (Γ, s) is the signed graph $(\Gamma, -s)$, that is, the signed graph where all edges have the opposite sign as on (Γ, s).

For $S \subset V$, we denote its complement in V by $\overline{S}$, that is, $\overline{S} = V \setminus S$.

When we speak of a signed graph Γ, we shall usually denote its vertex set by V, its edge set by E, the number of its vertices by N, its sign function by s, and its weight function by w. The edge connecting the vertices u and v is

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usually written as (uv), and since we are working with undirected graphs in this section, this is the same as (vu). We shall also usually write w_{uv} in place of $w(uv)$. We shall also say that an edge is positive (negative) if its sign is positive (negative).

Some special features of signed graphs are important. A *cycle* C_m of length m in a graph Γ consists of vertices $v_1, \dots, v_m \in V$ and edges $e_1 = (v_1, v_2), \dots, e_{m-1} = (v_{m-1}, v_m), e_m = (v_m, v_1) \in E$.

Definition 4.6.3. The signed cycle C_m is *balanced* if

$$\prod_{i=1}^{m} s(e_i) = 1. \tag{4.6.3}$$

A signed graph (Γ, s) is *balanced* if every cycle contained in it is balanced. (Γ, s) is *antibalanced* if $(\Gamma, -s)$ is balanced.

We have Harary's characterization of balanced graphs [124].

Lemma 4.6.1 (Harary)**.** *A signed graph Γ is balanced precisely if there is a partition $V = V_1 \cup V_2$, where one of these sets may be empty, such that all edges between points of the same subset have a positive sign and those between points of different subsets have a negative sign.*

Proof The idea of the proof consists in approaching Γ from two ends. For the sufficiency, we take the maximal graph K_N with the same vertex set and delete edges one by one until we are left with the edge set of Γ. For the necessity, we start with a minimally connected graph with the same vertex set, a tree, and add edges one by one until we arrive at the edge set of Γ.

Now the—easy—details. We first observe that a subgraph of a balanced graph is balanced itself, as follows trivially from the definition. For the sufficiency of the condition, we shall therefore show that when this condition holds, we can extend the sign function to the complete graph K_N with the same vertex set V as Γ and make K_N balanced. Thus, for any pair $u, v \in V$, we give the edge (uv) in K_N a positive sign if u and v are in the same subset and a negative sign when they are in different subsets, that is, one is in V_1 and the other in V_2. Since then every cycle in K_N has to contain an even number of edges between V_1 and V_2, K_N with this sign function is balanced, and hence so is our original graph.

Necessity is proved inductively on the number of edges. We may assume that our graph is connected. Therefore, it contains a tree T, that is, a connected graph without cycles, that contains all vertices of V as a subgraph. Take any $v_1 \in V$. Let V_1 be the set of those vertices that are connected in T by a path of positive sign, that is, a path containing an even number of negative edges, and

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let V_2 be its complement (possibly empty). If we add another edge of Γ to T, it has to be positive when it connects two vertices that are both in V_1 or both in V_2 and negative when it connects vertices in different subsets. We can iterate this and add the remaining edges of Γ one by one to see the necessity of the condition. □

Definition 4.6.4. Let (Γ, s) be a signed graph. A function $\theta\colon V \to \{+1, -1\}$ is called a *switching function*. It switches the sign function from s to s^θ by

$$s^\theta(vv') = \theta(v)s(vv')\theta(v'). \tag{4.6.4}$$

(Thus, the sign of an edge is changed precisely if θ has opposite signs on its two vertices.)

The sign functions s and s' are *switching equivalent* if there exists a switching function θ with $s' = s^\theta$. We write $s \approx s^\theta$ and denote the equivalence of s by $[s]$.

Let $S \subset V$. A *switching* of S is the sign function s^S obtained via the switching function

$$\theta^S(v) = \begin{cases} -1 & \text{if } v \in S \\ +1 & \text{if } v \notin S\,, \end{cases} \tag{4.6.5}$$

that is,

$$s^S(uv) := \begin{cases} -s(uv) & \text{when } u \in S, v \in \overline{S} \\ s(uv) & \text{else.} \end{cases} \tag{4.6.6}$$

(Note that we are discussing undirected graphs here; that is, the edge (uv) is the same as the edge (vu).)

We observe that

$$\theta^S = \prod_{v \in S} \theta^v. \tag{4.6.7}$$

When the vertices of our graph are divided into two groups, and an edge connecting members of different groups has a negative sign, whereas those remaining in the same group are positive, then switching a subset S means that its members switch the group they belong to. Edges connecting them with members of their former group become negative, while those connecting with members of their new group turn positive. (4.6.7) says that we can switch the members of S one by one.

Lemma 4.6.2. *A bipartite graph (Γ, s^+) with the positive sign function s^+, that is, $s^+(e) = 1$ for every edge, which thus is balanced, is also switching equivalent to an antibalanced graph.*

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Proof When $V = V_1 \cup V_2$, with no edges inside either subset, we can switch one of them, say V_1, and thereby make every edge negative. The resulting signed bipartite graph then is both balanced and antibalanced. □

In social terminology, we have two groups with two possible opinions, and connections only exist between members of different groups. Switching one of these groups means that all members of that group change their opinion, see [1].

A similar observation will now be used for Zaslavsky's switching lemma [275].

Lemma 4.6.3 (Zaslavsky)**.** *A signed graph (Γ, s) is balanced if and only if s is switching equivalent to the positive sign function, that is, the one that is $+1$ on every edge. It is antibalanced if and only if s is switching equivalent to the negative sign function.*

Proof Let (Γ, s) be balanced and take the partition $V = V_1 \cup V_2$ of Lemma 4.6.1. Switching one of these subsets, say V_2, keeps the graph balanced, and s^{V_2} is the positive sign function because it keeps the signs of all edges inside V_2 or V_1 and changes the signs of the edges between these two sets. Conversely, when s is switching equivalent to the positive sign function s^+, we let V_2 be the set of vertices on which the switching function θ is negative. That gives a partition as in Lemma 4.6.1.

The antibalanced case is treated by working with $-s$. □

Definition 4.6.5. Let Γ be a signed graph. Its (normalized) Laplacian is defined by

$$\begin{aligned}\Delta^s f(v) &:= f(v) - \frac{1}{\deg v} \sum_{v' \sim v} w_{vv'} s(vv') f(v') \\ &= \frac{1}{\deg v} \sum_{v' \sim v} w_{vv'} (f(v) - s(vv') f(v')) \end{aligned} \tag{4.6.8}$$

with $\deg v = \sum_{v' \sim v} w_{vv'}$, for functions $f : V \to \mathbb{R}$.
The spectrum of a signed graph is the spectrum of Δ^s, with the same conventions as in Section 4.1.

We directly observe

Lemma 4.6.4. *λ is an eigenvalue of the signed graph (Γ, s) precisely if $2 - \lambda$ is an eigenvalue of the opposite signed graph $(\Gamma, -s)$. And the corresponding eigenfunctions are the same.*

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In particular, λ is an eigenvalue of the signed graph (Γ, s^+) on which all signs are positive precisely if $2-\lambda$ is an eigenvalue of the signed graph (Γ, s^-) on which all signs are negative.

Proof If we write the Laplacian of (Γ, s) as

$$\Delta^s = \mathrm{Id} - P, \tag{4.6.9}$$

then

$$\Delta^{-s} = \mathrm{Id} + P, \tag{4.6.10}$$

we see that

$$\Delta^{-s} = 2 - \Delta^s. \tag{4.6.11}$$

This implies the desired relation between the eigenvalues. □

Let us consider examples; for simplicity, they are unweighted. The signed graph in Figure 4.16 has the eigenvalue $\lambda = 2$ with a constant eigenfunction, $\lambda = 1$ with an eigenfunction that is $+1$ on the left, -1 on the right, 0 on the top vertex, and $\lambda = 0$ with 1 on the two lower vertices and -1 on the top one. This is the same as for the corresponding unsigned graph, the complete bipartite graph $K_{1,2}$, but with the roles of the eigenvalues $\lambda = 2$ and $\lambda = 0$ exchanged. In fact, this is a consequence of Lemma 4.6.4.

If we add an edge and turn the graph of Figure 4.16 into a triangle, as indicated in Figure 4.17, then has the eigenvalue $\lambda = 2$ with a constant eigenfunction and the eigenvalue $\lambda = 1/2$ with multiplicity 2, with an eigenfunction that is $+1$ on one vertex, -1 on another, and 0 on the third. Again, this is a consequence of Lemma 4.6.4 and Lemma 4.1.8.

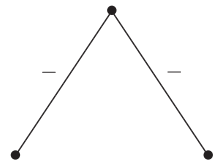


Figure 4.16 Simple signed graph A.

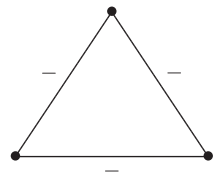


Figure 4.17 A signed graph with a frustrated triangle.

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Similarly, the graph of Figure 4.18 now again has $\lambda = 2$ and $\lambda = 1/2$ with multiplicity 3, with an eigenfunction that is ± 1 on the two upper vertices, or on the two lower vertices, and 0 elsewhere, or with 2 at the center and -1 at all other vertices. (Corollary 4.8.3 will provide an explanation for this eigenvalues and its multiplicity.) It has the eigenvalue $\lambda = 3/2$ with an eigenfunction that is $+1$ on the upper, -1 on the lower vertices, and 0 at the center. This follows from Lemma 4.6.4 and the computation of the spectrum of the petal graph in Section 4.1. We move on to the signed graph shown in Figure 4.19.

We again have $\lambda = 2$ with a constant eigenfunctions and $\lambda = 1/2$ with eigenfunctions that are ± 1 either on the two upper or on the two lower vertices. Two further eigenfunctions for that eigenvalue are indicated in Figure 4.20.

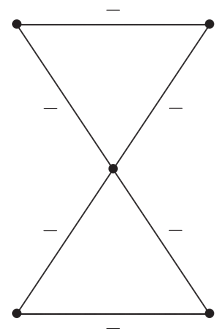


Figure 4.18 A signed graph with two frustrated triangles.

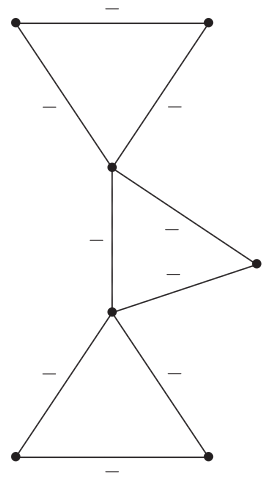


Figure 4.19 A signed graph whose eigenvalues and eigenfunctions will be computed in the main text; see also Figures 4.20 and 4.21.

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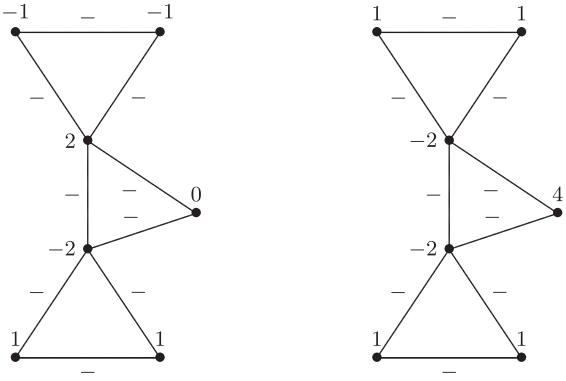


Figure 4.20 Two eigenfunctions on the signed graph of Figure 4.19.

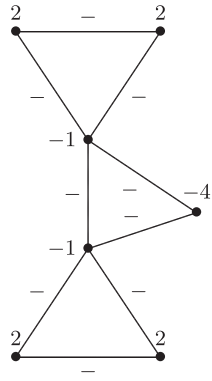


Figure 4.21 A third eigenfunction on the signed graph of Figure 4.19.

Altogether, the eigenvalue $\lambda = 1/2$ has multiplicity 4. We note that, here and in the previous examples, all eigenfunctions for $\lambda = 1/2$ sum to 0 on every loop.

In Figure 4.21, we get the eigenvalue $\lambda = 5/4$ with and in Figure 4.22, the eigenvalue $\lambda = 7/4$ with.

Lemma 4.6.5. *Δ^s is self-adjoint with respect to the product (4.1.32) $(f,g) = \sum_v \deg(v)\, f(v)g(v)$, and*

$$(\Delta^s f, g) = \sum_{(vv')} w_{vv'}(f(v) - s(vv')f(v'))(g(v) - s(vv')g(v')) = (f, \Delta^s g). \tag{4.6.12}$$

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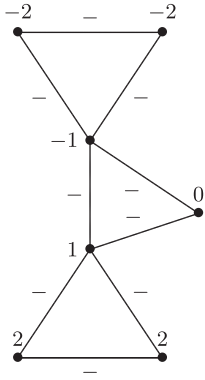


Figure 4.22 A fourth eigenfunction on the signed graph of Figure 4.19.

With the signed adjacency matrix (cf. (4.1.21))

$$A^s := (s(uv)w_{uv})_{u,v\in V} \tag{4.6.13}$$

and the switching matrix

$$M^\theta := \operatorname{diag}(\theta(v))_{v\in V}, \tag{4.6.14}$$

we have (cf. (4.1.22), (4.1.36))

$$\Delta^s = \mathrm{Id} - D^{-1}A^s \tag{4.6.15}$$

and

$$A^{s^\theta} = (M^\theta)^{-1}A^s M^\theta, \tag{4.6.16}$$

that is,

$$\Delta s^\theta = \mathrm{Id} - (M^\theta)^{-1}D^{-1}A^s M^\theta, \tag{4.6.17}$$

from which we conclude [276]

Lemma 4.6.6. *The spectrum of a signed graph is switching invariant.*

Thus, for instance, the signed graph of Figure 4.23 has the same spectrum as (Figure 4.18) ($\lambda = 2$ and $= 3/2$ with multiplicity 1 and $= 1/2$ with multiplicity 3), as it is obtained from the latter by switching the central vertex.

From the Lemmata 4.6.2, 4.6.4, and 4.6.6, we obtain another proof of Lemma 4.1.13.

From Theorem 2.6.1 and (4.6.12), we obtain

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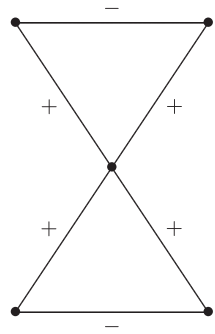


Figure 4.23 The signed graph obtained from that of Figure 4.18 by switching the central node.

Lemma 4.6.7. *The eigenvalues $\lambda_k, k = 1, \dots, N$ of a signed graph (that is, the eigenvalues of Δ^s) satisfy, when identifying the space of functions $g\colon V \to \mathbb{R}$ with $\mathbb{R}^N$,*

$$\begin{aligned}\lambda_k &= \min_{g\in\mathbb{R}^N,(g,g_j)=0 \text{ for } j=1,\dots,k-1} \frac{(\Delta^s g,g)}{(g,g)} = \max_{g\in\mathbb{R}^N,(g,g_\ell)=0 \text{ for } \ell=k+1,\dots,N} \frac{(\Delta^s g,g)}{(g,g)} \\ &= \min_{H_k\in\mathcal{H}_k} \max_{g(\neq 0)\in H_k} \frac{(\Delta^s g,g)}{(g,g)} = \max_{H_{m-k+1}\in\mathcal{H}_{N-k+1}} \min_{g(\neq 0)\in H_{N-k+1}} \frac{(\Delta^s g,g)}{(g,g)} \\ &= \min_{H_k\in\mathcal{H}_k} \max_{g(\neq 0)\in H_k} \frac{\sum_{(vv')} w_{vv'}(g(v) - s(vv')g(v'))^2}{(g,g)} \\ &= \max_{H_{N-k+1}\in\mathcal{H}_{N-k+1}} \min_{g(\neq 0)\in H_{N-k+1}} \frac{\sum_{(vv')} w_{vv'}(g(v) - s(vv')g(v'))^2}{(g,g)}\end{aligned} \tag{4.6.18}$$

where $\mathcal{H}_k$ is the family of all k-dimensional subspaces of $\mathbb{R}^N$.

Definition 4.6.6. We call the quotient appearing in (4.6.18),

$$R^s(g) := \frac{\sum_{(vv')} w_{vv'}(g(v) - s(vv')g(v'))^2}{\sum_v \deg v\, g(v)^2}, \tag{4.6.19}$$

the *signed Rayleigh quotient* of Γ, and

$$R^{-s}(g) = \frac{\sum_{(vv')} w_{vv'}(g(v) + s(vv')g(v'))^2}{\sum_v \deg v\, g(v)^2} \tag{4.6.20}$$

its *dual-signed Rayleigh quotient*.

Corollary 4.6.1. *The eigenvalues λ of a signed graph satisfy*

$$0 \le \lambda \le 2. \tag{4.6.21}$$

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Proof Because of the characterization of the eigenvalues by Rayleigh quotients, as stated in Lemma 4.6.7, the proof is the same as that of Lemma 4.1.12. □

Lemma 4.6.8. *Let θ be a switching function. Then,*

$$R^{s^\theta}(g) = R^s(\theta g). \tag{4.6.22}$$

Proof We have

$$\begin{aligned} R^s(\theta g) &= \frac{\sum_{(vv')} w_{vv'}(\theta(v)g(v) - s(vv')\theta(v')g(v'))^2}{\sum_v \deg v\, g(v)^2} \\ &= \frac{\sum_{(vv')} w_{vv'}(g(v) - \theta(v)s(vv')\theta(v')g(v'))^2}{\sum_v \deg v\, g(v)^2} \\ &= \frac{\sum_{(vv')} w_{vv'}(g(v) - s^\theta(vv')g(v'))^2}{\sum_v \deg v\, g(v)^2} \\ &= R^{s^\theta}(g). \end{aligned}$$

□

Lemmata 4.6.7 and 4.6.8 provide another proof of Lemma 4.6.6.

Corollary 4.6.2. *There exists a function g with $R^s(g) = 0$ precisely if s is balanced.*

Proof $R^s(g) = 0$ for a nontrivial g if and only if $g(v) - s(vv')g(v') = 0$ for every pair $v \sim v'$. Without loss of generality, $g(v) = \pm 1$ for all v. We then have the two subsets $V_1 := \{v\colon g(v) = 1\}$ and $V_2 := \{v\colon g(v) = -1\}$ satisfying the conditions of Theorem 4.6.1. Conversely, when we have such V_1, V_2, we can put $g(v) = 1$ (-1) on V_1 (V_2) to get $R^s(g) = 0$. □

We had observed in Lemma 4.6.4 that

$$\lambda_k(\Delta^{-s}) = 2 - \lambda_{N-k+1}(\Delta^s) \text{ for } k = 1, \ldots, N. \tag{4.6.23}$$

In particular, from Lemma 4.6.7,

Lemma 4.6.9.

$$\lambda_1(\Delta^s) = \min_{g \neq 0} R^s(g) \text{ and } 2 - \lambda_N(\Delta^s) = \lambda_1(\Delta^{-s}) = \min_{g \neq 0} R^{-s}(g). \tag{4.6.24}$$

From Corollary 4.6.2 and Lemma 4.6.9, we have

Corollary 4.6.3. *The following conditions are equivalent for a signed graph (Γ, s).*

1. *(Γ, s) is balanced.*
2. *s is switching equivalent to the positive sign function.*
3. $$\lambda_1 = 0. \tag{4.6.25}$$

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Similar to Corollaries 4.6.2 and 4.6.3, we have

Corollary 4.6.4. *There exists a function g with $R^{-s}(g) = 0$ precisely if s is antibalanced.*

The following conditions are equivalent for a signed graph (Γ, s).

1. *(Γ, s) is antibalanced.*
2. *s is switching equivalent to the negative sign function.*
3. $$\lambda_N = 2. \tag{4.6.26}$$

We shall now describe a relation, established in [30], between the spectrum of a 2-covering of a graph and that of a signed graph associated to that covering.

Let Γ be a finite graph with vertex set V, again unweighted, not out of necessity, but for simplicity. Let Γ' be an isomorphic copy of Γ, with vertex v' of Γ' corresponding to vertex v of Γ. For the construction of a 2-covering $\hat{\Gamma}$ of Γ, we can take the union of V and V', and for each pair $u \sim v$ of neighbors in Γ (and $u' \sim v'$ then are neighbors in Γ'), we either connect u and v and hence also u' and v' also in $\hat{\Gamma}$ (parallel connections), or we connect u with v' and v with u' (cross connections). When Γ has N vertices, there are 2^N different possible choices and hence that many different such 2-coverings. In Figure 4.24, we only have parallel connections whereas in Figure 4.25, some of them are replaced by cross connections.

In Figure 4.25, the covering graph is connected.

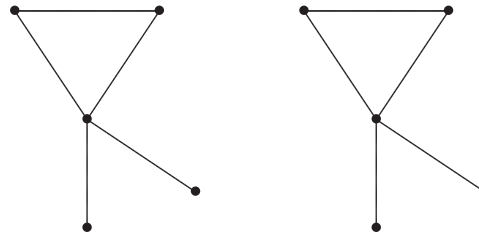


Figure 4.24 Only parallel connections.

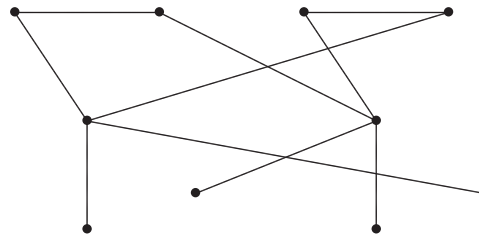


Figure 4.25 Parallel and cross connections.

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Theorem 4.6.1. *The spectrum of* $\hat{\Gamma}$ *is the union of the spectrum of* Γ *and that of the signed graph* (Γ, s) *obtained from* Γ *by assigning—to precisely those edges that are replaced by cross connections*.

In Figure 4.26, this is shown for the example of Figure 4.25.

Proof The operation $\tau\colon V \to V', \tau(v) = v', \tau(v') = v$ for all v, v' induces an automorphism of $\hat{\Gamma}$. As in Section 2.7, we have symmetric and antisymmetric eigenfunctions. The symmetric ones are obtained by taking an eigenfunction f of Γ and putting $f(v') = f(v)$ for all v, v'. This is an eigenfunction of $\hat{\Gamma}$ because if u is connected with v' instead of v, the value of $\Delta f(u)$ does not change.

Likewise, if g is an eigenfunction of (Γ, s), that is,

$$\Delta^s g(v) = g(v) - \frac{1}{\deg v} \sum_{u \sim v} s(uv) g(u) = \lambda g(v),$$

then putting $g(v') = -g(v)$ for all v, v' yields an antisymmetric eigenfunction. □

For instance, identifying v_i and v_i' for $i = 0, 1, 2$ in Figure 4.27 yields a 2-cover of the triangle, and therefore, also a book graph with an even number of pages is a 2-cover of a petal graph. Hence, by Theorem 4.6.1 and a generalization of the spectral analysis of (Figure 4.23), the spectrum of such a book

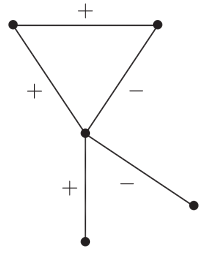


Figure 4.26 An illustration of Theorem 4.6.1.

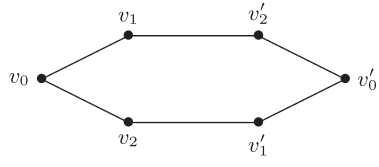


Figure 4.27 A special book graph illustrating the application of Theorem 4.6.1.

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graph is obtained from that of the petal graph. It thus consists of the eigenvalues $0, 1/2, 3/2, 2$, as directly determined before Theorem 4.1.2.

Finally, we want to discuss Cheeger constants of signed graphs. Following [11], the constructions and estimates of Section 4.4 and Chapter 8 can be unified by introducing a signed Cheeger constant. For that purpose, let $E^+(V_1, V_2)$ the positively signed and $E^-(V_1, V_2)$ the negatively signed edges between $V_1, V_2 \subset V$. We assume that V_1 and V_2 are not both empty. The *signed Cheeger constant* of the signed graph (Γ, s) then is

$$h^s(\Gamma) := \min_{V_1, V_2} \frac{2|E^+(V_1,V_2)| + 2|E^-(V_1,V_1)| + 2|E^-(V_2,V_2)| + |E(V_1 \cup V_2, \overline{V_1 \cup V_2})|)}{\mathrm{vol}(V_1) + \mathrm{vol}(V_2)}. \tag{4.6.27}$$

With the techniques of the proofs of Theorems 4.3.1 and 4.4.1, one can obtain

Theorem 4.6.2. *The smallest eigenvalue of the signed Laplacian Δ^s of the signed graph (Γ, s) satisfies*

$$1 - \sqrt{1 - (h^s)^2} \leq \lambda_1 \leq 2h^s. \tag{4.6.28}$$

Of course, when the graph is balanced, then by Corollary 4.6.3, $\lambda_1 = 0$, and consequently, also $h^s(\Gamma) = 0$. We can then find vertex sets V_1, V_2 with $V_1 \cup V_2 = V, |E^+(V_1, V_2)| = |E^-(V_1, V_1)| = |E^-(V_2, V_2) = 0$. For instance, when the sign function is positive on all edges, we can simply take $V_1 = V$. In particular, the signed Cheeger constant on this graph does not reduce to the ordinary Cheeger constant. It rather generalizes the constant h_1 introduced in 4.3.7.

4.7 The General Case: Directed Graphs with Arbitrary Weights

In this section, we shall briefly outline the spectral theory of directed graphs with arbitrary real edge weights. In particular, we also allow the weights to be negative. We do not develop the theory in detail, however, as these general structures will not come up in the rest of the book, except for Chapter 12.

For a directed graph, the spectrum in general is no longer real, and in this book, we only investigate real spectra. As already indicated, there is one exception, the nonbacktracking Laplacian treated in Chapter 12. This Laplacian can be seen as a Laplacian of a directed graph and therefore typically will also possess nonreal eigenvalues. A general spectral theory of Laplacians has been

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developed by Bauer [23], and we shall reproduce here only the basic setting of that theory, referring to [23] for deeper results and to [25, 26] for applications for the synchronization of dynamical networks. The reader should be alerted that we do not adopt all the conventions of [23]. For instance, there the Laplacian is defined in terms of incoming edges at a node, but here, we use the outgoing edges. The two different versions are of course formally completely analogous.

In this section, $\Gamma = (V, E, w)$ is a weighted directed graph on N vertices. The weight function $w\colon V \times V \to \mathbb{R}$ is not assumed to be symmetric and can take arbitrary real values. A directed edge from v to v' is denoted by $e = (v, v') \in E$. $w_{vv'}$ is the weight of $e = (v, v')$. $w_{vv'} = 0$ if and only if $e = (v, v') \notin E$. And Γ is undirected precisely if $w_{vv'} = w_{v'v}$ for all v, v'. $W := (w_{vv'})$ is the *weighted adjacency matrix*. A path from v to v' is a sequence of directed edges $(v, v_1), (v_1, v_2), \ldots, (v_k, j)$, that is, if one gets from v to v' along a sequence of directed edges.

The in-degree and the out-degree of vertex v are defined as

$$\deg_{\text{in}} v := \sum_{v'} w_{v'v} \quad \text{and } \deg_{\text{out}} v := \sum_{v'} w_{vv'}. \tag{4.7.1}$$

A graph is called *balanced* if $\deg_{\text{in}} v = \deg_{\text{out}} v$ for all $v \in V$. Obviously, undirected graphs are balanced.

Definition 4.7.1. The vertex v is a *dead end* if $w_{vv'} = 0$ for all $v' \in V$. The vertex v is *ambiguous* if $\deg_{\text{out}} v = \sum_{v'} w_{vv'} = 0$.

Every dead-end vertex is ambiguous, but not vice versa because we are allowing for both positive and negative weights.

Definition 4.7.2. A directed graph Γ is *weakly connected* if for any pair of distinct vertices v and v', there is a path from v to v' or from v' to v in Γ. A directed graph Γ is *strongly connected* if for any pair of distinct vertices v and v', there exist both a path from v to v' and one from v' to v.

Strongly connected graphs are weakly connected, but the converse need not hold. But for undirected graphs, the two notions coincide.

Definition 4.7.3. The *normalized graph Laplacian* for a directed graph Γ operates on a function $f\colon V \to \mathbb{C}$ via

$$\Delta f(v) := \begin{cases} f(v) - \frac{1}{\deg_{\text{out}} v} \sum_{v'} w_{vv'} f(v') & \text{if } \deg_{\text{out}} v \neq 0. \\ 0 & \text{else.} \end{cases} \tag{4.7.2}$$

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The *algebraic graph Laplacian* operates via

$$\Lambda f(v) \coloneqq (\deg_{\text{out}} v)\, f(v) - \sum_{v'} w_{vv'} f(v') \tag{4.7.3}$$

In the rest of this section, we shall only treat the normalized Laplacian Δ, although Λ enjoys similar results.

If $\deg_{\text{out}} v \neq 0$ for all $v \in V$, then Δ is given by

$$\Delta = \mathrm{Id} - D^{-1}W,$$

where D is the diagonal matrix of vertex out-degrees, and W is the weighted adjacency matrix of the graph Γ. When restricted to undirected graphs with non-negative weights, Definition 4.7.3 reduces to the definitions given earlier in (4.1.2), (4.1.20), (4.1.33), and (4.1.35).

Let $V_R \subseteq V$ be the set of all vertices that are not ambiguous. We can define the reduced Laplacian Δ_R on V_R as

$$\Delta_R = \mathrm{Id}_R - D_R^{-1} W_R,$$

where the subscript R simply denotes the restriction to V_R.

Every graph that is not strongly connected can be decomposed into its strongly connected components. We observe that if Γ_k and Γ_ℓ are two different strongly connected components, then there can exist directed edges between them in only one direction. Namely, if there were both a directed edge from a vertex $v_k \in \Gamma_k$ to a vertex $v_\ell \in \Gamma_\ell$, and one from $w_\ell \in \Gamma_\ell$ to $w_k \in \Gamma_k$, then $\Gamma_k \cup \Gamma_\ell$ would also be strongly connected.

Therefore, using this decomposition, after a permutation of the vertices, the Laplacian Δ can then be written in the Frobenius normal form

$$\Delta = \begin{pmatrix} \Delta_1 & \Delta_{12} & \dots & \Delta_{1r} \\ 0 & \Delta_2 & \dots & \Delta_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \Delta_r \end{pmatrix}, \tag{4.7.4}$$

where $\Delta_1, \dots \Delta_r$ are square matrices corresponding to the strongly connected components $\Gamma_1, \dots, \Gamma_r$ of Γ. The off-diagonal elements of Δ_k are of the form $\frac{w_{vv'}}{\deg_{\text{out}} v}$ for $v, v' \in \Gamma_k$, and the diagonal elements are either zero (if the out-degree of the corresponding vertex is equal to zero) or one (if it is nonzero). If Γ_k does not contain an ambiguous vertex, then Δ_k is irreducible. Furthermore, the submatrices Δ_{kl}, $1 \leq k < l \leq r$ are determined by the connectivity structure between different strongly connected components. Δ_{kl} contains all elements of the form $\frac{w_{vv'}}{\deg_{\text{out}} v}$ for $v \in \Gamma_k, v' \in \Gamma_l$. We summarize the preceding considerations in

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Lemma 4.7.1. *The spectrum of Δ consists of the eigenvalues of Δ_R and the eigenvalue 0 with multiplicity $|V \setminus V_R|$, and it is the union of the spectra of the Laplacians Δ_{Γ_i} of the strongly connected components Γ_i of Γ.*

Proof The first claim follows from (4.7.2) since $\deg_{\text{out}} = 0$ on $|V \setminus V_R|$. The second claim follows from (4.7.4) since Δ_i, $i = 1, \ldots, r$, is the Laplacian of the strongly connected component Γ_i. □

We shall now present basic spectral properties of the Laplacian Δ, following [23]. While for undirected graphs with non-negative weights, the Laplacian is self-adjoint and non-negative, and hence the eigenvalues of Δ are real and non-negative, the Laplacian considered here is neither self-adjoint nor non-negative, and thus the eigenvalues are in general complex and can have negative real parts.

Theorem 4.7.1. *(i) The Laplacian Δ has always an eigenvalue $\lambda = 0$ with eigenvector $e = (1, \ldots, 1)^\top$.*

(ii) The non-real eigenvalues of Δ appear in complex conjugate pairs.

(iii) The eigenvalues of Δ satisfy

$$\sum_{i=1}^{N} \lambda_i = \sum_{i=1}^{N} \Re(\lambda_i) = |V_R|.$$

(iv) The spectrum of Δ is invariant under multiplying all weights $w_{vv'}$ for some fixed v and all v' by a nonzero constant c. In particular, it is invariant if we multiply all weights by a nonzero constant c.

Proof *(i)* Δ has zero row sums, and so $e = (1, \ldots, 1)^\top$ is an eigenvector with eigenvalue 0.

(ii) Since Δ is a real matrix, the characteristic polynomial is given by

$$\det(\Delta - \lambda I) = a_0 + a_1\lambda + \ldots + a_{N-1}\lambda^{N-1},$$

with all $a_i \in \mathbb{R}$. Therefore, the roots occur in complex conjugate pairs.

(iii) This follows from *(ii)* and by considering the trace of Δ.

(iv) This follows from the definition of Δ and $\deg_{\text{out}}$.

□

By Lemma 4.7.1, it suffices to consider strongly connected graphs.

We shall now apply Gershgorin's circle theorem [108], formulated here as

Lemma 4.7.2. *Let $A = (a_{ij})_{i,j=1,\ldots M}$ be a matrix with entries $a_{ij} \in \mathbb{C}$ and*

$$\rho_i = \sum_{j \neq i} \left| a_{ij} \right|.$$

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Let $D(z,r)$ denote the closed disk in $\mathbb{C}$ with center z and radius r.

Then, every eigenvalue of A lies in one of the Gershgorin discs $D(a_{ii}, \rho_i)$.

Proof Let λ be an eigenvalue of A with eigenvector $x = (x^1, \dots, x^M)$. Then, for all i,

$$\sum_{j=1}^{M} a_{ij} x^j = \lambda x^i,$$

hence also

$$\sum_{j \neq i} a_{ij} x^j = (\lambda - a_{ii}) x^i.$$

We take a component x^i with the largest absolute value (which is $\neq 0$, as an eigenvector cannot vanish identically). Thus, $|x^j| \leq |x^i|$ for all j, and

$$|\lambda - a_{ii}| = \left| \sum_{j \neq i} \frac{a_{ij} x^j}{x^i} \right| \leq \sum_{j \neq i} \left| \frac{a_{ij} x^j}{x^i} \right| \leq \sum_{j \neq i} \left| a_{ij} \right| = R_i.$$

□

Theorem 4.7.2. *Let $V_{R,1}, \dots, V_{R,r}$ be the strongly connected components of the induced subgraph Γ_R with vertex set V_R. In our formulas, we put $\frac{1}{|\deg_{\text{out}} v|} = 0$ when $\deg_{\text{out}} v = 0$.*

The spectrum of Δ then satisfies

$$\sigma(\Delta) \subseteq D(1, \rho_1) \cup \{0\} \subseteq D(1, \rho_2) \cup \{0\} \subseteq D(1, \rho) \cup \{0\},$$

where $D(1,r)$ is the closed disk in the complex plane with center 1 and radius r, and

$$\rho_1 := \max_{i=1,\dots,r} \max_{v \in V_{R,i}} \frac{\sum_{v' \in V_{R,i}} |w_{vv'}|}{|\deg_{\text{out}} v|}$$

$$\rho_2 := \max_{v \in V_R} \frac{\sum_{v' \in V_R} |w_{vv'}|}{|\deg_{\text{out}} v|}$$

$$\rho := \max_{v \in V} \rho(v) := \max_{v \in V} \frac{\sum_{v' \in V} |w_{vv'}|}{|\deg_{\text{out}} v|}.$$

Proof $\rho_1 \leq \rho_2 \leq \rho$ and the proof follows from Lemmas 4.7.2 and 4.7.1. □

For undirected graphs with non-negative weights, Theorem 4.7.2 reduces to (4.1.51).

The radius ρ in Theorem 4.7.2 is ≥ 1 if and only if there is at least one vertex that is not ambiguous. And if no vertex is ambiguous, then $\rho = 1$ if and only if for every vertex v the weights $w_{vv'}$ have the same sign for all v'.

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From this observation and Theorem 4.7.1 (iv), we conclude that if Γ is a graph without ambiguous vertices, that is, $V_R = V$, and with $\rho = 1$, then the graph Γ^+ where we have replaced all weights by their absolute values $|w_{vv'}|$ has the same spectrum as Γ.

Corollary 4.7.1. *The nonzero eigenvalues of* Δ *satisfy*

$$1 - \rho \leq \min_{i\colon \lambda_i \neq 0} \Re(\lambda_i) \leq \frac{|V_R|}{N - m_0} \leq \max_{i\colon \lambda_i \neq 0} \Re(\lambda_i) \leq 1 + \rho, \tag{4.7.5}$$

where m_0 *is the multiplicity of the eigenvalue* 0. *In particular,*

$$1 \leq \max_{i\colon \lambda_i \neq 0} \Re(\lambda_i).$$

Proof The estimates follow from Theorem 4.7.1 (iii) and Theorem 4.7.2 and the fact that $N - m_0 \leq |V_R|$. □

4.8 Simplicial Complexes

We return to symmetric operators.

For a simplicial complex, the multiplicities of the eigenvalue 0 of the Laplacians L^q contain topological information. This is the content of Eckmann's Theorem [86], which is a discrete version of the Hodge theorem.

Theorem 4.8.1. *For a simplicial complex* Σ,

$$\ker L^q(\Sigma) \cong H^q(\Sigma).$$

Thus, the multiplicity of the eigenvalue 0 *of the operator* $L^q(\Sigma)$ *is equal to the Betti number* b_q, *the dimension of* $H^q(\Sigma)$.

Proof By (2.5.15),

$$\begin{aligned} \ker L^q(\Sigma) &= \ker \delta^q \cap \ker \delta^{q-1^*} \\ &= \ker \delta^q \cap (\operatorname{im} \delta^{q-1})^{\perp} \\ &\cong H^q(\Sigma, \mathbb{R}). \end{aligned} \tag{4.8.1}$$

□

Corollary 4.8.1.

$$C^q = \operatorname{im} \delta^{q-1} \oplus \operatorname{im} (\delta^q)^* \oplus \ker L^q. \tag{4.8.2}$$

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Proof This follows from (2.5.6) and (4.8.1). □

While cohomology groups are defined as quotients, that is, as equivalence classes of elements of C^q, Theorem 4.8.1 provides us with concrete representatives in C^q of those equivalence classes, the so-called *harmonic cocycles*.

We note that Eckmann's Theorem does not depend on the choice of scalar products on the spaces C^q (although the harmonic cocycles do). That theorem is concerned with the eigenvalue 0 of the Laplacian. We shall now investigate the non zero part of the spectrum.

Since $\delta^q \delta^{q-1} = 0$ and $\delta^{q-1^*} \delta^{q^*} = 0$ (recall (2.5.2)),

$$\operatorname{im} L^q_{down}(\Sigma) \subset \ker L^q_{up}(\Sigma), \tag{4.8.3}$$

$$\operatorname{im} L^q_{up}(\Sigma) \subset \ker L^q_{down}(\Sigma). \tag{4.8.4}$$

Therefore, λ is a nonzero eigenvalue of $L_i(\Sigma)$ if and only if it is a nonzero eigenvalue of either $L^q_{up}(\Sigma)$ or $L^q_{down}(\Sigma)$. Therefore, the nonzero parts of the spectra satisfy

$$\operatorname{spec}_{\neq 0}(L^q(\Sigma)) = \operatorname{spec}_{\neq 0}(L_i^{up}(\Sigma)) \cup \operatorname{spec}_{\neq 0}(L_i^{down}(\Sigma)). \tag{4.8.5}$$

The multiplicity of the eigenvalue 0 may be different, however.

Since $\operatorname{spec}_{\neq 0}(AB) = \operatorname{spec}_{\neq 0}(BA)$, for linear operators A and B on Hilbert spaces, we get the following equality.

$$\operatorname{spec}_{\neq 0}(L^q_{up}(\Sigma)) = \operatorname{spec}_{\neq 0}(L^{q+1}_{down}(\Sigma)). \tag{4.8.6}$$

From (4.8.5) and (4.8.6), we conclude that each of the three families of multisets

$$\{\operatorname{spec}_{\neq 0}(L^q(\Sigma)) \mid 0 \leq q \leq m\}, \{\operatorname{spec}_{\neq 0}(L^q_{up}(\Sigma)) \mid 0 \leq q \leq m-1\}$$

$$\text{or } \{\operatorname{spec}_{\neq 0}(L^q_{down}(\Sigma)) \mid 1 \leq q \leq m\}$$

determines the other two. Therefore, it suffices to consider only one of them. In the sequel, we shall often omit the argument Σ from our Laplace operators.

We now apply the constructions of Section 4.6. This is partly based on discussions with Bobo Hua.

The results here are taken from [160]. We recall the formula (2.5.21) for the combinatorial normalized up-Laplacian of a simplicial complex Σ,

$$(L^q_{up} f)([\sigma]) = f([\sigma]) - \frac{1}{\deg \sigma} \sum_{\substack{\sigma' \in \Sigma_q \,:\, \sigma \neq \sigma', \\ \sigma, \sigma' \in \partial \rho}} w_{\sigma\sigma'} s([\sigma], [\sigma']) f([\sigma']), \tag{4.8.7}$$

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where we have put

$$w_{\sigma\sigma'} := w(\rho) \text{ for } \sigma, \sigma' \in \partial\rho,$$
$$s([\sigma],[\sigma']) := -\operatorname{sgn}([\sigma],\partial[\rho])\operatorname{sgn}([\sigma'],\partial[\rho]). \tag{4.8.8}$$

Thus, we may express L^q_{up} in terms of the Laplacian $\Delta_{(\Gamma_q,s)}$ for the signed graph (Γ_q, s) with vertex set consisting of the q-simplices of our simplicial complex, and where two different such vertices σ, σ' are connected by an edge, $\sigma \sim \sigma'$, if there exists a $(q+1)$-simplex ρ in Σ with $\sigma, \sigma' \in \partial\rho$. For instance, when we have a 2-simplex, then the signed graph corresponding to its three boundary edges is given in Figure 4.17, and when we have two adjacent 2-simplices, we get that in Figure 4.18.

Theorem 4.8.2.

$$L^q_{up} = (q+1)\Delta_{(\Gamma_q,s)} - q\,\mathrm{Id}. \tag{4.8.9}$$

Proof In order to get that relation, we have to observe that

$$\sum_{\substack{\sigma'\in\Sigma_q:\,\sigma\neq\sigma',\\ \sigma,\sigma'\in\partial\rho}} w_{\sigma\sigma'} = (q+1)\deg\sigma, \tag{4.8.10}$$

since according to (2.5.19)

$$\deg\sigma = \sum_{\rho\in\Sigma_{q+1}(\Sigma):\,\sigma\in\partial\rho} w(\rho), \tag{4.8.11}$$

and each such ρ has $q+1$ other facets σ'. Hence,

$$\begin{aligned}(L^q_{up}f)([\sigma]) &= \sum_{\substack{\sigma'\in\Sigma_q:\,\sigma\neq\sigma',\\ \sigma,\sigma'\in\partial\rho}} \frac{w_{\sigma\sigma'}}{\deg\sigma}(f([\sigma]) - s([\sigma],[\sigma'])f([\sigma'])) - qf([\sigma])\\ &= (q+1)\Delta_{(\Gamma_q,s)}f([\sigma]) - qf([\sigma]).\end{aligned}$$

□

Remark 4.8.1. The condition (2.5.20) is set up in such a way that it simplifies the up-Laplacian (2.5.17) by making the coefficient of $f([\sigma])$ equal to 1 in (2.5.21). This allows us to derive the relation (4.8.9). Since (2.5.20) does not lead to such a simplification for the down-Laplacian (2.5.18), we do not have a corresponding formula for the down-Laplacian. That would only be obtained if instead of (2.5.20), we had required that the weight of a simplex be equal to the sum of the weights of its facets. Since, however, we already know from (4.8.6) that the nonzero eigenvalues of the down-Laplacians coincide with those of the up-Laplacians, we can concentrate on the latter for investigating the spectra of simplicial complexes.

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By Theorem 4.8.2, the eigenvalues μ_j of L^q_{up} and the eigenvalues λ_j of $\Delta_{(\Gamma_q,s)}$ are related by

$$\mu_j = (q+1)\lambda_j - q. \tag{4.8.12}$$

and we obtain

Corollary 4.8.2. *The eigenvalues of L^q_{up} lie in the interval $[0, q+2]$.*

Proof The eigenvalues are non-negative because L^q_{up} is a non-negative operator, see (2.5.10). The upper bound follows from (4.8.9) and the fact that the spectrum of $\Delta_{(\Gamma_q,s)}$ is contained in the interval $[0,2]$, see (4.6.21). □

Corollary 4.8.3. *The eigenvalues of $\Delta_{(\Gamma_q,s)}$ are $\geq \frac{q}{q+1}$. Equality holds if and only if there is some nontrivial f with $\partial^q f = 0$. More precisely, the multiplicity of the eigenvalue $\frac{q}{q+1}$ of $\Delta_{(\Gamma_q,s)}$ equals the dimension of the kernel of the coboundary operator δ^q.*

In particular, for $q > 0$, the graph (Γ_q, s) is never balanced.

The geometric intuition for the last statement can be seen in Figure 4.17, which is the signed graph corresponding to the boundary of a 2-simplex. More generally, when Γ_q comes from the boundary of a single $(q+1)$-simplex, then it is the complete graph with $q+1$ vertices and a $-$ sign on every edge.

Proof The inequality follows again from (4.8.9) and the fact that L^q_{up} is a non-negative operator, that is, all its eigenvalues are non-negative. The equality case is handled in Corollary 2.5.2. The last claim follows from Corollary 4.6.4. □

Later, we shall study the eigenvalues of L^q_{up}, and the results are taken from [138, 160].

We now try to characterize those simplicial complexes where the spectrum of L^q_{up} contains the maximal value $q+2$, following [138]. As before, we use (4.8.9). According to Corollary 4.6.4 or the proof of Corollary 4.6.1, the dual-signed Rayleigh quotient (4.6.20) of $\Delta_{(\Gamma_q,s)}$ must assume the value 0, and for that, we need some function g with (in the notation employed in (4.6.20))

$$g(v) = -s(vv')g(v') \text{ for any pair } v \sim v'. \tag{4.8.13}$$

In the notation currently employed, see (4.8.7) and (4.8.8), this means that we need

$$\operatorname{sgn}([\sigma], \partial[\rho]) f(\sigma) = \operatorname{sgn}([\sigma'], \partial[\rho]) f(\sigma') \tag{4.8.14}$$

whenever σ, σ' are different facets of some ρ. We may then assume that $f(\sigma) = \pm 1$ for all σ, that is, f assigns an orientation to every σ. We observe

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Lemma 4.8.1. *The existence of a function f satisfying (4.8.14) means that there exists an orientation on the $(q+1)$-simplices of Σ for which any two $(q+1)$-simplices intersecting in a common q-face induce the same orientation on the intersecting simplex.*

□

Definition 4.8.1. A pure simplicial complex of dimension p is called a *p-path of length m* if and only if there is an ordering of its p-simplices $\rho_1, \rho_2 \ldots \rho_m$, such that ρ_i and ρ_j are $(p-1)$-down neighbors, that is, share a facet, if and only if $\mid j - l \mid = 1$. When ρ_m coincides with ρ_1, we speak of a *q-circuit* of length $(m-1)$.

We say that a path or circuit is *orientable* if and only if it is possible to assign an orientation to all its p-simplices in such a way that any two simplices that intersect in an $(p-1)$-face induce a different orientation on that face. We say that such simplices are oriented *coherently*.

Note that some or all the p-simplices of a path or circuit could intersect in some simplices of dimension $\leq p-2$.

A graph possesses the eigenvalue 2 if and only if it is bipartite, that is, does not contain cycles of odd length; see Lemma 4.1.11. The following is the higher-dimensional generalization of this fact [138].

Theorem 4.8.3. *For a q-connected (that is, any two q-simplices can be connected by a path) simplicial complex Σ, the following statements are equivalent*

1. *The spectrum of L^q_{up} contains the eigenvalue $q+2$.*
2. *There are no $(q+1)$-orientable circuits of odd length nor $(q+1)$-nonorientable circuits of even length in Σ.*

Proof (1) $\Rightarrow$ (2) proceeds by contradiction: Assume that there exists a $(q+1)$-orientable circuit of odd length, whose q-simplices $\sigma_1, \ldots, \sigma_{2n+1}$ are ordered increasingly, as suggested in Definition 4.8.1. Then, it is possible to orient these simplices in such a way that every two neighboring simplices induce different orientations on their intersecting face. Denote these oriented simplices by $[\sigma_1], \ldots, [\sigma_{2n+1}]$. In order to have the same orientation induced on the intersecting face, we reverse the orientation of every simplex $[\sigma_k]$, for k even. Thus, $[\sigma_l]$ and $-[\sigma_{l+1}]$ induce the same orientation on $[\sigma_l \cap \sigma_{l+1}]$, for every $1 \leq l \leq 2n$. However, $[\sigma_1]$ and $[\sigma_{2n+1}]$ remain coherently oriented, which contradicts Lemma 4.8.1. The analysis for the case of $(q+1)$-nonorientable circuits is analogous.

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(2) $\Rightarrow$ (1): Let σ_1 be an arbitrary $(q+1)$-face of Σ. Consider its positive orientation $[\sigma_1]$ and call it an *initial* oriented face. Let $[\sigma_{i_1 i_2 \ldots i_n}]$ be a $(q+1)$-face of Σ which shares a q-face with $[\sigma_{i_1 i_2 \ldots i_{n-1}}]$, and both faces induce the same orientation on their intersecting face. Now, assume the opposite: The eigenvalue $q+2$ is not in the spectrum, that is, it is not possible to choose an orientation on the $(q+1)$-faces of Σ satisfying the conditions of Lemma 4.8.1. This means that after some number of steps in the construction earlier, two faces $[\sigma_{i_1 i_2 \ldots i_n}]$, $[\sigma_{i_1 i_2 \ldots i_m}]$, which are the same but differently oriented are obtained. Obviously, there exists a circuit containing $[\sigma_{i_1 i_2 \ldots i_n}]$ which does not admit an orientation as in Lemma 4.8.1. This is possible only in the case when a circuit is orientable and odd or nonorientable and even. This is a contradiction; hence, $q+2$ is contained in the spectrum. □

As a supplement of Theorem 4.8.3, we have:

Proposition 4.8.1. *The spectrum of L^q_{up} contains the eigenvalue $q+2$ if and only if the signed graph (Γ_q, s) has an antibalanced component. Moreover, the multiplicity of $q+2$ equals the number of antibalanced components of (Γ_q, s).*

We consider the opposite $(\Gamma_q, -s)$ of the signed graph (Γ_q, s), and we simply use $\Delta_{(\Gamma_q,-s)}$ to denote the Laplacian for the signed graph $(\Gamma_q, -s)$. Then, the eigenvalues of the three Laplacians L^q_{up}, $\Delta_{(\Gamma_q,s)}$ and $\Delta_{(\Gamma_q,-s)}$ satisfy the relation:

Spectrum of L^q_{up}		Spectrum of $\Delta_{(\Gamma_q,s)}$		Spectrum of $\Delta_{(\Gamma_q,-s)}$
0		$\frac{q}{q+1}$		$\frac{q+2}{q+1}$
$\vdots$		$\vdots$		$\vdots$
λ	$\Longleftrightarrow$	$\frac{\lambda+q}{q+1}$	$\Longleftrightarrow$	$\frac{q+2-\lambda}{q+1}$
$\vdots$		$\vdots$		$\vdots$
$q+2$		2		0

that is, λ is an eigenvalue of L^q_{up} if and only if $\frac{\lambda+q}{q+1}$ is an eigenvalue of $\Delta_{(\Gamma_q,s)}$ if and only if $\frac{q+2-\lambda}{q+1}$ is an eigenvalue of $\Delta_{(\Gamma_q,-s)}$.

In addition, the multiplicity of the eigenvalue 0 of L^q_{up} is larger than or equal to $q+1$ (when the simplicial complex is pure, the multiplicity of the eigenvalue 0 of L^q_{up} is $q+1$ if and only if the simplicial complex is a simplex of dimension $q+1$). And, the multiplicity of the eigenvalue $q+2$ of L^q_{up} agrees with the number of balanced components of $\Delta_{(\Gamma_q,-s)}$.

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4.9 Oriented Hypergraphs

We consider an (oriented) hypergraph $\Gamma = (V, E, \varphi)$, as defined in Section 2.4.3, and we assume that it has no isolated vertices, that is, all vertices have degree > 0. We let $v_1, \dots, v_N$ denote its vertices and we let $e_1, \dots, e_M$ denote its hyperedges. We recall, from Section 2.5.4, that the Laplacian L^0 is the operator

$$L^0 \colon \{f \colon V \to \mathbb{R}\} \to \{f \colon V \to \mathbb{R}\}$$

such that, given $f \colon V \to \mathbb{R}$ and $v \in V$,

$$L^0 f(v) = \frac{\sum_{e_{\text{in}} \colon v \text{ input}} \left(\sum_{v' \text{ input of } e_{\text{in}}} f(v') - \sum_{z' \text{ output of } e_{\text{in}}} f(z') \right)}{\deg v} - \frac{\sum_{e_{\text{out}} \colon v \text{ output}} \left(\sum_{\hat{v} \text{ input of } e_{\text{out}}} f(\hat{v}) - \sum_{\hat{z} \text{ output of } e_{\text{out}}} f(\hat{z}) \right)}{\deg v}.$$

Similarly, the Laplacian L^1 is the operator

$$L^1 \colon \{\gamma \colon E \to \mathbb{R}\} \to \{\gamma \colon E \to \mathbb{R}\}$$

such that, given $\gamma \colon E \to \mathbb{R}$ and $e \in E$,

$$L^1 \gamma(e) = \sum_{v_i \text{ input of } e} \frac{\sum_{e_{\text{in}} \colon v_i \text{ input}} \gamma(e_{\text{in}}) - \sum_{e_{\text{out}} \colon v_i \text{ output}} \gamma(e_{\text{out}})}{\deg v_i} - \sum_{v^j \text{ output of } e} \frac{\sum_{e'_{\text{in}} \colon v^j \text{ input}} \gamma(e'_{\text{in}}) - \sum_{e'_{\text{out}} \colon v^j \text{ output}} \gamma(e'_{\text{out}})}{\deg v^j}.$$

We want to consider the matrix formulations of L^0 and L^1. We need some preliminary definitions:

Definition 4.9.1. The *degree matrix* of Γ is the $N \times N$ diagonal matrix

$$D \coloneqq \operatorname{diag}(\deg v_1, \dots, \deg v_N). \tag{4.9.1}$$

The *incidence matrix* of Γ is the $N \times M$ matrix $\mathcal{I} \coloneqq (\varphi(v_i, e_j))_{ij}$.

Given a hyperedge $e \in E$, we say that two vertices v_i and v_j are *co-oriented in* e if

$$\varphi(v_i, e) = \varphi(v_j, e) \neq 0.$$

We say that v_i and v_j are *antioriented in* e if

$$\varphi(v_i, e) = -\varphi(v_j, e) \neq 0.$$

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The *adjacency matrix* of Γ is the $N \times N$ matrix $A := (A_{ij})_{ij}$, where $A_{ii} := 0$ for each $i = 1, \dots, N$ and, for $i \neq j$,

$$A_{ij} := \Big|\{\text{hyperedges in which } v_i \text{ and } v_j \text{ are antioriented}\}\Big| - \Big|\{\text{hyperedges in which } v_i \text{ and } v_j \text{ are co-oriented}\}\Big|.$$

The above matrices allow us to write

$$L^0 = \mathrm{Id} - D^{-1}A = D^{-1}\mathcal{I}\mathcal{I}^\top$$

and

$$L^1 = \mathcal{I}^\top D^{-1}\mathcal{I},$$

in a matrix form. Moreover, we can also write

$$L^0 f(v_i) = f(v_i) - \frac{1}{\deg v_i} \sum_{j \neq i} A_{ij} f(v_j),$$

for a given function $f : V \to \mathbb{R}$ and a vertex v_i.

Remark 4.9.1. We make an important observation. When we consider an oriented hypergraph, if a vertex v belongs to a hyperedge e, then v is either an input or an output for e but not both. This is true also if e is a self-loop, that is, it contains only v. On the other hand, when we consider a self-loop $e = \{v\}$ in Section 4.1, that is, in the case of graphs, the vertex v is treated both as input and as output of e. Therefore, self-loops in this chapter are conceptually different, and, as a consequence, also the Laplacians are different. In particular, while in the context of Section 4.1, the Laplacian matrix L^0 does not only have 1's in the diagonal in the presence of self-loops, the Laplacian L^0 for oriented hypergraphs always has only 1's in the diagonal.

Our aim is to investigate the spectral properties of L^0 (and L^1) and to understand, in particular, which spectral properties from Section 4.1 can be generalized to the hypergraph case and how. We start with the following lemma, which generalizes part of Lemma 4.1.7.

Lemma 4.9.1. *The Laplacians L^0 and L^1 are self-adjoint and non-negative operators. Hence, in particular, their eigenvalues are real and non-negative.*

Proof By the construction in Section 2.5.4, L^0 and L^1 are the two compositions of δ and δ^*, which are adjoint to each other. Therefore, they are both self-adjoint, which implies that their eigenvalues are real.

Moreover, given $f : V \to \mathbb{R}$,

$$(L^0 f, f)_V = (\delta^* \delta f, f)_V = (\delta f, \delta f)_E \geq 0.$$

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Analogously, for $\gamma\colon E \to \mathbb{R}$,

$$(L^1\gamma,\gamma)_E = (\delta\delta^*\gamma,\gamma)_E = (\delta^*\gamma,\delta^*\gamma)_V \geq 0.$$

Hence, L^0 and L^1 are non-negative operators. In particular, this implies that their eigenvalues are non-negative.

□

Now, as for the graph case, we order the eigenvalues of L^0 as

$$\lambda_1 \leq \ldots \leq \lambda_N$$

and we observe that they always sum to N, since the trace of $L^0 = \mathrm{Id} - D^{-1}A$ is clearly N. Using the min–max principle (Theorem 2.6.1) and the construction of L^0 and L^1 in Section 2.5.4, we can characterize these eigenvalues using the following Rayleigh quotients.

Definition 4.9.2. The *Rayleigh quotient* of $f\colon V \to \mathbb{R}$ with respect to Γ is

$$\begin{aligned} R(f) &:= \frac{(\delta f,\delta f)_E}{(f,f)_V} \\ &= \frac{\sum_{e\in E}\left(\sum_{v_i \text{ input of } e} f(v_i) - \sum_{v^j \text{ output of } e} f(v^j)\right)^2}{\sum_{v\in V} \deg v\, f(v)^2}. \end{aligned}$$

Similarly, the *Rayleigh quotient* of $\gamma\colon E \to \mathbb{R}$ with respect to Γ is

$$\begin{aligned} R(\gamma) &:= \frac{(\delta^*\gamma,\delta^*\gamma)_V}{(\gamma,\gamma)_E} \\ &= \frac{\sum_{v\in V} \frac{1}{\deg v} \cdot \left(\sum_{e_{\text{in}}\colon v \text{ input}} \gamma(e_{\text{in}}) - \sum_{e_{\text{out}}\colon v \text{ output}} \gamma(e_{\text{out}})\right)^2}{\sum_{e\in E} \gamma(e)^2}. \end{aligned}$$

Lemma 4.9.2. *The nonzero eigenvalues of L^0 and L^1 are the same, counted with multiplicity. Moreover, the N eigenvalues of L^0 can be characterized, by the min–max principle, via the Rayleigh quotients $R(f)$ of functions $f\colon V \to \mathbb{R}$. Similarly, the M eigenvalues of L^1 can be characterized, by the min–max principle, via the Rayleigh quotients $R(\gamma)$ of functions $\gamma\colon E \to \mathbb{R}$.*

In particular,

$$\lambda_1 = \min_{f\colon V\to\mathbb{R},\, f\neq\mathbf{0}} R(f)$$

and

$$\lambda_N = \max_{f\colon V\to\mathbb{R}} R(f) = \max_{\gamma\colon E\to\mathbb{R}} R(\gamma).$$

Proof It follows from the construction of L^0 and L^1 in Section 2.5.4. □

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From here on, following the usual notation, we let $\Delta := L^0$.

Next, we consider some examples of hypergraphs for which we compute the spectrum. As a consequence, we will see that several properties from Section 4.1 that hold for the spectra of graphs do not hold for the general case.

Example 4.9.1. Let $\Gamma = (V, E, \varphi)$ with $V = \{v_1, \dots, v_N\}$ and $E = \{\{v_1\}, \dots, \{v_N\}\}$, that is, the vertices are only contained in self-loops. Then, $\Delta = \mathrm{Id}$, implying that 1 is the only eigenvalue in this case.

Example 4.9.2. Assume that $\Gamma = (V, E, \varphi)$ has only one hyperedge, and this contains all vertices as inputs. Then, the Laplacian Δ can be seen as the matrix whose entries are all equal to 1, implying that a nonzero function $f : V \to \mathbb{R}$ is an eigenfunction with eigenvalue λ if and only if

$$f(v_i) = \sum_{j=1}^{N} f(v_j), \quad \forall i = 1, \dots, N.$$

Hence, N is an eigenvalue with multiplicity 1, and the corresponding eigenfunctions are constant. All other $N-1$ eigenvalues are 0, and the corresponding eigenfunctions satisfy $\sum_{j=1}^{N} f(v_j) = 0$.

The two examples above show, in particular, that the third part of Lemma 4.1.7 does no longer hold in the general case of hypergraphs. In fact, for graphs, 0 is always an eigenvalue, and its multiplicity equals the number of connected components of Γ. In the general case, there could be both cases in which 0 is not an eigenvalue (as in Example 4.9.1) and cases in which the multiplicity of 0 is higher than the number of connected components of Γ (as in Example 4.9.2). Moreover, the third part of Lemma 4.1.7 shows that, for a connected graph, the eigenfunctions of 0 are precisely the constant functions. Interestingly, for the hypergraph in Example 4.9.2, the constant functions are precisely the eigenfunctions of the only nonzero eigenvalue. The underlying reason is that, while the graph Laplacian satisfies a maximum principle, this no longer holds for the hypergraph Laplacian. As we have seen in Section 4.1, the maximum principle says that solutions of $\Delta u = 0$ on a connected graph are constant, and hence, the eigenvalue $\lambda = 0$ has multiplicity 1. On a general hypergraph, due to the possibility of the presence of co-oriented vertices in hyperedges, such a maximum principle can no longer hold for Δ on a hypergraph, and consequently, the multiplicity of $\lambda = 0$ can be different from 1.

Both Examples 4.9.1 and 4.9.2 are particular cases of complete hypergraphs:

Definition 4.9.3. A hypergraph $\Gamma = (V, E, \varphi)$ is *c-complete* if E is the set of all possible $\binom{N}{c}$ subsets of V of cardinality c.

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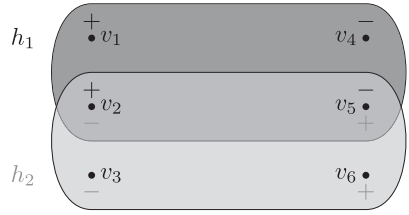


Figure 4.28 A bipartite hypergraph with $V_1 = \{v_1, v_2, v_3\}$ and $V_2 = \{v_4, v_5, v_6\}$.

Clearly, the complete graph is a 2-complete hypergraph, the hypergraph in Example 4.9.1 is 1-complete, and the one in Example 4.9.2 is N-complete.

Now, there are different ways of generalizing the notion of a bipartite graph to the case of hypergraphs. In this chapter, we consider the following definition.

Definition 4.9.4. A hypergraph $\Gamma = (V, E, \varphi)$ is *bipartite* (Figure 4.28) if one can decompose the vertex set as a disjoint union $V = V_1 \sqcup V_2$ such that, for every $e \in E$, either e has all its inputs in V_1 and all its outputs in V_2, or vice versa.

For instance, the underlying hypergraph of any hypergraph is bipartite:

Definition 4.9.5. The *underlying hypergraph* of $\Gamma = (V, E, \varphi)$ is the oriented hypergraph $\Gamma^+ := (V, E, \varphi^+)$ obtained from Γ by letting each vertex be an input for all hyperedges in which it is contained. The *signless Laplacian* of Γ, denoted Δ^+, is the Laplacian of its underlying hypergraph, that is,

$$\Delta^+(\Gamma) := \Delta(\Gamma^+).$$

Remark 4.9.2. If Γ is a simple graph, then

$$\Delta(\Gamma) = \mathrm{Id} - D(\Gamma)^{-1} A(\Gamma)$$

and

$$\Delta^+(\Gamma) = \Delta(\Gamma^+) = \mathrm{Id} + D(\Gamma)^{-1} A(\Gamma) = 2 \cdot \mathrm{Id} - \Delta(\Gamma).$$

Therefore, λ is an eigenvalue for Δ if and only if $2 - \lambda$ is an eigenvalue for Δ^+.

For example, as a consequence of the last remark, we can equivalently reformulate Lemma 4.1.8 by saying that the spectrum of Δ^+ for the complete graph K_N consists of the eigenvalue 2 with multiplicity 1 and the eigenvalue $\frac{N-2}{N-1}$ with multiplicity $N - 1$. This can be generalized as follows.

Lemma 4.9.3. *Let Γ be a c-complete hypergraph, with $c \geq 2$. Then, the spectrum of Δ^+ is given by c, with multiplicity 1, and $\frac{N-c}{N-1}$, with multiplicity $N - 1$.*

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Proof Let Γ^+ be the underlying hypergraph of Γ, and let $A^+ \coloneqq A(\Gamma^+)$.

It is easy to see that the constant functions are eigenfunctions for $\Delta^+(\Gamma) = \Delta(\Gamma^+)$ with eigenvalue c. Now, observe that each vertex has degree $d \coloneqq \binom{N-1}{c-1}$, while $a \coloneqq A^+_{ij} = -\binom{N-2}{c-2}$ is constant for all $i \neq j$. Therefore, $\frac{a}{d} = -\frac{c-1}{N-1}$ and

$$\Delta^+ f(v) = f(v) - \frac{a}{d}\left(\sum_{v' \neq v} f(v')\right) = f(v) + \frac{c-1}{N-1}\left(\sum_{v' \neq v} f(v')\right),$$

for all $v \in V$.

For each $i = 2, \dots, N$, let $f_i(v_1) \coloneqq 1$, $f_i(v_i) \coloneqq -1$ and $f_i \coloneqq 0$ otherwise. Then,

- $\Delta^+ f_i(v_1) = 1 - \frac{c-1}{N-1} = \frac{N-c}{N-1} \cdot f_i(v_1)$,
- $\Delta^+ f_i(v_i) = -1 + \frac{c-1}{N-1} = \frac{N-c}{N-1} \cdot f_i(v_i)$, and
- $\Delta^+ f_i(v_j) = 0 = \frac{N-c}{N-1} \cdot f_i(v_j)$ for all $j \neq 1, i$.

Therefore, the f_i's are $N-1$ linearly independent eigenfunctions with eigenvalue $\frac{N-c}{N-1}$. □

We now prove that the spectrum of a bipartite hypergraph coincides with the spectrum of its underlying hypergraph.

Proposition 4.9.1. *If Γ is bipartite, it is isospectral to its underlying hypergraph; therefore, in particular, also to every other bipartite hypergraph that has the same underlying hypergraph as Γ.*

Proof Since Γ is bipartite, up to switching (without loss of generality) the orientations of some hyperedges, we can assume that all the inputs are in V_1 and all the outputs are in V_2, with $V = V_1 \sqcup V_2$. Furthermore, by definition of L^1, which has the same nonzero spectrum as Δ, we can move a vertex from V_1 to V_2 or vice versa by letting it be always an output or always an input without affecting the spectrum. In particular, if we move all vertices to V_1, we obtain the underlying hypergraph of Γ. □

Now, by Corollary 4.1.4, Lemmas 4.1.12, 4.1.13, and 4.1.10, we have that, if Γ is a connected graph, then

$$\frac{N}{N-1} \leq \lambda_N \leq 2, \tag{4.9.2}$$

and $\lambda_N = \frac{N}{N-1}$ if and only if Γ is complete, while $\lambda_N = 2$ if and only if Γ is bipartite. In Theorem 4.9.1, we generalize this result to the case of hypergraphs. Before that, we give the preliminary Definition 4.9.6.

Definition 4.9.6. A hypergraph $\hat{\Gamma} = (\hat{V}, \hat{E}, \hat{\varphi})$ is a *sub-hypergraph* of $\Gamma = (V, E, \varphi)$, denoted $\hat{\Gamma} \subset \Gamma$, if:

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1. $\hat{V} \subseteq V$,
2. $\hat{E} \subseteq \{e \cap \hat{V} : e \in E\}$,
3. $\hat{\varphi}(v,e) = \varphi(v,e)$ for all $v \in \hat{V}$ and $e \in \hat{E}$.

Given a sub-hypergraph $\hat{\Gamma} \subset \Gamma$, we let

$$\eta(\hat{\Gamma}) := \frac{\sum_{v \in \hat{V}} \frac{\deg_{\hat{\Gamma}}(v)^2}{\deg v}}{|\hat{E}|},$$

where $\deg_{\hat{\Gamma}}(v)$ denotes the degree of v in $\hat{\Gamma}$ and $|\hat{E}|$ is the number of hyperedges in $\hat{\Gamma}$.

Theorem 4.9.1. *For every connected hypergraph $\Gamma = (V, E, \varphi)$,*

$$\lambda_N \leq \max_{e \in E} |e|, \tag{4.9.3}$$

with equality if and only if Γ is bipartite and $|e|$ is constant for all $e \in E$, and

$$\lambda_N \geq \max_{\hat{\Gamma} \subset \Gamma \text{ bipartite}} \eta(\hat{\Gamma}). \tag{4.9.4}$$

Proof We first prove (4.9.3). Let $f : V \to \mathbb{R}$ be an eigenfunction for λ_N. Then,

$$\begin{aligned}\lambda_N &= \frac{\sum_{e \in E} \left(\sum_{v_i \text{ input of } e} f(v_i) - \sum_{v^j \text{ output of } e} f(v^j) \right)^2}{\sum_{v \in V} \deg v f(v)^2} \\ &\leq \frac{\sum_{e \in E} \left(\sum_{v \in e} |f(v)| \right)^2}{\sum_{i \in V} \deg v f(v)^2},\end{aligned}$$

with equality if and only if f has its nonzero values on a bipartite sub-hypergraph. Now, for each $e \in E$,

$$\begin{aligned}\left(\sum_{v \in e} |f(v)| \right)^2 &= \sum_{v \in e} f(v)^2 + \sum_{\{v,v'\} :\, v \neq v' \in e} 2 \cdot |f(v)| \cdot |f(v')| \\ &\leq \sum_{v \in e} f(v)^2 + \sum_{\{v,v'\} :\, v \neq v' \in e} \left(f(v)^2 + f(v')^2 \right) \\ &= \sum_{v \in e} f(v)^2 + \sum_{v \in e} (|e| - 1) f(v)^2 \\ &= |e| \cdot \sum_{v \in e} f(v)^2,\end{aligned}$$

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with equality if and only if $|f|$ is constant on all $v \in e$. Therefore,

$$\begin{aligned}\frac{\sum_{e\in E}\left(\sum_{v\in h}|f(v)|\right)^2}{\sum_{i\in V}\deg v f(v)^2} &\leq \frac{\sum_{e\in E}\sum_{v\in e}|e|\cdot f(v)^2}{\sum_{i\in V}\deg v f(v)^2}\\ &= \frac{\sum_{v\in V}\sum_{e\ni v}|e|\cdot f(v)^2}{\sum_{i\in V}\deg v f(v)^2}\\ &\leq \left(\max_{e\in E}|e|\right)\cdot\frac{\sum_{v\in V}\deg v f(v)^2}{\sum_{i\in V}\deg v f(v)^2}\\ &= \max_{e\in E}|e|,\end{aligned}$$

where the first inequality is an equality if and only if $|f|$ is constant (since we are assuming that Γ is connected), and the last inequality is an equality if and only if $|e|$ is constant for all e. Putting everything together, we have that

$$\lambda_N \leq \max_{e\in E}|e|,$$

with equality if and only if $|e|$ is constant for all $|e|$, while $|f|$ is constant, and it is defined on a bipartite sub-hypergraph (i.e., $|f|$ is constant and Γ is bipartite). This proves the first claim.

It is left to prove (4.9.4). Given a bipartite sub-hypergraph $\hat{\Gamma} \subset \Gamma$, let $\gamma' \colon E \to \mathbb{R}$ be 1 on $\hat{E}$ and 0 otherwise. Then, up to changing (without loss of generality), the orientations of the hyperedges,

$$\begin{aligned}\lambda_N &= \max_{\gamma\colon E\to\mathbb{R}}\frac{\sum_{v\in V}\frac{1}{\deg v}\cdot\left(\sum_{e_{\text{in}}\colon v \text{ input}}\gamma(e_{\text{in}})-\sum_{e_{\text{out}}\colon v\text{ output}}\gamma(e_{\text{out}})\right)^2}{\sum_{e\in E}\gamma(h)^2}\\ &\geq \frac{\sum_{v\in V}\frac{1}{\deg v}\cdot\left(\sum_{e_{\text{in}}\colon v \text{ input}}\gamma'(e_{\text{in}})-\sum_{e_{\text{out}}\colon v\text{ output}}\gamma'(e_{\text{out}})\right)^2}{\sum_{e\in E}\gamma'(e)^2}\\ &\geq \frac{\sum_{v\in \hat{V}}\frac{1}{\deg v}\cdot\left(\sum_{e_{\text{in}}\colon v \text{ input}}\gamma'(e_{\text{in}})-\sum_{e_{\text{out}}\colon v\text{ output}}\gamma'(e_{\text{out}})\right)^2}{\sum_{e\in E}\gamma'(e)^2}\\ &= \frac{\sum_{v\in\hat{V}}\frac{\deg_{\hat{\Gamma}}(v)^2}{\deg v}}{|\hat{E}|}.\end{aligned}$$

Since the above inequality is true for all $\hat{\Gamma}$, this proves (4.9.4). □

Remark 4.9.3. Theorem 4.9.1 generalizes the inequalities in (4.9.2). In fact, while this is clear for the upper bound, to see it for the lower bound, consider

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a graph Γ. Fix a vertex v and let $\hat{\Gamma}$ be the bipartite sub-graph of Γ given by the edges that have v as endpoint. Then, (4.9.4) implies

$$\lambda_N \geq \eta(\hat{\Gamma}) = 1 + \sum_{v' \sim v} \frac{1}{\deg v' \cdot \deg v}$$
$$\geq 1 + \sum_{v' \sim v} \frac{1}{(N-1) \cdot \deg v} = 1 + \frac{1}{N-1} = \frac{N}{N-1}.$$

An immediate consequence of Theorem 4.9.1 is the following

Corollary 4.9.1. *If Γ is c-uniform and bipartite, then c is an eigenvalue for the Laplacian Δ, and its multiplicity equals the number of connected components of Γ.*

If Γ is c-uniform, then c is an eigenvalue for the signless Laplacian Δ^+, and its multiplicity equals the number of connected components of Γ.

Notably, Corollary 4.9.1 can be seen as a generalization of the fact that the multiplicity of 0 for Δ, in the case of simple graphs, equals the number of connected components of Γ. In fact, if Γ is a simple graph, then by Remark 4.9.2, λ is an eigenvalue for Δ if and only if $2 - \lambda$ is an eigenvalue for Δ^+. Hence, the fact that the multiplicity of 0 for Δ, in this case, equals the number of connected components of Γ, can be equivalently reformulated in terms of the multiplicity of 2 for Δ^+.

We now generalize the notion of duplicate vertices to the case of hypergraphs.

Definition 4.9.7. Two vertices v_i and v_j are *duplicates* of each other if the corresponding rows/columns of the adjacency matrix are the same, that is,

$$A_{il} = A_{jl} \quad \text{for each } l = 1, \ldots, N.$$

In particular, $A_{ij} = A_{jj} = 0$.

Lemma 4.9.4. *Let v_i and v_j be duplicates of each other. Let $f : V \to \mathbb{R}$ satisfy $f(v_i) = -f(v_j) \neq 0$ and $f = 0$ otherwise. Then, 1 is an eigenvalue for Δ and f is a corresponding eigenfunction.*

Proof By definition of f, we have that:

- $\Delta f(v_i) = f(v_i)$,
- $\Delta f(v_j) = f(v_j)$, and
- For each $l \neq i, j$,

$$\Delta f(v_l) = -\frac{1}{\deg v_l}\left(A_{li} f(v_i) + A_{lj} f(v_j)\right)$$

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$$= -\frac{1}{\deg v_l}\left(A_{li} f(v_i) - A_{li} f(v_i)\right)$$
$$= 0 = f(v_l).$$

Therefore, $\Delta f = f$, that is, 1 is an eigenvalue for Δ and f is a corresponding eigenfunction.

□

Corollary 4.9.2. *If there are n duplicate vertices, 1 is an eigenvalue with multiplicity at least $n-1$.*

Proof Assume, without loss of generality, that $v_1, \ldots, v_n$ are duplicates of each other. For each $i = 1, \ldots, n-1$, let $f_i : V \to \mathbb{R}$ such that $f_i(v_i) = 1$, $f_i(v_{i+1}) = -1$, and $f_i = 0$ otherwise. Then, by Lemma 4.9.4, the f_i's are eigenfunctions corresponding to the eigenvalue 1. Also, $\dim(\operatorname{span}(f_1, \ldots, f_{n-1})) = n-1$; therefore, the multiplicity of 1 is at least $n-1$. □

Similarly, we introduce twin vertices:

Definition 4.9.8. Two vertices v_i and v_j are *twins* of each other if they belong exactly to the same hyperedges, with the same orientations. In particular, $A_{ij} = -\deg v_i = -\deg v_j$ and $A_{il} = A_{jl}$ for all $l \neq i, j$.

Note that, while duplicate vertices exist for graphs, twin vertices cannot exist for graphs. Also, two vertices v_i and v_j cannot be both duplicates and twins of each other. In fact, if they are duplicates, then $A_{ij} = 0$, while, if they are twins, then $A_{ij} < 0$.

We now compute the spectrum of the signless Laplacian for the hyperflowers, which generalize star graphs.

Definition 4.9.9. Given $t \geq 1$, a hypergraph $\Gamma = (V, E, \varphi)$ is a *hyperflower with t twins* if (Figure 4.29):

- The vertex set can be decomposed as $V = C \sqcup P$, where C is the *core*, containing c vertices, and P is given by tM *peripheral vertices* $v_{11}, \ldots, v_{t1}, \ldots, v_{1M}, \ldots, v_{tM}$;
- The hyperedges are

$$e_j = C \sqcup \bigsqcup_{i=1}^{t} v_{ij}, \quad \text{for } j = 1, \ldots, M.$$

Thus, the hyperflower contains a core of c vertices and M leaves with t vertices each. Each hyperedge contains the core and one of the leaves.

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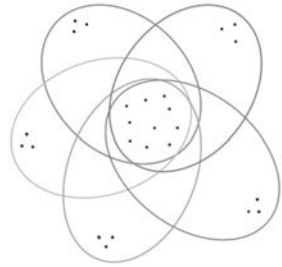


Figure 4.29 A hyperflower with 3 twins, 5 hyperedges, and 10 central vertices.

Proposition 4.9.2. *Given $t \geq 1$, let Γ be a hyperflower with t twins. Then, the spectrum of Δ^+ is given by:*

- 0, *with multiplicity* $N - M$;
- t, *with multiplicity* $M - 1$;
- $N - tM + t$, *with multiplicity* 1.

Proof We want to compute the spectrum of $\Delta(\Gamma^+)$. Since all hyperedges have cardinality $N - tM + t$, by Theorem 4.9.1,

$$\lambda_N = N - tM + t,$$

and the constant functions are the corresponding eigenfunctions.

Furthermore, t is an eigenvalue with multiplicity at least $M - 1$. To see this, consider the functions $f : V \to \mathbb{R}$ that are $= +1$ on one leaf, $= -1$ on another leaf, and 0 elsewhere. This construction gives $M - 1$ linearly independent functions for the eigenvalue t.

We have therefore listed M eigenvalues whose sum is N. Since $\Delta(\Gamma^+)$ has, in total, N eigenvalues whose sum is N, this implies that 0 has multiplicity $N - M$. □

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