Chapter 1
Graphs, Simplicial Complexes and Hypergraphs: Spectral Theory and Topology

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Abstract In this chapter we discuss the spectral theory of discrete structures such as graphs, simplicial complexes and hypergraphs. We focus, in particular, on the corresponding Laplace operators. We present the theoretical foundations, but we also discuss the motivation to model and study real data with these tools.

Keywords Simplicial complexes · Hypergraphs · Laplace operators · Eigenvalues · Topology

1.1 Introduction

1.1.1 Motivating Examples

Example 1 Consider scientists A, B, C, D that work in the same field and assume that there exists a joint publication of A, B, C, a single author paper of A, a joint paper of B, C and one of C, D. What are formal structures that model these relations?

(a) A **graph**: We take A, B, C, D as the vertices of a graph and connect vertices by an edge when the two scientists are coauthors. Thus, there are edges (A, B), (B, C), (A, C), (C, D).

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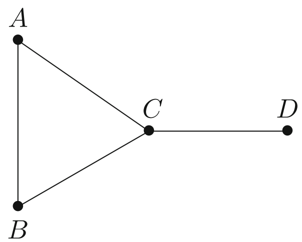
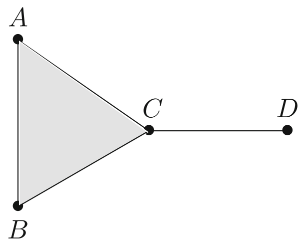


(b) A **simplicial complex**: The preceding model does not distinguish the fact that there is a 3-author paper between A, B, C from the possibility that there might be three 2-author papers between A, B, between B, C and between A, C. The latter would yield the same graph as the former. We therefore add a 2-dimensional simplex (A, B, C) to represent the 3-author paper.



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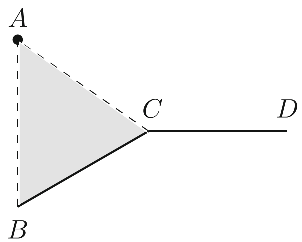
(c) A **hypergraph**: Still, this does not account for the facts that while there is a joint paper between B, C, there are no 2-author papers involving A, B only or A, C only. Nor does it account for the fact that only A has a single author paper. We therefore consider the hypergraph with hyperedges (A), (B, C), (C, D), (A, B, C) that represents the full information about the collaboration pattern.



Example 2 We consider a metric space (X, d). For simplicity, we assume that it is finite, although that is not needed for the construction. Thus, we have points $x_1, \ldots, x_N$ with mutual distances $d(x_i, x_j)$ that are positive for $x_i \neq x_j$, symmetric ($d(x_i, x_j) = d(x_j, x_i)$) and satisfy the triangle inequality ($d(x_i, x_j) \leq d(x_i, x_k) + d(x_k, x_j)$). For $x \in X$ and $\rho \geq 0$, we consider the closed ball $B(x, \rho) := \{y \in X : d(x, y) \leq \rho\}$ of radius ρ. For radii $r_i > 0, i = 1, \ldots .N$, we then form a complex

by associating a $(d-1)$-dimensional simplex to every family $(x_{i_1}, r_{i_1}), \ldots, (x_{i_d}, r_{i_d})$ that satisfies

$$\bigcap_{j=1,\ldots,d} B(x_{i_j}, r_{i_j}) \neq \emptyset, \tag{1.1}$$

that is, whenever these d balls have some point in common, for $d = 0, \ldots, N$. This is a simplicial complex (see the definition below), because whenever some collections of balls has a nonempty intersection, then this also holds for any subcollection. Such a complex is called a *Čech complex*, and it will play an important role in our discussion of topology. When we take all $r_i \equiv r$ and then let r vary, we get the family of complexes whose topology yields the bar codes of topological data analysis (TDA).

Example 3 We consider a system of chemical reactions with substances A, B, C, D, E. Reaction 1 transforms A, B into C, with E acting as a catalyst. Reaction 2 has B, C as inputs and A, D as outputs.

(a) We represent this by a **directed hypergraph** with one hyperedge $(A, B, E; C, E)$ going from the inputs A, B, E to the outputs C, E (note that the catalyst E appears both as an input and as an output) and another hyperedge $(B, C; A, D)$.
(b) Alternatively, we construct a **(directed) bipartite graph** with vertices $A, B, C, D, E, 1, 2$, with edges from A, from B and from E to 1, from 1 to C and to E, from B and from C to 2, and from 2 to A and to D.

1.1.2 How Can We Handle the Data?

While the preceding describes some modelling options, we should keep in mind that the real data sets are much larger. There are probably millions of scientists, with intricate patterns of collaborations. And by now, more than 20 million chemical substances and 40 million reactions have been reported in the chemical literature (see [1, 2]).

Therefore, we need not only mathematical concepts to model the data, but also mathematical tools to extract qualitative or quantitative information from the models about the data. Since (hyper)graphs and simplicial complexes are combinatorial objects, we may have to face the danger of combinatorial explosion, that the effort needed to analyze them grows exponentially with their size. For instance, the question whether two (unlabelled) graphs are isomorphic to each other is known to be in the complexity class NP [3]. That is, we cannot easily decide whether two data structures modelled as graphs are abstractly the same or different. And, of course, since simplicial complexes or hypergraphs are more complicated structures than graphs, the difficulties become even more severe.

But when we look at the global structures, for instance the collaboration pattern of all scientists in some field, or the chemical hypergraph consisting of all known substances and reactions, perhaps we are not so much interested in local details, but rather wish to extract some global qualitative information that identifies characteristic features of the data sets. And the methods to extract that kind of information should scale nicely with the data size.

Here, we describe one such method, the spectral analysis (for networks modelled as graphs, this has been systematically applied in [4–6]). This can be seen as some kind of Fourier transform. We define a linear operator (or several in the case of simplicial complexes) acting on functions on the vertices (or more generally, the simplices) and consider its spectrum, that is, the collection of its eigenvalues. There exist quick and robust numerical schemes to compute these eigenvalues (or possibly only those that are most interesting for our purposes). And as we shall explain in this contribution, from these eigenvalues we can read off many important qualitative properties of the underlying structure. This requires some mathematical theory, as we shall describe. The rewards are high, as we shall see.

Of course, the spectrum cannot provide full information about the underlying structure. That is, two (hyper)graphs or two simplicial complexes with the same spectra need not be isomorphic. In fact, it is not surprising that graphs cannot always be distinguished by their spectra, since, as mentioned, the graph isomorphism problem is in the complexity class NP, and therefore, according to current belief, is unlikely to be possible to solve it in polynomial time. However, spectra provide important information about many qualitative properties.

We should point out that there are also other geometric quantities that are on one hand readily computed and on the other yield useful qualitative information about the underlying structure. We should mention in particular the so-called *Ricci curvatures* whose statistics reveal important patterns (see for instance [7]). The name *curvature*, while perhaps not being very appropriate for a discrete structure, reveals its origin in Riemannian geometry (see [8]). In fact, also the spectral theory of Laplace operators was originally explored in Riemannian geometry (see [9]), and many ideas developed there are also useful here.
In any case, in this contribution, in line with the purpose of the present volume, we only discuss the spectral theory of discrete structures.

1.1.3 Definitions of Structures

We shall begin with the simplest structures before we shall subsequently enrich or decorate them. Keeping real data in mind, all objects will be assumed *finite*.

The starting point is a finite collection V of elements. As such, such a collection is amorphous. But we want to assume that these elements stand in certain discrete relations, and these relations then provide us with the structure to work with. The basic definition shall now identify some such structures that we shall explore in this contribution.

Definition 1.1.1

- A *graph* consists of a set V of *vertices* and a set E of *edges* which are unordered pairs of different vertices. When $e = (i, j)$ is an edge between the vertices $i, j \in V$, we say that i and j are *neighbors* and write $i \sim j$. The *degree* $\deg i$ is the number of neighbors of i.
- A *hypergraph* consists of a set V of *vertices* and a set H of *hyperedges* which are nonempty sets of vertices. An *oriented hypergraph* has hyperedges consisting of two disjoint sets of vertices, called the inputs and the outputs of the corresponding hyperedge. Either of them, but not both might be empty.
- A *simplicial complex* is defined on a set of vertices V as a subset of its power set, i.e. $\mathcal{C} \subset \mathcal{P}(V)$ that is closed under taking subsets, i.e. for a *simplex* $C \in \mathcal{C}$, any of its subsets $C' \subset C$ is also a simplex in $\mathcal{C}$. In contrast to the previous two definitions, the empty set is a simplex. A simplex c with $d + 1$ vertices is called a d-simplex (with d being considered as its dimension), its subsimplices are called its *faces*, and its $(d - 1)$-dimensional faces are called its *facets*. The *down degree* of c is the number of its facets, and its *up degree* is the number of $(d + 1)$-simplices of which c is a facet.

Every simplicial complex is a hypergraph when we consider every simplex (except the empty one) as a hyperedge. As it turns out, however, this is not a very useful perspective, and it is much better to develop the theories for these two concepts differently.

We can enrich this definition by providing additional structure.

Definition 1.1.2

- The graph (V, E) is *directed* when the edge set E contains ordered pairs of vertices. Likewise, the oriented hypergraph (V, H) is directed when we consider each hyperedge $h = (h_1; h_2)$ as going from the input set h_1 to the output set h_2.
- We may allow the graph (V, E) to contain self-loops, that is, edges of the form $e = (i, i)$ with $i \in V$.
- The (hyper)graph or simplicial complex is *weighted* when each vertex, (hyper)edge, simplex is allowed to carry some real number as its weight. When, for instance, the edges $e = (i, j)$ of a graph (V, E) carry weights $w_e = w_{ij}$, we put $\deg i = \sum_j w_{ij}$. Here, $w_{ij} = 0$ may simply express the fact that i and j are not connected by an edge.

In most cases, the weights are assumed to be nonnegative (so as to make also the vertex degrees nonnegative), but in certain cases, also negative weights might be permitted. Since subsequently, we want to normalize by the degree, we may want to assume that $\deg i \neq 0$ for all i.

1.1.4 Conventions

The conventions for the sign and the eigenvalues of Laplacians vary in the literature, and even in our own papers. This is partly due to the fact that in different circumstances, different conventions seem to be most natural and convenient.

Here, we make the Laplacian into a positive operator. Since the Laplacian is also selfadjoint, its spectrum is real and nonnegative. We denote its smallest eigenvalue by λ_1, and not by λ_0, as often done in the literature, as in the basic case of a graph, that smallest eigenvalue is $= 0$. For a simplicial complex or a hypergraph, that smallest eigenvalue, however, in general is no longer 0, or in contrast, there might be several eigenvalues $= 0$ while for a connected graph, there is only one such eigenvalue.

1.2 Graphs

While this contribution is not about graphs, we nevertheless develop their theory first, because both simplicial complexes and hypergraphs can be advantageously treated as generalizations of graphs. This is particularly true for the Laplacians and their spectra.
We shall develop the theory in such a manner that the generalizations appear most natural. We should also point out that the theory to be developed here is inspired by the corresponding theory in Riemannian geometry, see [9]. Systematic presentations of the spectral theory of graphs can be found in [10, 11]. While we shall partly use those references, we develop the theory here somewhat differently, in order to motivate and to facilitate the generalizations to simplicial complexes [12, 13] and hypergraphs [14] which is the main interest of this contribution.

1.2.1 The Laplacian

We start with the formula for the Laplace operator on an unweighted and undirected graph.

Definition 1.2.1 Let Γ be a graph with vertex set V and edge set E without isolated vertices (i.e., $\deg v > 0$ for every $v \in V$). Its *(vertex) Laplace operator* (or *Laplacian* for short) operates on functions $f : V \to \mathbb{R}$ via

$$L^0 f(v) := f(v) - \frac{1}{\deg v} \sum_{w \sim v} f(w) \quad \text{for } v \in V. \tag{1.2}$$

This definition is easy to understand: The Laplacian takes the value of the function f at the vertex v in question and subtracts from it the average of the values of the neighbors of v. It can also be interpreted as the negative of the generator of a random walk on the vertex set, where the random walker, when it finds herself at the vertex v, randomly selects one of the neighbors of v for her next position.

Warning: The Laplacian L^0 is **not** the *algebraic Laplacian* used in classical graph theory. That latter operator is given by

$$\mathcal{L}f(v) := \deg v\ f(v) - \sum_{w \sim v} f(w) \quad \text{for } v \in V. \tag{1.3}$$

When the graph is *regular*, that is $\deg v \equiv const$, then L^0 and $\mathcal{L}$ differ only by a constant factor. For general graphs, their theory is different, however. L^0 has better mathematical properties than $\mathcal{L}$ and, in particular, generalizes much more readily to both simplicial complexes and hypergraphs. That is why we take L^0 as our basic object.

We are interested in the spectrum, that is, the eigenvalues of L^0. In order to derive properties of that spectrum, we need to introduce some more mathematical structure. Perhaps somewhat surprisingly, we shall begin by introducing another operator that operates on functions on oriented edges. Here, the oriented edge $e = [v, w]$ is considered as going from the tail or input v to the head or output w. A change of orientation corresponds to reversing the ordering and considering $e^- = [w, v]$. That is, $e^+ = [v, w]$ and $e^- = [w, v]$ carry opposite orientations. We shall understand below why this is a natural construction. From now on, we let E denote the set of *oriented* edges of our graph. We then consider functions γ defined on oriented edges that are required to satisfy

$$\gamma(e^-) = -\gamma(e^+) \tag{1.4}$$

for all oriented edges. (A reader knowledgable in Riemannian geometry [9] might be reminded of exterior 1-forms.) We then define a Laplacian operating on such functions.

Definition 1.2.2 The Laplacian for functions on oriented edges is

$$L^1\gamma(e) := \frac{1}{\deg v_0} \cdot \sum_{v_0 \in e' = [v_0, w]} \gamma(e') - \frac{1}{\deg v_1} \cdot \sum_{v_1 \in e'' = [v_1, w]} \gamma(e''), \tag{1.5}$$

where $e = [v_0, v_1]$, and γ has to satisfy 1.4.

Again, this Laplacian is easy to understand. When we consider γ as a flow along oriented edges, then it compares the difference between out- and inflow at the tail with the difference between in- and outflow at the head. That is, it compares the flow in the direction of the edge, what comes in at the tail and what goes out at the head, with that in the opposite direction, what goes out at the tail and what comes in at the head. That is, $\gamma(e)$ measures the net flow of γ through the oriented edge e. Changing the orientation of e changes the sign of this Laplacian, that is,

$$L^1\gamma(e^-) = -L^1\gamma(e^+), \tag{1.6}$$

in accordance with 1.4.

As we shall see in a moment, the two operators L^0 and L^1 are intimately related. In particular, they have the same spectrum, apart from possibly the multiplicity of the eigenvalue 0.

We first define the boundary operator for a function $f : V \to \mathbb{R}$. Let $e = [v_0, v_1]$ be an oriented edge, then

$$\delta f(e) := f(v_0) - f(v_1). \tag{1.7}$$

In order to define an adjoint of δ, we shall utilize a scalar product for functions $f, g : V \to \mathbb{R}$ on vertices, defined by

$$(f, g)_V := \sum_{v \in V} \deg v \cdot f(v) \cdot g(v) \tag{1.8}$$

and a scalar product for functions $\omega, \gamma : E \to \mathbb{R}$ on oriented edges

$$(\omega, \gamma)_E := \sum_{e \in E} \omega(e) \cdot \gamma(e). \tag{1.9}$$

Lemma 1.2.1 *The operator*

$$\delta^* : \{\gamma : E \to \mathbb{R}\} \longrightarrow \{f : V \to \mathbb{R}\}$$

defined as

$$\delta^*(\gamma)(v) := \frac{\sum_{e'=[v,w]} \gamma(e') - \sum_{e''=[w,v]} \gamma(e'')}{2 \deg v} \tag{1.10}$$

is the adjoint of δ *in the sense that*

$$(\delta f, \gamma)_E = (f, \delta^* \gamma)_V \text{ for all } f, \gamma. \tag{1.11}$$

Proof

$$\begin{aligned}
(\delta f, \gamma)_E &= \sum_{e=[v_0,v_1]} \gamma(e) \cdot (f(v_0) - f(v_1)) \\
&= \frac{1}{2} \sum_{v \in V} f(v) \cdot \left(\sum_{e'=[v,w]} \gamma(e') - \sum_{e''=[w,v]} \gamma(e'') \right) \\
&= \sum_{v \in V} \deg v \cdot f(v) \cdot \frac{\sum_{e'=[v,w]} \gamma(e') - \sum_{e''=[w,v]} \gamma(e'')}{2 \deg v} \\
&= \sum_{v \in V} \deg v \cdot f(v) \cdot \delta^*(\gamma)(v) \\
&= (f, \delta^* \gamma)_V .
\end{aligned}$$

□

Lemma 1.2.2 *We have*

$$L^0 = \delta^* \delta \tag{1.12}$$

and

$$L^1 = \delta \delta^*. \tag{1.13}$$

Proof

$$\begin{aligned}
\delta^*(\delta f)(v) =& \frac{\sum_{e'=[v,w']} \delta f(e') - \sum_{e''=[w'',v]} \delta f(e'')}{2 \deg v} \\
=& \frac{\sum_{e'=[v,w']}(f(v) - f(w'))}{2 \deg v} + \\
& - \frac{\sum_{e''=[w'',v]}(f(w'') - f(v))}{2 \deg v} \\
& = L^0 f(v)
\end{aligned}$$

and for $e = [v_0, v_1]$

$$\begin{aligned}
\delta(\delta^* \gamma)(e) =& \delta^* \gamma(v_0) - \delta^* \gamma(v_1) \\
=& \frac{\sum_{e'=[v_0,w]} \gamma(e') - \sum_{e''=[w,v_0]} \gamma(e'')}{2 \deg v_0} \\
& - \frac{\sum_{f'=[v_1,w]} \gamma(f') - \sum_{f''=[w,v_1]} \gamma(f'')}{2 \deg v_1} \\
& = L^1 \gamma(e).
\end{aligned}$$

□

Corollary 1.2.1 *We have*

$$(f, L^0 f)_V = (\delta f, \delta f)_E = (L^0 f, f)_V \tag{1.14}$$

and

$$(\gamma, L^1 \gamma)_E = (\delta^* \gamma, \delta^* \gamma)_V = (L^1 \gamma, \gamma)_E \tag{1.15}$$

for all f, γ.
In particular, the operators L^0 *and* L^1 *are self-adjoint and nonnegative, and all their eigenvalues are real and nonnegative.*
L^0 *and* L^1 *have the same spectrum, except possibly for the multiplicity of the eigenvalue 0.*

Proof 1.14 and 1.15 follow from Lemmas 1.2.1 and 1.2.2, and these relations then imply the next claim. Finally, two operators AB and BA have the same eigenvalues except possibly for the multiplicity of the eigenvalue 0. □

Remark The algebraic Laplacian $\mathcal{L}$ from 1.3 is self-adjoint w.r.t. the product

$$(f, g)_{\mathrm{alg}} := \sum_v f(v)g(v).$$

1.2.2 The Spectrum

We consider a graph $\Gamma = (V, E)$ with N vertices.

Definition 1.2.3 We say that Γ is *connected* if for any $v', v'' \in V$, there exist vertices $v_1, \ldots, v_k$ and (unoriented) edges $e_0 = (v', v_1)$, $e_1 = (v_1, v_2)$,..., $e_{k-1} = (v_{k-1}, v_k)$, $e_k = (v_k, v'')$, that is, if v' and v'' can be connected by a sequence of edges. Such a sequences of edges is called a *path* from v' to v''.

We shall usually assume that our graphs are connected, even though we may not always say so explicitly. For a graph that is not connected, we can simply treat its connected components individually. We shall also usually assume that our graph (or, if not connected, every connected component) has more than one vertex. Thus, every vertex is assumed to support at least one edge, and hence have positive degree.

Lemma 1.2.3 *Let $v_0 \in V$ be a local maximum of $f : V \to \mathbb{R}$, that is $f(v) \geq f(w)$ for all $w \sim v$. Then*

$$L^0 f(v) \geq 0, \tag{1.16}$$

and in fact $L^0 f(v) > 0$ unless $f(w) = f(v)$ for all $w \sim v$.

Proof If $f(v) \geq f(w)$ for all $w \sim v$, then also $f(v) \geq \frac{1}{\deg v} \sum_{w \sim v} f(w)$. The last claim then is obvious. □

Corollary 1.2.2 *If Γ is connected, then $L^0 f = 0$ implies $f \equiv const$.*

Proof Let v_0 be a local maximum of f. Then by the Lemma, $f(w) = f(v)$ for all $w \sim v$. Thus, all neighbors of v are also local maxima, with the same value of f. Iterating the argument, also all the neighbors of those neighbors have the same (maximal) value of f, and so on. Since Γ is connected, we can reach each vertex from v through a path connecting local neighbors, and therefore f is constant. □

Corollary 1.2.3 *If Γ is connected, then $\lambda = 0$ is a simple eigenvalue of L^0, and it is an eigenvalue of L^1 with multiplicity $|E| - |V| + 1$.*

Proof By Corollary 1.2.2, the only solutions of $L^0 f = 0 \cdot f$ are the constants. Therefore, the corresponding Eigenspace is 1-dimensional. The vector space on which L^0

operates is $|V|$-dimensional, and that of L^1 is $|E|$-dimensional. Hence they have $|V|$ and $|E|$ eigenvalues counted with multiplicity. In particular, by what we have already proved, L^0 has $|V|-1$ nonzero eigenvalues. By Corollary 1.2.1, these are also the nonzero eigenvalues of L^1. Hence the eigenvalue 0 of L^1 must have multiplicity $|E|-|V|+1$. □

Lemma 1.2.4 *All eigenvalues of L^0 and L^1 satisfy*

$$0 \leq \lambda \leq 2. \tag{1.17}$$

Proof The eigenvalues are nonnegative by Corollary 1.2.1. Let f_λ be an eigenfunction for the eigenvalue $\lambda > 0$. Then

$$\lambda f(v) = f(v) - \frac{1}{\deg v} \sum_{w \sim v} f(w). \tag{1.18}$$

Let v be a vertex where $|f|$ assumes its maximum. Then

$$\lambda |f(v)| \leq |f(v)| + \frac{1}{\deg v} \sum_{w \sim v} |f(w)| \leq 2|f(v)| \tag{1.19}$$

which implies $\lambda \leq 2$. □

Corollary 1.2.4 *The eigenvalue $\lambda = 2$ is attained for an eigenfunction that satisfies*

$$f(w) = -f(v) \text{ whenever } w \sim v. \tag{1.20}$$

Such an eigenfunction exists if and only if the graph is bipartite, that is, has two classes V_1, V_2 of vertices and allows only connections between vertices from different classes.

Proof 1.20 is the condition for equality in 1.19. And we can construct such an f only in the bipartite case, where we can take $f(v) = 1$ for $v \in V_1$, $f(v) = -1$ for $v \in V_2$. □

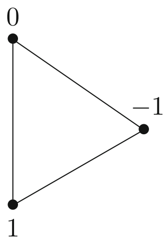
It is often convenient to reformulate the eigenvalue Eq. 1.18 as

$$(1-\lambda) f(v) = \frac{1}{\deg v} \sum_{w \sim v} f(w). \tag{1.21}$$

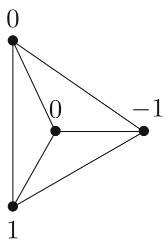
Thus, not only are the eigenvalues 0 and 2 extremal, but also the eigenvalue 1 is special as in that case, the right hand side of 1.21 vanishes, that is, the average of the values of f over the neighbors of any vertex vanishes.

Let us consider some simple **examples** where we can determine the eigenvalues of L^0 (and hence also infer those of L^1 by Corollary 1.2.3). Further examples can be found in Sect. 1.3.4.

is an eigenfunction for the eigenvalue 2 for the two-vertex graph K_2.



is an eigenfunction for the complete graph K_3 with three vertices, for the eigenvalue $\frac{3}{2}$. By permuting the vertices, we obtain another linearly independent such eigenfunction with the same eigenvalue. Hence the spectrum of K_3 is $(0, \frac{3}{2}, \frac{3}{2})$.



is an eigenfunction for the complete graph K_4 with four vertices, for the eigenvalue $\frac{4}{3}$. By permuting the vertices, we obtain two further linearly independent such eigenfunction with the same eigenvalue. Hence the spectrum of K_4 is $(0, \frac{4}{3}, \frac{4}{3}, \frac{4}{3})$.

Inductively, we see that the complete graph K_N has the eigenvalue 0 with multiplicity 1 and the eigenvalue $\frac{N}{N-1}$ with multiplicity $N-1$.

We can also see a principle here that will also be useful for determining the spectra of simplicial complexes and hypergraphs. Whenever we have two vertices v_1, v_{-1} with the same other neighbors, we obtain an eigenfunction when we put

$$f(v) := \begin{cases} 1 & \text{for } v = v_1 \\ -1 & \text{for } v = v_{-1} \\ 0 & \text{else} \end{cases} \tag{1.22}$$

as is readily checked from 1.2.

Let us explore this observation a bit more. First of all, such a graph possesses an automorphism ι that exchanges v_1 and v_{-1} and leaves all other vertices fixed. Secondly, as will become clear below, we may assume that all other eigenfunctions f' satisfy

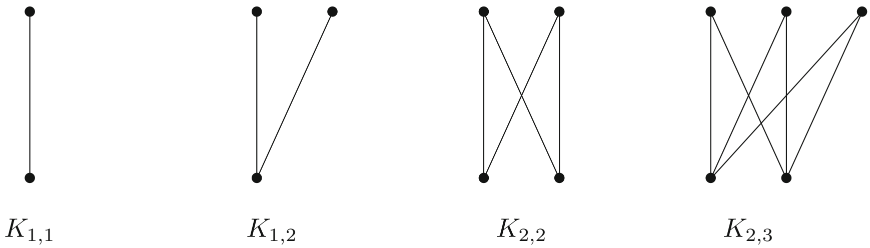
$$f'(v_1) = f'(v_{-1}). \tag{1.23}$$

This is useful for an iterative determination of the eigenvalues and eigenfunctions. Third, when v_1 and v_{-1} are not neighbors, then the eigenvalue for f from 1.22 is $= 1$, because then, by 1.21, for every vertex u

$$\sum_{w \sim u} f(w) = 0. \tag{1.24}$$

We may then say that v_1 and v_{-1} are *duplicates* of each other.

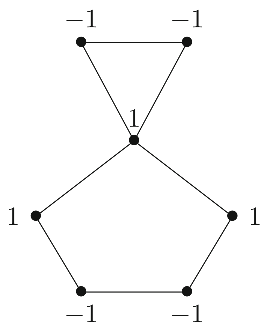
With this principle [15], we can iteratively determine the entire spectrum of the *complete bipartite graph* $K_{m,n}$. That graph has two groups V_1, V_{-1} of m and n vertices, resp., such that every vertex in one group is connected to every vertex in the other group, but there are no connections inside either group. This graph is obtained from $K_{1,1} = K_2$ by the repeated duplication of nodes



$K_{m,n}$ then has the eigenvalue 0 with multiplicity 1 and the eigenvalue 1 with multiplicity $m + n - 2$. The remaining eigenvalue is 2. In fact, every graph that is *bipartite*, meaning that it has two groups V_1, V_{-1} of vertices without any connections inside either group, has that eigenvalue, with an eigenfunction that is $= 1$ on V_1 and $= -1$ on V_{-1}. In fact, only bipartite graphs can carry the eigenvalue 2, as the condition 1.20 of Corollary 1.2.4 can only be satisfied on such graphs.

An example of a complete bipartite graph is the *star graph* $K_{1,n}$ that has one central vertex connected to n peripheral ones.

Remark While the presence of the eigenvalue 1, as in 1.24, can be seen as an indication of vertex duplication in empirical spectra [16], we should point out that this eigenvalue can also arise in other graphs:



Here, the eigenfunction for the eigenvalue 1 is invariant under the automorphisms of the graph.

We now develop a more abstract perspective on symmetries and spectra, following [17].

Definition 1.2.4 An *automorphism* of the graph $\Gamma = (V, E)$ consists of bijections $\sigma : V \to V$ and $\sigma : E \to E$ such that $\sigma(v) \in \sigma(e)$ if and only if $v \in e$.
For $f : V \to \mathbb{R}$, we then put $\sigma_* f(v) = f(\sigma(v))$.

The Laplace operator commutes with automorphisms.

Lemma 1.2.5 *If σ is an automorphism of $\Gamma = (V, E)$, then*

$$L^0(\sigma_* f)(v) = \sigma_*(L^0 f)(v) \tag{1.25}$$

for all $v \in V$ and $f : V \to \mathbb{R}$.

The *proof* is obvious.

We can use Lemma 1.2.5 to decompose the spectrum of L^0. Let τ be an automorphism of $\Gamma = (V, E)$ with

$$\tau^2 = \mathrm{id}. \tag{1.26}$$

Then τ has two possible eigenvalues, ± 1, on the space of functions $f : V \to \mathbb{R}$, and L^0 leaves those two Eigenspaces $L_\pm$ invariant. Also, $V = V_0 \cup V_1$ where V_0 is the set of those vertices that are fixed by τ. Thus $\tau(v_0) = v_0$ if and only if $v_0 \in V_0$. We write $V_1 = V' \cup V''$ where V', V'' are disjoint and $\tau(V') = V''$. Since also $\tau(V'') = V'$ because of (1.26), V' and V'' play symmetric roles.

Without loss of generality, we assume that V' (and hence also V'') is connected, as otherwise we can rearrange the decomposition of V_1 and/or write τ as the composition of several such automorphisms.

Lemma 1.2.6 *We can decompose V into spaces generated by symmetric and antisymmetric eigenfunctions. More precisely, we have a $|V'|$-dimensional space of functions $f : V \to \mathbb{R}$ generated by eigenfunctions of L^0 that vanish on V_0 and that are antisymmetric on V' and V'', $f(v'') = -f(v')$ if $v'' = \tau(v') \in V''$ for $v' \in V'$. The remaining $(|V'| + |V_0|)$-dimensional space is generated by eigenfunctions that are symmetric on V' and V'', that is, $f(v'') = f(v')$.*

Proof The first class of functions are those that are eigenfunctions of τ for the eigenvalue -1, and the second class has eigenvalue 1. By Lemma 1.2.5, these are unions of Eigenspaces of L^0. Since $|V''| = |V'|$ and $V = V_0 \cup V' \cup V''$, this generates the space of all functions on V.

Definition 1.2.5 Let $\Gamma = (V, E)$ be a graph. An *induced subgraph*, also called a *motif*, $\hat{\Gamma}$ has some nonempty vertex set $\hat{V} \subset V$ and an edge set $\hat{E} \subset E$ such that any two $v_1, v_2 \in \hat{V}$ are contained in an edge $e \in \hat{E}$ whenever they are contained in e in Γ.

Let $\hat{\Gamma}$ be a motif in Γ. We then have the induced Laplacian

$$L^0_{\Gamma,\hat{\Gamma}} f(v) = f(v) - \frac{1}{\deg_\Gamma v} \cdot \left(\sum_{v' \in \hat{V}, v' \sim v} f(v') \right) \tag{1.27}$$

where $\deg_\Gamma v$ denotes the degree of v in Γ.

Definition 1.2.6 We say that the motif Γ' with vertex set V' is a *duplicated motif* if V' and V'' are disconnected, that is, when there is no edge containing elements from both V' and V''.
We say that Γ' and Γ'' with vertex sets V' and V'' are *twin motives* if for every $e \in E$ we have that $v' \in e$ if and only if $v'' = \tau(v') \in e$.

Lemma 1.2.7 *Let Γ' be a duplicated motif in Γ, and let $v_0 \in V_0$ be a neighbor of some $v' \in V'$. Then v_0 is also a neighbor of $v'' = \tau(v') \in V''$.*

Proof Since $v_0 \in V_0$ is fixed by the automorphism τ, and since τ maps the edge e containing v_0 and v' onto an edge $\tau(e)$ containing $v'' = \tau(v')$ and $v_0 = \tau(v_0)$, the claim follows.

Lemma 1.2.8 *Let Γ' be a duplicated motif in Γ. Then we find a basis of eigenfunctions of the Laplacian L^0 of Γ of functions f satisfying either*

1.

$$L^0_{\Gamma,\Gamma'} f(v) = \begin{cases} \lambda f(v) & \textit{for } v \in V' \cup V'' \\ -\lambda f(\tau(v)) & \textit{for } v \in V'' \\ 0 & \textit{for } v \in V_0 \end{cases} \tag{1.28}$$

2. or

$$f(\tau(v)) = f(v) \textit{ for } v \in V'. \tag{1.29}$$

The latter eigenfunctions are those of the graph Γ^τ obtained as the quotient of Γ by τ, that is, the graph with vertex set $V_0 \cup V'$ and all edges induced by Γ.

Proof If $v_0 \in V_0$ and $f(v_0) = 0$ and if f is antisymmetric, then also $L^0 f(v_0) = 0$, since by Lemma 1.2.7 the contributions from its neighbors v' and $v'' = \tau(v')$ cancel in $L^0 f(v_0)$. The result then follows from Lemma 1.2.6, since a neighbor w of $v \in V'$ is contained either in V' or in V_0, in which case for an antisymmetric f, $f(w) = 0$, and therefore, we can restrict the computation in (1.28) to the induced Laplacian, that is, consider only the vertices in V'.

Examples:

1. We had already looked at the example of a duplicated vertex, that is, where v' and v'' are not connected, but have the same neighbors.

2. Let V' consist of a single vertex v' connected to $v'' = \tau(v')$ by an edge. Then 1.28 becomes
$$f(v') - \frac{1}{\deg_\Gamma v'} f(v'') = \lambda f(v'),$$
that is, since $f(v'') = -f(v')$,
$$\lambda = 1 + \frac{1}{\deg_\Gamma v'}.$$
3. We next duplicate an edge $e = (v'_1, v'_2)$. Then two eigenvalues and eigenfunctions of L^0 are obtained by solving
$$\begin{aligned} f(v'_1) - \frac{1}{\deg_\Gamma v'_1} f(v'_2) &= \lambda f(v'_1) \\ f(v'_2) - \frac{1}{\deg_\Gamma v'_2} f(v'_1) &= \lambda f(v'_2) \\ f(v) &= 0 \qquad \text{for all other } v. \end{aligned}$$
This yields [15]
$$\lambda = 1 \pm \frac{1}{\sqrt{\deg_\Gamma v'_1 \deg_\Gamma v'_2}}.$$
4. It should now be clear how to analyze the duplication or twinning of other motives.

1.2.3 Rayleigh Quotients and the Courant-Fischer-Weyl Scheme

We now want to develop a more systematic approach for studying Laplacian spectra. We shall employ the fundamental

Theorem 1.2.1 *(Courant-Fischer-Weyl min-max principle) Let H be an N-dimensional vector space with a positive definite scalar product $(.,.)$. Let $\mathcal{H}_k$ be the family of all k-dimensional subspaces of H. Let $A : H \to H$ be a self adjoint linear operator. Then the eigenvalues $\lambda_1 \leq \ldots \leq \lambda_N$ of A can be obtained by*
$$\lambda_k = \min_{H_k \in \mathcal{H}_k} \max_{g(\neq 0) \in H_k} \frac{(Ag, g)}{(g, g)} = \max_{H_{N-k+1} \in \mathcal{H}_{N-k+1}} \min_{g(\neq 0) \in H_{N-k+1}} \frac{(Ag, g)}{(g, g)}. \tag{1.30}$$
The vectors g_k realizing such a min-max or max-min then are corresponding Eigenvectors, and the min-max spaces $\mathcal{H}_k$ are spanned by the Eigenvectors for the eigenvalues $\lambda_1, \ldots, \lambda_k$, and analogously, the max-min spaces $\mathcal{H}_{N-k+1}$ are spanned by the Eigenvectors for the eigenvalues $\lambda_k, \ldots, \lambda_N$.

Thus, we also have

$$\begin{aligned}\lambda_k &= \min_{g(\neq 0)\in H, (g,g_j)=0 \text{ for } j=1,\dots,k-1} \frac{(Ag,g)}{(g,g)} \\ &= \max_{g(\neq 0)\in H, (g,g_\ell)=0 \text{ for } \ell=k+1,\dots,N} \frac{(Ag,g)}{(g,g)}.\end{aligned} \tag{1.31}$$

In particular,

$$\lambda_1 = \min_{g(\neq 0)\in H} \frac{(Ag,g)}{(g,g)}, \qquad \lambda_N = \max_{g(\neq 0)\in H} \frac{(Ag,g)}{(g,g)}. \tag{1.32}$$

A *prf* can for instance be found in [18].

Definition 1.2.7 $\frac{(Ag,g)}{(g,g)}$ is called the *Rayleigh quotient* of g.

According to Theorem 1.2.1, the eigenvalues of L^0 are given by minimax values of

$$\frac{(L^0 g,g)}{(g,g)} = \frac{(\delta g,\delta g)}{(g,g)} = \frac{\sum_{e=(v,w)}(g(v)-g(w))(g(v)-g(w))}{\sum_v \deg v\; g(v)^2}, \tag{1.33}$$

that is, when we denote an eigenfunction for the eigenvalue λ_k by f_k,

$$\lambda_k = \min_{f:(f,f_j)=0 \text{ for } j=1,\dots,k-1} \frac{\sum_{e=(v,w)}(f(v)-f(w))^2}{\sum_v \deg v\; f(v)^2}. \tag{1.34}$$

It is not difficult, for instance, to read off Lemma 1.2.4 from this formula.

Theorem 1.2.1 will play a fundamental role in our analysis of the spectra of simplicial complexes and hypergraphs below. In order to see its usefulness, let us look here at the following result.

Corollary 1.2.5 *A graph with N vertices is complete if and only if its spectrum consists of* 0 *as a simple eigenvalue and* $\frac{N}{N-1}$ *with multiplicity* $N-1$.
For a graph with N vertices that is not complete, we have

$$\lambda_2 \leq 1 \text{ and } \lambda_N > \frac{N}{N-1}. \tag{1.35}$$

Proof By Theorem 1.2.1,

$$\lambda_2 = \min_{g:\ \sum_v \deg v\ g(v)=0} \frac{(L^0 g,g)}{(g,g)}. \tag{1.36}$$

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

$$\deg v_1\; g(v_1) + \deg v_2\; g(v_2) = 0 \text{ and } g(v) = 0 \text{ for all other } v. \tag{1.37}$$

Inserting this into the Rayleigh quotient 1.36 makes that expression 1, and the minimum therefore is ≤ 1. We leave the second inequality of 1.35 as an exercise.

From Corollary 1.2.5 we see that the complete graphs K_N are completely determined by their spectrum. Thus, there are no other graphs that are isospectral with K_N. There do not even exist graphs whose spectrum is very close to that of K_N. In fact, not only do we have $\lambda_2 \leq 1 = \frac{N-1}{N-1}$ for non-complete graphs, but Das and Sun [19] proved that for all non-complete graphs we also have

$$\lambda_N \geq \frac{N+1}{N-1}, \tag{1.38}$$

with equality if and only if the complement graph (that is, the graph that connects precisely those vertices that are not neighbors in the graph under consideration) is a single edge or a complete bipartite graph with both parts of size $\frac{N-1}{2}$. More precise results in this direction can be found in [20].

Corollary 1.2.6 *Eigenfunctions for different eigenvalues of L^0 are orthogonal to each other w.r.t. $(.,.)_V$. In particular, all the eigenfunctions f for λ_k with $k \geq 2$ are orthogonal to the constants (the eigenfunctions for $\lambda_1 = 0$) and satisfy therefore*

$$\sum_v \deg v f(v) = 0. \tag{1.39}$$

1.2.4 Cheeger-Type Estimates

In this section, we only provide a survey of results, but no proofs. As we have seen, the spectrum of a graph can tell us its number of connected components (the multiplicity of the eigenvalue 0), whether it is bipartite (if and only if it has the eigenvalue 2) or complete (see Corollary 1.2.5), and it can indicate node duplications [15]. In fact, the spectrum reflects the general symmetries of a graph [17].

But the spectrum controls many further qualitative properties of a graph by inequalities relating eigenvalues to other quantities characterizing graphs. In particular, we have the so-called Cheeger-type estimates, the first of which were discovered by Dodziuk [21] and Alon and Milman [22].

In fact, these estimates concern a quantity that had already been introduced by Pólya and Szegö [23] into graph theory, but the estimate was inspired by Cheeger's estimate for an analogous constant in Riemannian geometry. The *(Polya)-Cheeger constant* is defined as

$$h := \min_S \frac{|E(S, \overline{S})|}{\min(\mathrm{vol}(S), \mathrm{vol}(\overline{S}))}, \tag{1.40}$$

where $|E(S, \overline{S})|$ denotes the number of edges between the two complementary subsets $S, \overline{S}$ of the vertex set V, and

$$\mathrm{vol}(S) := \sum_{v \in S} \deg v. \tag{1.41}$$

Thus, the aim is to cut the graph into two large vertex sets with few connections between them. That is, we want to *cluster* the vertex set. The result of [21, 22] then is

Theorem 1.2.2 *The eigenvalue λ_2 of a connected graph satisfies*

$$\frac{1}{2}h^2 \leq 1 - \sqrt{1-h^2} \leq \lambda_2 \leq 2\,h. \tag{1.42}$$

We do not provide the proof here which can be found, for instance, also in [10, 11]. A systematic general treatment will be given in [24].

The inequality 1.42 tells us that the first nonzero eigenvalue λ_2 of a connected graph measures how different that graph is from a disconnected one (where both that eigenvalue and h would be 0). We also recall that the largest eigenvalue λ_N is $= 2$ if and only if the graph is bipartite. We may therefore ask whether in general $2 - \lambda_N$ could also tell us how different a graph is from being bipartite. That works, indeed, and there is a *dual Cheeger constant* that bounds the largest eigenvalue [25, 26] (or a bipartiteness ratio [27]). It is defined as

$$\bar{h} := \max_{\text{partitions } V = V_1 \sqcup V_2 \sqcup V_3} \frac{|E(V_1, V_2)|}{\mathrm{vol}(V_1) + \mathrm{vol}(V_2)}. \tag{1.43}$$

This constant is $= 1$ if and only if the graph is bipartite (we take V_1, V_2 as the two classes of the bipartite graph and $V_3 = \emptyset$). It satisfies an analogue of (1.42),

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

The two constants h and $\bar{h}$ are related to each other [26].

We also have another characterization of h.

Theorem 1.2.3 *For every connected graph,*

$$h = \min_{f: V \to \mathbb{R} \text{ non constant}} \max_{t \in \mathbb{R}} \frac{\sum_{v \sim w} \left| f(v) - f(w) \right|}{\sum_{v \in V} \deg v \cdot \left| f(v) - t \right|}$$

and

$$\frac{1}{2}h \leq \min_{f: V \to \mathbb{R} \text{ s.t. } \sum_{v \in V} \deg v \cdot f(v) = 0} \frac{\sum_{v \sim w} \left| f(v) - f(w) \right|}{\sum_{v \in V} \deg v \cdot \left| f(v) \right|} \leq h.$$

For background on this result and the relation of the Cheeger constant with Rayleigh quotients, we refer to [28–35]. The nodal sets of an eigenfunction f_2 for λ_2, that is $V_\pm := \{v \in V : \pm f_2 > 0\}$ are connected and, according to the characterization in Theorem 1.2.3, there are only few edges between V_+ and V_-. Thus, they provide natural clusters for the graph. A general survey of spectral clustering of graphs is found in [36].

There is, however, no analogue for $\bar{h}$ of Theorem 1.2.3, although optimal sets V_1, V_2 in 1.43 should have few internal connections and therefore yield some structure that approaches a bipartite one. Therefore, in [37], another quantity was introduced,

$$Q := \max_{e=(v,w)} \left(\frac{1}{\deg v} + \frac{1}{\deg w} \right).$$

We also need

$$\tau := \max_{e=(v,w):\deg w \geq \deg v} \left(\frac{(\deg w - \deg v + N) \cdot \deg v}{\deg v + \deg w} \right).$$

We then have the result of [37] which draws upon the duality between L^0 and L^1.

Theorem 1.2.4 *For every graph,*

$$Q = \max_{\gamma : E \to \mathbb{R}} \frac{\sum_{v \in V} \frac{1}{\deg v} \cdot \left| \sum_{e_{in}:v \text{ input}} \gamma(e_{in}) - \sum_{e_{out}:v \text{ output}} \gamma(e_{out}) \right|}{\sum_{e \in E} |\gamma(e)|}$$

and

$$Q \leq \lambda_N \leq Q \cdot \tau.$$

We also have

$$Q = \max_{\hat{\Gamma} \subset \Gamma \text{ bipartite}} \frac{\sum_{v \in V} \frac{\deg_{\hat{\Gamma}}(v)}{\deg_{\Gamma}(v)}}{|E(\hat{\Gamma})|}.$$

The last equation shows why Q is related to bipartiteness.

1.2.5 Generalizations and Extensions

1.2.5.1 Weighted Graphs

We can put weights on the vertices and/or the edges of a graph. When the vertex weights are denoted by w_i and the edge weights by w_e or w_{ij} for $e = (i, j)$, and we then require the symmetry

$$w_{ij} = w_{ji}, \tag{1.44}$$

$$(f, g)_V := \sum_i w_i f(i)g(i) \quad \text{for } f, g : V \to \mathbb{R} \tag{1.45}$$

$$(\gamma, \omega)_E := \sum_e w_e \gamma(e)\omega(e) \quad \text{for } \gamma, \omega : E \to \mathbb{R}. \tag{1.46}$$

In order to avoid problems, it might be good to require that all weights are nonnegative and every vertex supports at least one edge with a positive weight. (Formally, we could put $w_e = 0$ to indicate that the edge e is not present, that is, $e \notin E$. Thus, an ordinary graph has weight 1 for all $e \in E$ and weight 0 for all $e \notin E$.) In order to define an adjoint δ^* of the boundary operator δ as above, these two products have to be compatible in the sense that

$$w_i = \sum_j w_{ij}. \tag{1.47}$$

In fact, from this perspective, for a graph without edge weights, as considered above, deg i are the natural weights for the vertices i. In some situations, like neural networks, it might be natural to also admit negative edge weights (for inhibitory connections). In that case, we need to assume that $w_i \neq 0$ in 1.47 for all vertices, in order to be able to define our Laplacian.

That definition then is a simple and natural generalization of 1.2:

$$L^0 f(i) := f(i) - \frac{1}{w_i} \sum_j w_{ij} f(j). \tag{1.48}$$

And the preceding scheme can then be used to define L^1 analogously. We don't spell out the details here as such a scheme will come up again when we discuss simplicial complexes.

In summary, the spectral theory for weighted graphs (with the restrictions that we have imposed here) is not principally different from that of unweighted graphs.

1.2.5.2 Directed Graphs

When we allow for directed edges, going for instance from i to j, but not back from j to i, or more generally, give up the symmetry 1.44 in the weighted case, the theory becomes very different. The Laplacians, defined as in 1.2 or in 1.48, then are no longer self-adjoint, and consequently, their spectrum need no longer be real. Complex eigenvalues may occur. A corresponding theory has been developed in [38]. So far, however, this has not yet been pursued much, and systematic applications to real data have not yet been carried out, although many networks are naturally directed. Examples range from neural networks to weblinks or citations.

Importantly, chemical reaction networks should be modelled by *directed hypergraphs*. This calls for the development of the corresponding theory.

1.2.5.3 Signed Graphs

There is another version that, in contrast to directed graphs, supports a Laplacian with a real spectrum.

Definition 1.2.8 A *signed graph* Γ consists of a vertex set V and a set E of undirected edges with a sign function

$$s : E \to \{+1, -1\}. \tag{1.49}$$

A reference on the spectral theory of signed graphs is [39].
Such a signed graph may also carry a weight function

$$w : E \to \mathbb{R}_+, \tag{1.50}$$

but as we discussed the easy incorporation of weights into the theory already above, we neglect that possibility here.

The sign distinguishes between positive and negative relations, like friendship vs. hostility in a social network.

Definition 1.2.9 Let Γ be a signed graph. Its Laplacian is defined by

$$L_s^0 f(v) := f(v) - \frac{1}{\deg v} \sum_{v' \sim v} s(vv') f(v') = \frac{1}{\deg v} \sum_{v' \sim v} (f(v) - s(vv') f(v')) \tag{1.51}$$

with $\deg v$ defined as before as the number of neighbors of v, for functions $f : V \to \mathbb{R}$.

Lemma 1.2.9 *L_s^0 is selfadjoint w.r.t. the product 1.8 $(f, g) = \sum_v \deg v \ f(v)g(v)$, and*

$$(L_s^0 f, g) = \sum_{v \sim v'} (f(v) - s(vv') f(v'))(g(v) - s(vv') g(v')) = (f, L_s^0 g). \tag{1.52}$$

1.2.5.4 Self-Loops

We had excluded self-loops, that is, edges of the form $e = (i, i)$ for some vertex i. There is no deeper reason for such an exclusion, except perhaps historical contingencies in graph theory. The theory works as before when we allow for self-loops at some or all vertices.

To see what happens, let us consider the graph K_N^0 where each vertex i is connected with all vertices j, including itself. We then have

$$L^0_{K_N^0} f(i) = f(i) - \frac{1}{N} \sum_j f(j) = \left(1 - \frac{1}{N}\right) f(i) - \frac{1}{N} \sum_{j \neq i} f(j), \tag{1.53}$$

which we may compare to the Laplacian on the complete graph K_N,

$$L^0_{K_N} f(i) = f(i) - \frac{1}{N-1} \sum_{j \neq i} f(j). \tag{1.54}$$

The spectrum of $L^0_{K^0_N}$ has the eigenvalue 0 and the eigenvalue 1, the latter with multiplicity $N-1$, whereas the corresponding eigenvalue of $L^0_{K_N}$ was $\frac{N}{N-1}$.

1.3 Simplicial Complexes

1.3.1 Homology of Simplicial Complexes

Definition 1.3.1 Let $\Sigma \subset \mathcal{P}(V)$ be a simplicial complex with vertex set $V = \{v_1, \ldots, v_N\}$. A collection of subsets of V, with $\emptyset \in \Sigma$, $S \in \Sigma$ is called a *q-simplex* if it contains precisely $q+1$ vertices.
When $S = \{v_{\sigma_0}, \ldots, v_{\sigma_q}\}$ is a q-simplex, then the ordered set $[v_{\sigma_0}, \ldots, v_{\sigma_q}]$ is called an *oriented q-simplex*. Changing the ordering by an odd permutation of the vertices induces the opposite orientation.
Let G be an abelian group. A *q-chain* is a formal linear combination

$$c_q = \sum_{i=1}^{m} g_i \sigma_q^i \tag{1.55}$$

for elements g_i of G and q-simplices σ_q^i.

Definition 1.3.2 The *boundary* of an oriented q-simplex $\sigma_q = [v_0, v_1, \ldots, v_q]$ is the $(q-1)$-chain

$$\partial \sigma_q := \sum_{i=0}^{q} (-1)^i (v_0, \ldots, \hat{v}_i, \ldots, v_q) \text{ for } q > 0, \tag{1.56}$$

and, of course, $\partial \sigma_0 = 0$ for a 0-chain. Here, $\hat{v}_i$ means that the vertex v_i is omitted. The boundary of the q-chain $c_q = \sum_{i=1}^m g_i \sigma_q^i$ then is, by linearity,

$$\partial c_q := \sum_{i=1}^{m} g_i \partial \sigma_q^i. \tag{1.57}$$

When we want to emphasize that ∂ operates on q-chains, we shall write ∂_q.

Definition 1.3.3 The q-chain c_q is called *closed* or, equivalently, a cycle, if

$$\partial_q c_q = 0. \tag{1.58}$$

The q-chain c_q is called a *boundary* if there exists some $(q+1)$-chain γ_{q+1} with

$$\partial_{q+1}\gamma_{q+1} = c_q. \tag{1.59}$$

Theorem 1.3.1

$$\partial_{q-1}\partial_q = 0 \textit{ for all } q. \tag{1.60}$$

We shall usually abbreviate this fundamental relation as

$$\partial^2 = 0. \tag{1.61}$$

Proof Because of 1.57, it suffices to show that

$$\partial\partial\sigma_q = 0 \tag{1.62}$$

for any oriented q-simplex. Since $C_s = 0$ for $s < 0$, we only need to consider the case $q \geq 2$. For $\sigma_q = [v_0, \dots, v_q]$, we have

$$\begin{aligned}
\partial\partial\sigma_q &= \partial \sum_{i=0}^{q} (-1)^i (v_0, \dots, \hat{v}_i, \dots, v_q) \\
&= \sum_{i=0}^{q} (-1)^i \partial (v_0, \dots, \hat{v}_i, \dots, v_q) \\
&= \sum_{i=0}^{q} (-1)^i \left(\sum_{j=0}^{i-1} (-1)^j (v_0, \dots, \hat{v}_j, \dots, \hat{v}_i, \dots, v_q) \right. \\
&\quad \left. + \sum_{j=i+1}^{q} (-1)^{j-1} (v_0, \dots, \hat{v}_i, \dots, \hat{v}_j, \dots, v_q) \right) \\
&= \sum_{j<i} (-1)^{i+j} (v_0, \dots, \hat{v}_j, \dots, \hat{v}_i, \dots, v_q) \\
&\quad + \sum_{j>i} (-1)^{i+j-1} (v_0, \dots, \hat{v}_i, \dots, \hat{v}_j, \dots, v_q),
\end{aligned}$$

and exchanging i and j in the last sum gives the result.

Definition 1.3.4 The quotient group

$$H_q(\Sigma, G) := \ker \partial_q / \mathrm{im}\partial_{q+1} \tag{1.63}$$

is called the *qth homology group* (with coefficients in G) of the simplicial complex Σ.

When Σ is a simplicial complex and G is an abelian group G, we can define the group of q-cochains

$$C^q(\Sigma, G) := \mathrm{Hom}(C_q(\Sigma), G). \tag{1.64}$$

We then get the coboundary operators

$$\begin{aligned}\delta^q : C^q(\Sigma, G) &\to C^{q+1}(\Sigma, G)\\ \phi &\mapsto \phi \circ \partial_q.\end{aligned}$$

Explicitly,

$$(\delta^q f)([v_0, \ldots, v_{q+1}]) = \sum_{j=0}^{q+1} (-1)^j f([v_0, \ldots, \hat{v}_j \ldots v_{q+1}]). \tag{1.65}$$

From Theorem 1.3.1, it follows that

$$\delta^q \circ \delta^{q-1} = 0. \tag{1.66}$$

We can therefore proceed to

Definition 1.3.5 The qth cohomology group of the simplicial complex Σ with coefficients in the abelian group G is

$$H^q(\Sigma, G) := \ker \delta^q / \mathrm{im}\delta^{q-1}. \tag{1.67}$$

1.3.2 Laplace Operators on Simplicial Complexes

In this section, we develop the theory of [13]. Σ is a simplicial complex. $[F]$ will denote an oriented simplex, that is, an ordered set $[v_0, \ldots, v_q]$ of vertices. Also, for the abelian group G of the previous section, we take the real field $\mathbb{R}$. The cochain groups $C^q(\Sigma, \mathbb{R})$ then are vector spaces over $\mathbb{R}$.

Definition 1.3.6 The dimension $b_q(\Sigma)$ of $H^q(\Sigma, \mathbb{R})$ is called the qth Betti number of Σ.

Also, concerning the orientations, we have for any $\phi \in C^q(\Sigma, \mathbb{R})$,

$$\phi(-\sigma_q) = -\phi(\sigma_q), \tag{1.68}$$

that is, changing the orientation yields a minus sign.

Definition 1.3.7 The adjoint $(\delta^q)^* : C^{q+1}(\Sigma, \mathbb{R}) \to C^q(\Sigma, \mathbb{R})$ of the coboundary operator δ^q is defined by

$$(\delta^q f, g)_{C^{q+1}} = (f, (\delta^q)^* g)_{C^q},$$

for $f \in C^q(\Sigma, \mathbb{R})$ and $g \in C^{q+1}(\Sigma, \mathbb{R})$, where $(\ ,\ )_{C^q}$ denotes the inner product on the $C^q(\Sigma, \mathbb{R}) = C^q$ for short.

We then have the arrows

$$C^{q-1}(\Sigma, \mathbb{R}) \underset{\delta^{q-1*}}{\overset{\delta^{q-1}}{\rightleftarrows}} C^q(\Sigma, \mathbb{R}) \underset{\delta^{q*}}{\overset{\delta^q}{\rightleftarrows}} C^{q+1}(\Sigma, \mathbb{R}), \tag{1.69}$$

enabling us to define the following three operators on $C^q(\Sigma, \mathbb{R})$:

Definition 1.3.8 (i) The *q-dimensional combinatorial up Laplace operator* or simply q-up Laplace operator of the simplicial complex Σ is

$$L^q{}_{up} := (\delta^q)^* \delta^q,$$

(ii) the *q-dimensional combinatorial down Laplace operator* or q-down Laplace operator

$$L^q{}_{down} := \delta^{q-1}(\delta^{q-1})^*,$$

(iii) the *q-dimensional combinatorial Laplace operator* or q-Laplace operator

$$L^q := L^q{}_{up} + L^q{}_{down} = (\delta^q)^* \delta^q + \delta^{q-1}(\delta^{q-1})^*.$$

For $q = 0$, that is, when we look at the operators on the vertices of a simplicial complex, we have $L^0{}_{down} = 0$, and hence

$$L^0 = L^0{}_{up}. \tag{1.70}$$

Similarly, for $q = \dim \Sigma$, the up-Laplacian vanishes, and

$$L^{\dim \Sigma} = L^{\dim \Sigma}{}_{down}. \tag{1.71}$$

The operators L^q_{up}, L^q_{down} and L^q are obviously self-adjoint. Also

Lemma 1.3.1 *The operators $L = L^q_{up}, L^q_{down}, L^q$ are nonnegative, that is, they satisfy*

$$(Lf, f) \geq 0 \, \textit{for all } f \in C^q. \tag{1.72}$$

Proof We have, generalizing (1.14),

$$(L^q_{up} f, f) = ((\delta^q)^* \delta^q f, f) = (\delta^q f, \delta^q f) \geq 0 \tag{1.73}$$

$$(L^q_{down} f, f) = (\delta^{q-1}(\delta^{q-1})^* f, f) = ((\delta^{q-1})^* f, (\delta^{q-1})^* f) \geq 0 \tag{1.74}$$

$$(L^q f, f) = (\delta^q f, \delta^q f) + ((\delta^{q-1})^* f, (\delta^{q-1})^* f) \geq 0. \tag{1.75}$$

In particular, from 1.73-1.75

Corollary 1.3.1

$$L^q_{up} f = 0 \ \text{ if and only if } \ \delta^q f = 0 \tag{1.76}$$
$$L^q_{down} f = 0 \ \text{ if and only if } \ (\delta^{q-1})^* f = 0 \tag{1.77}$$
$$L^q f = 0 \ \text{ if and only if } \ \delta^q f = 0 \text{ and } (\delta^{q-1})^* f = 0. \tag{1.78}$$

Since the operators L^q_{up}, L^q_{down} and L^q are self-adjoint, nonnegative operators on finite-dimensional Hilbert spaces, we have

Theorem 1.3.2 *The eigenvalues of the operators $L^q_{up}(\Sigma)$, $L^q_{down}(\Sigma)$ and $L^q(\Sigma)$ are real and nonnegative.*

Corollary 1.3.1 characterizes the eigenvalue 0. The other eigenvalues then are positive. Furthermore, Theorem 1.2.1 tells us that the eigenvalues admit a variational characterization

We can easily prove Eckmann's theorem [40], which is a discrete version of the Hodge theorem.

Theorem 1.3.3 *For a simplicial complex Σ,*

$$\ker L^q(\Sigma) \cong H^q(\Sigma, \mathbb{R}).$$

Thus, the multiplicity of the eigenvalue 0 of the operator $L^q(\Sigma)$ equals the dimension of $H^q(\Sigma, \mathbb{R})$, that is, the Betti number b_q.

Proof By 1.78,

$$\begin{aligned} \ker L^q(\Sigma) &= \ker \delta^q \cap \ker \delta^{q-1^*} \\ &= \ker \delta^q \cap (\mathrm{im}\delta^{q-1})^{\perp} \\ &\cong H^q(\Sigma, \mathbb{R}). \end{aligned}$$

Also, one readily checks that $\dim H^q(\Sigma, \mathbb{R}) = \dim H_q(\Sigma, \mathbb{R}) = b_q$.

While cohomology groups, like homology groups, were defined as quotients, that is, as equivalence classes of elements of C^q, Theorem 1.3.3 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 nonzero part of the spectrum.

Since $\delta^q \delta^{q-1} = 0$ and $\delta^{q-1^*} \delta^{q*} = 0$ (recall 1.69),

$$\mathrm{im} L^q_{down}(\Sigma) \subset \ker L^q_{up}(\Sigma), \tag{1.79}$$
$$\mathrm{im} L^q_{up}(\Sigma) \subset \ker L^q_{down}(\Sigma). \tag{1.80}$$

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

$$\mathrm{spec}_{\neq 0}(L^q(\Sigma)) = \mathrm{spec}_{\neq 0}(L_i^{up}(\Sigma)) \cup \mathrm{spec}_{\neq 0}(L_i^{down}(\Sigma)). \tag{1.81}$$

The multiplicity of the eigenvalue 0 may be different, however.

Since $\mathrm{spec}_{\neq 0}(AB) = \mathrm{spec}_{\neq 0}(BA)$, for linear operators A and B on Hilbert spaces, we get the following equality.

$$\mathrm{spec}_{\neq 0}(L^q_{up}(\Sigma)) = \mathrm{spec}_{\neq 0}(L^{q+1}_{down}(\Sigma)). \tag{1.82}$$

From (1.81) and (1.82) we conclude that each of the three families of multisets

$$\begin{aligned}&\{\mathrm{spec}_{\neq 0}(L^q(\Sigma)) \mid 0 \le q \le m\}, \{\mathrm{spec}_{\neq 0}(L^q_{up}(\Sigma)) \mid 0 \le q \le m-1\}\\ &\text{or } \{\mathrm{spec}_{\neq 0}(L^q_{down}(\Sigma)) \mid 1 \le q \le m\}\end{aligned}$$

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 look at scalar products on the spaces of cochains, as needed for the definition of the Laplace operators. Here, we only consider positive inner products, and when we shall speak about a scalar product in the sequel, we shall always assume that it be positive definite.

Each simplex generates a cochain, consisting of its real multiples. We assume that the cochains generated by different simplices are orthogonal to each other. This restricts the possible scalar products. A scalar product with this property can be obtained from a *weight function* w that associates to every simplex σ a positive real number. In fact, any such positive inner product on the space $C^q(\Sigma, \mathbb{R})$ can be written in terms of a weight function w as

$$(f, g)_{C^q} = \sum_{\sigma \in S_q} w(\sigma) f([\sigma]) g([\sigma]), \tag{1.83}$$

where S_q is the space of q-simplices by S_q. In the sequel, we shall write $\mathrm{sgn}([\sigma], [\sigma']) = \pm 1$ for two orientations of a simplex when those orientations coincide/differ. We also write $\partial\sigma$ for the cellular boundary of a simplex, that is, for the collection of its facets.

By simple linear algebra, the q-up Laplace operator is then given by

$$\begin{aligned}(L^q_{up} f)([\sigma]) &= \sum_{\substack{\rho \in S_{q+1}: \\ \sigma \in \partial\rho}} \frac{w(\rho)}{w(\sigma)} f([\sigma])\\ &+ \sum_{\substack{\sigma' \in S_q : \sigma \neq \sigma', \\ \sigma, \sigma' \in \partial\rho}} \frac{w(\rho)}{w(\sigma)} \mathrm{sgn}([\sigma], \partial[\rho]) \mathrm{sgn}([\sigma'], \partial[\rho]) f([\sigma']),\end{aligned} \tag{1.84}$$

and the q-down Laplace operator is

$$(L^q_{down} f)([\sigma]) = \sum_{\tau \in \partial\sigma} \frac{w(\sigma)}{w(\tau)} f([\sigma]) + \sum_{\sigma' : \sigma \cap \sigma' = \tau} \frac{w(\sigma')}{w(\tau)} \mathrm{sgn}([\tau], \partial[\sigma]) \mathrm{sgn}([\tau], \partial[\sigma']) f([\sigma']). \tag{1.85}$$

For our purposes, however, we need some relation between the weights in different dimensions.

Definition 1.3.9 *The degree* of a q-simplex σ of Σ is

$$\deg \sigma := \sum_{\rho \in S_{q+1}(\Sigma) : \sigma \in \partial\rho} w(\rho). \tag{1.86}$$

Definition 1.3.10 If the weight function w on Σ satisfies

$$w(\sigma) = \deg \sigma, \tag{1.87}$$

for every $\sigma \in S_q(\Sigma)$, we call the Laplace operator defined on the cochain complex of Σ the *weighted normalized combinatorial Laplace operator*. If in addition the weights of the facets of Σ are equal to 1, then the Laplace operator is called the *normalized combinatorial Laplace operator*.

When 1.87 holds, 1.84 simplifies to become

$$(L^q_{up} f)([\sigma]) = f([\sigma]) + \frac{1}{\deg \sigma} \sum_{\substack{\sigma' \in S_q : \sigma \neq \sigma', \\ \sigma, \sigma' \in \partial\rho}} w(\rho) \mathrm{sgn}([\sigma], \partial[\rho]) \mathrm{sgn}([\sigma'], \partial[\rho]) f([\sigma']). \tag{1.88}$$

In the following, we discuss only the results related to the normalized combinatorial Laplace operator; the results for a more general case can be found in [12, 13].

1.3.3 Spectra of Simplicial Complexes

In the following, we restrict our analysis of $L^q_{up}(\Sigma)$ to pure, $(q + 1)$-dimensional simplicial complexes. It follows from the definition that simplices of dimension lower than $q - 1$ and higher than $q + 1$ will have no influence on the non-zero spectrum of $L^q_{up}(\Sigma)$.

We could refine the class of relevant simplicial complexes even further, without any loss of generality , by limiting our attention to q-path connected components.

Definition 1.3.11 A simplicial complex Σ is q-path connected if and only if for any two q-faces E, F of Σ there exists a sequence of q-simplices $E = F_0, F_1, \dots, F_n = F$, such that every two neighbouring simplices intersect in a $(q-1)$-face, i.e., they are $(q-1)$-down neighbours. The maximal q-path connected subcomplexes of Σ are called *q-path connected components*.

Any two q-path connected components share faces of dimension $q-2$, at most, therefore $\operatorname{spec}_{\neq 0}(L^q_{up}(\Sigma))$ is a multiset union of its q-path connected components. Hence, without loss of generality we shall assume that simplicial complexes in the subsequent analysis are pure and $q+1$- path connected.

We first generalize Lemma 1.2.4

Lemma 1.3.2 *All eigenvalues of L^q_{up} satisfy*

$$0 \leq \lambda \leq q+2. \tag{1.89}$$

Proof The spectrum of any bounded symmetric operator on a Hilbert space is real. Operator L^q_{up} is self-adjoint, thus symmetric, hence its eigenvalues are real. The non-negativity follows from the Courant-Fischer-Weyl theorem and non-negative weights.

Furthermore, for every $f \in C^q(\Sigma, \mathbb{R})$

$$\begin{aligned}
(L^q_{up} f, f) &= (\delta f, \delta f) \\
&= \Big(\sum_{\bar F \in S_{q+1}(\Sigma)} f(\partial[\bar F])\, \mathrm{e}_{[\bar F]}, \sum_{\bar F \in S_{q+1}(K)} f(\partial[\bar F])\, \mathrm{e}_{[\bar F]} \Big) \\
&= \sum_{\bar F \in S_{q+1}(K)} f(\partial[\bar F])^2 w(\bar F) \\
&\leq (q+2) \sum_{F \in S_q(K)} f([F])^2 \sum_{\bar F \in S_{q+1}(K): F \in \partial \bar F} w(\bar F) && (1.90) \\
&= (q+2) \sum_{F \in S_q(K)} f([F])^2 \deg F && (1.91) \\
&= (q+2)(f, f). && (1.92)
\end{aligned}$$

Here $\mathrm{e}_{\bar F}$ denotes the elementary functional and (1.90) is obtained by using the Cauchy-Schwarz inequality. From (1.92) and the Courant-Fischer-Weyl min-max principle (Theorem 1.2.1) it follows that $\lambda \leq q+2$ for all $\lambda \in \operatorname{spec}(L^q_{up})$

The exact number of zero eigenvalues in the spectrum of L^q_{up} is given in the following theorem.

Theorem 1.3.4 *The multiplicity of the eigenvalue zero in* $\operatorname{spec}(L^q_{up})$ *is*

$$\dim C^q - \sum_{i=0}^{q} (-1)^{i+q} (\dim C^i - \dim H^i), \tag{1.93}$$

or equivalently

$$\dim C^q + \sum_{i=1}^{\dim K - q} (-1)^i (\dim C^{q+i} - \dim H^{q+i}). \tag{1.94}$$

Proof The following are short exact sequences that split

$$0 \to \ker \delta_q \to C^q \to \operatorname{im} \delta_q \to 0,$$

$$0 \to \operatorname{im} \delta_{q-1} \to \ker \delta_q \to H^q \to 0.$$

This is a direct consequence of the fact that $\operatorname{im} \delta_q$ and H^q are projective modules. Therefore,

$$\dim C^q = \dim \ker \delta_q + \dim \operatorname{im} \delta_q, \tag{1.95}$$

and

$$\dim \ker \delta_q = H^q + \dim \operatorname{im} \delta_{q-1}. \tag{1.96}$$

From (1.95) and (1.96)

$$\dim \operatorname{im} \delta_q = \sum_{i=0}^{q} (-1)^{q+i} (\dim C^i - \dim H^i).$$

The number of zeros in the spectrum of L^q_{up} is equal to the dimension of its kernel, thus

$$\begin{aligned} \dim \ker L^q_{up} &= \dim \ker \delta_q \\ &= \dim C^q - \sum_{i=0}^{q} (-1)^{q+i} (\dim C^i - \dim H^i). \end{aligned}$$

The expression (1.94) for the number of zeros in $\operatorname{spec}(L^q_{up})$ is easily obtained by using the Euler characteristic and the equality $\chi = \sum_{i=0}^{\dim \Sigma} (-1)^i \dim C^i = \sum_{i=0}^{\dim \Sigma} (-1)^i \dim H^i$.

Corollary 1.3.2 *Let Σ be a pure simplicial complex of dimension $q+1$, then the number of zero eigenvalues in the spectrum of $L^q_{up}(\Sigma)$ is $\dim C^q - \dim C^{q+1} + \dim H^{q+1}$.*

Using the above results, we can derive some lower bounds for the maximal eigenvalue of $L^q_{up}(\Sigma)$.

Theorem 1.3.5 *Let Σ be a pure simplicial complex of dimension $q+1$; let λ_m be the maximum eigenvalue in the spectrum of L^q_{up}, then*

$$\frac{\dim C^q}{(\dim C^{q+1} - \dim H^{q+1})} \leq \lambda_m. \tag{1.97}$$

Proof The sum of all eigenvalues is equal to the trace of the Laplace matrix, and in the case of the normalized Laplacian, the trace of the q-dimensional upper Laplacian equals the number of q-simplices.

The number of zero eigenvalues in the spectrum of L^q_{up} according to Corollary 1.3.2 is $\dim C^q - \dim C^{q+1} + \dim H^{q+1}$. Thus, the number of non-zero eigenvalues in L^q_{up} is exactly $\dim C^{q+1} - \dim H^{q+1}$. Hence,

$$\frac{\dim C^q}{(\dim C^{q+1} - \dim H^{q+1})} \leq \lambda_m,$$

which proves the theorem. □

Note that for $q = 0$ (i.e., for graphs) inequality (1.97) reduces to $\frac{V}{(E-\dim H^1)} = \frac{V}{(V-1)} \leq \lambda_m$, and it attains the lower bound when the underlying graph is complete. Interestingly, when Σ is a $q+1$-dimensional simplex, then from 1.97 it follows that $q + 2 \leq \lambda_m$; together with the inequality from Lemma 1.3.2 we conclude $\lambda_m = q + 2$.

The upper bound for the spectrum of the normalized graph Laplacian ($q = 0$) is 2 and is attained for bipartite graphs. There are many possible characterisations of bipartite graphs, the one that we will consider in this section is

Definition 1.3.12 A 1-dimensional simplicial complex (a graph) is bipartite if and only if it has no cycles of odd length.

We shall then see that we can generalize the characterization of bipartite graphs, as attaining the upper bound 2 for the largest eigenvalue, for the upper bound $q + 2$ of $\text{spec}(L^q_{up}(\Sigma))$. We shall start with the definition of high dimensional cycles, which we shall refer to as circuits, to avoid the confusion with co-chain cycles.

Definition 1.3.13 A pure simplicial complex Σ of dimension q is called a *q-path of length m* if there is an ordering of its q-simplices $F_1 < F_2 < \ldots < F_m$, such that F_i and F_j are $(q-1)$-down neighbours if and only if $| j - l |= 1$; Σ is an *i-circuit* of length $(m-1)$ when $F_m = F_1$.

Theorem 1.3.6 *Let Σ be a pure q-connected simplicial complex, then the following statements are equivalent:*

(1) $q + 2$ is an eigenvalue of $L^{up}_q(\Sigma)$,
(2) There are no $(q+1)$-orientable circuits of odd length nor $(q+1)$-non orientable circuits of even length in Σ.

The following holds

$$(L^q_{up}(\Sigma)f, f) = \sum_{\bar{F}\in S_{q+1}(\Sigma)} f(\partial[\bar{F}])^2 w(\bar{F})$$
$$\leq (q+2) \sum_{F\in S_q(\Sigma)} f([F])^2 \deg(F). \tag{1.98}$$

The equality in (1.98) is reached if and only if there exists a function $f \in C^q(\Sigma, \mathbb{R})$, such that

$$\operatorname{sgn}([F_i], \partial[\bar{F}]) f([F_i]) = \operatorname{sgn}([F_j], \partial[\bar{F}]) f([F_j]),$$

for every $\bar{F}$ in S_{q+1} and every $F_i, F_j \in \partial\bar{F}$. Thus, $|f([F])|$ is a constant for every $F \in S_q(\Sigma)$; without loss of generality we shall assume further that $|f([F])|= 1$, then $f([F])$ is equal either to $\operatorname{sgn}([F], \partial[\bar{F}])$ or $-\operatorname{sgn}([F], \partial[\bar{F}])$, for every $F \in \partial\bar{F}$. Therefore, f could be viewed as a choice of orientation on the $(q + 1)$-skeleton of Σ.

Theorem 1.3.7 *The existence of a function f satisfying the equality in (1.98) is equivalent to the existence of an orientation on the $(q + 1)$-skeleton of Σ, for which any two $(q + 1)$-simplices intersecting in a common q-face induce the same orientation on the intersecting simplex (This condition is opposite to the condition of coherently oriented simplices).*

Proof (**Proof of Theorem** 1.3.6) (1) $\Rightarrow$ (2) proceeds by contradiction.
Assume that there exists a $(q + 1)$-orientable circuit of odd length, whose q-simplices $F_1,\ldots, F_{2m+1}$ are ordered as suggested in Definition 1.3.13. Then it is possible to orient these simplices in such a way that every two neighbouring simplices induce different orientations on their intersecting face. Denote these oriented simplices by $[F_1], \ldots, [F_{2m+1}]$. In order to have the same orientation induced on the intersecting face, we reverse the orientation of every simplex $[F_k]$, for k even. Thus, $[F_i]$ and $-[F_{i+1}]$ induce the same orientation on $[F_i \cap F_{i+1}]$, for every $1 \leq i \leq 2m$. However, $[F_1]$ and $[F_{2m+1}]$ remain coherently oriented, which contradicts Theorem 1.3.7. The analysis for the case of $(n + 1)$-non-orientable circuits is analogous.

(2) $\Rightarrow$ (1) proceeds by contradiction. We shall assume (2) and $\neg$(1), i.e. $q + 2 \notin \operatorname{spec}(L^q_{up}(\Sigma))$; by Theorem 1.3.7 the former is equivalent to non-existence of an orientation which induces incoherent orientations on neighbouring q-simplices. Namely, any attempt to assign incoherent orientations to neighbouring simplices would eventually result in two neighbouring simplices with coherent orientations.

More precisely, let F_{i_1} be an arbitrary $(q + 1)$-face of Σ; and let $[F_{i_1}]$ be the *initial* positively oriented face. Let $[F_{i_1 i_2 \ldots i_m}]$ be a $(q + 1)$-face of Σ which shares a q-face with $[F_{i_1 i_2 \ldots i_{m-1}}]$; assume both faces induce the same orientation on their intersecting face and are oriented incoherently. Then by $\neg$(1) this construction will eventually lead us to a point where $F_{i_1 i_2 \ldots i_m} \equiv F_{i_1 i_2 \ldots i_k}$, but $[F_{i_1 i_2 \ldots i_m}] = -[F_{i_1 i_2 \ldots i_k}]$. Notice that by construction, $\{F_{i_1 i_2 \ldots i_m}, F_{i_1 i_2 \ldots i_{m+1}}, \ldots, F_{i_1 i_2 \ldots i_k}\}$ is a circuit. However, the only circuits which do not admit incoherent orientations are odd orientable or even non-orientable circuits, which contradicts (2).

1.3.4 Spectra of Some Special Classes of Simplicial Complexes

In this section we shall fully describe the spectrum of $L^q_{up}(\Sigma)$ for some basic classes of simplicial complexes:

- $(n-1)$-simplex
- n- path
- n-circuit
- n-star

Theorem 1.3.8 *Let Σ be a simplex on n vertices, i.e., an $(n-1)$-dimensional simplex. Then*

$$\operatorname{spec}(L^q_{up}(\Sigma)) = \left\{0^{(\binom{n-1}{q})}, \frac{n}{n-q-1}^{(\binom{n-1}{q+1})}\right\}.$$

Proof We shall proceed to construct an eigenfunction $f \in C^q(\Sigma, \mathbb{R})$, corresponding to the Eigenvalue $\frac{n}{n-q-1}$. In particular,

$$f = f_{[\bar{F}]}([F]) = \begin{cases} \operatorname{sgn}([F], \partial[\bar{F}]) \text{ if } F \text{ is facet of } (q+1)\text{-face } \bar{F} \\ \quad 0 \qquad\qquad \text{otherwise.} \end{cases}$$

There are exactly $\binom{n-1}{q+1}$ linearly independent functions of this form. In the following, we shall verify that the equality

$$(L^q_{up} f_{[\bar{F}]})[F] = \frac{n}{n-q-1} f([F])$$

holds for every q-dimensional face F of Σ. We shall distinguish three possibilities for F and $\bar{F}$:
(i) F is an arbitrary facet of $\bar{F}$. Then,

$$\begin{aligned}
(L^q_{up} f_{[\bar{F}]})([F]) = & \sum_{\substack{\bar{E}\in S_{q+1}: \\ F\in\partial\bar{E}}} \frac{w(\bar{E})}{w(F)} f_{[\bar{F}]}([F]) \\
& + \sum_{\substack{F'\in S_q(L): \\ (\exists \bar{E}\in S_{q+1}(L)) F, F'\in\partial\bar{E}}} \frac{w(\bar{E})}{w(F)} \operatorname{sgn}([F], \partial[\bar{E}]) \operatorname{sgn}([F'], \partial[\bar{E}]) f_{[\bar{F}]}([F']) \\
= & \frac{1}{n-q-1} \sum_{\substack{\bar{E}\in S_{q+1}: \\ F\in\partial\bar{E}}} f_{[\bar{F}]}(F) \\
& + \frac{1}{n-q-1} \sum_{\substack{F'\in S_q(L): \\ (\exists \bar{E}\in S_{q+1}(L)) F, F'\in\partial\bar{E}}} \operatorname{sgn}([F], \partial[\bar{E}]) \operatorname{sgn}([F'], \partial[\bar{E}]) f_{[\bar{F}]}([F']) \\
= & f_{[\bar{F}]}([F]) + \frac{q+1}{n-q-1} \operatorname{sgn}([F], \partial[\bar{F}]) \\
= & \frac{n}{n-q-1} f([F]).
\end{aligned}$$

(ii) F and $\bar{F}$ have q vertices in common, i.e., their intersection is a face of dimension $q-1$.
Then by definition $f_{\bar{F}}([F]) = 0$. Let $v_0, v_1, \ldots, v_{q+2} \in [n]$ be arbitrary vertices of Σ; then we shall assume without loss of generality that $\bar{F} = [v_0, \ldots, \hat{v}_l, \ldots, v_{q+2}]$ and $[F] = [v_0, \ldots, \hat{v}_j, \ldots, \hat{v}_k, \ldots, v_{q+2}]$ for $0 \leq j < k < l \leq q+2$. Therefore, there are exactly two q-faces, F_1 and F_2, in the boundary of $\bar{F}$, and two $(i+1)$-simplices, $\bar{F}_1$ and $\bar{F}_2$, of Σ, such that $F, F_1 \in \partial \bar{F}_1$ and $F, F_2 \in \partial \bar{F}_2$. In particular, $F_1 = [v_0, \ldots, \hat{v}_k, \ldots, \hat{v}_l, \ldots, v_{i+2}]$, $F_2 = [v_0, \ldots, \hat{v}_j, \ldots, \hat{v}_l, \ldots, v_{i+2}]$ and $\bar{F}_1 = [v_0, \ldots, \hat{v}_k, \ldots, v_{i+2}]$, $\bar{F}_2 = [v_0, \ldots, \hat{v}_j, \ldots, v_{i+2}]$. Now it is straightforward to calculate

$$\begin{aligned}
(L^q_{up} f_{[\bar{F}]})([F]) &= 0 + \operatorname{sgn}([F], \partial[\bar{F}_1])\operatorname{sgn}([F_1], \partial[\bar{F}_1]) f_{[\bar{F}]})([F_1]) \\
&\quad + \operatorname{sgn}([F], \partial[\bar{F}_2])\operatorname{sgn}([F_2], \partial[\bar{F}_2]) f_{[\bar{F}]})([F_2]) \\
&= \operatorname{sgn}([F], \partial[\bar{F}_1])\operatorname{sgn}([F_1], \partial[\bar{F}_1])\operatorname{sgn}([F_1], \partial[\bar{F}]) \\
&\quad + \operatorname{sgn}([F], \partial[\bar{F}_2])\operatorname{sgn}([F_2], \partial[\bar{F}_2])\operatorname{sgn}([F_2], \partial[\bar{F}]) \\
&= (-1)^j(-1)^{l-1}(-1)^k + (-1)^{k-1}(-1)^{l-1}(-1)^j \\
&= 0.
\end{aligned}$$

(iii) F and $\bar{F}$ have less than q vertices in common.
Obviously, there are no faces in the boundary of $\bar{F}$ which are $(q+1)$-up neighbours of F. This implies that $L^q_{up} f([F]) = 0$, which completes the proof.

Remark Let K be a $q+1$-combinatorial manifold, possibly with boundary. Then, by orienting it, that is by orienting its $(q+1)$-simplices coherently, we in fact choose a basis $B_{q+1}(\Sigma)$ of the vector space $C_{q+1}(\Sigma, \mathbb{R})$ consisting of elementary $(q+1)$-chains $[\bar{F}]$ that are oriented *coherently*.

For the subsequent calculations, the following elementary result will be useful.

Lemma 1.3.3 *When two matrices M and P commute, i.e., $MP = PM$, and when λ is a simple eigenvalue of P, then its corresponding eigenvector v is also an eigenvector of M.*

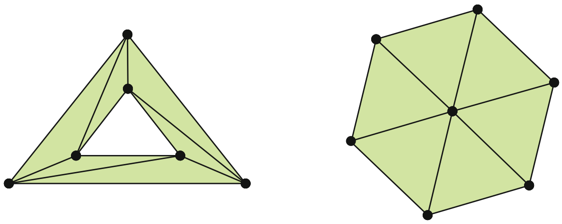
Proof Let $Pv = \lambda v$. Then $PMv = MPv = \lambda Mv$, and so, Mv is an eigenvector of P for λ. Since λ is simple, it must be a multiple of v.

Theorem 1.3.9 *Let Σ be an orientable n-circuit of length m. Then the eigenvalues of $L^n_{down}(\Sigma)$ are $n - \cos(2\pi i/m)$, $i = 0, 1, \ldots m-1$.*

Proof Let $F_1 < F_2 < \ldots < F_m$ be the ordering of n-simplices of Σ satisfying the conditions of Definition 1.3.13; and let $[F_1], [F_2], \ldots, [F_m]$ be a coherent orientatation. Let $p : C^n(\Sigma, \mathbb{R}) \to C^n(\Sigma, \mathbb{R})$ be a map, such that $p([F_i]) = [F_{i+1}]$, for all $1 \leq i < m$, and $p([F_m]) = [F_1]$.

It is not difficult to check that

Fig. 1.1 Examples of 2-circuits



(a) 2-circuit of length 6 (b) 2-circuit of length 6

$$pL^n_{down} = L^n_{down}p \tag{1.99}$$

Let P be the matrix associated to the mapping p. P is a permutation matrix and its characteristic polynomial is $\lambda^m - 1 = 0$. Eigenvectors of P are $U_\theta = (1,\ \theta,\ \theta^2, \dots \theta^{m-1})^T$, where θ is the m-th root of unity. Thus, the eigenfunctions of the map p are $u_\theta([F_i]) = \theta^{i-1}$.

With Lemma 1.3.3, we can now easily calculate the eigenvalues of L^n_{down}. Let $E_i := F_{i-1} \cap F_i$ for $2 \le i \le m-1$ and let $E_m := F_m \cap F_1$. We have

$$\begin{aligned}
L^n_{down}u_\theta([F_i]) = &\sum_{\substack{E \in S_{n-1}(L):\\ E \in \partial F_i}} \frac{w(F_i)}{w(E)}\theta^{i-1} \\
&+ \frac{w(F_i)}{w(E_i)}\mathrm{sgn}([E_i], \partial[F_i])\mathrm{sgn}([E_i], \partial F_{i-1})\theta^{i-2} \\
&+ \frac{w(F_i)}{w(E_{i+1})}\mathrm{sgn}([E_{i+1}], \partial[F_i])\mathrm{sgn}([E_{i+1}], \partial[F_{i+1}])\theta^{i} \\
= &(\frac{2}{2} + n - 1)\theta^{i-1} - \frac{1}{2}\theta^{i-2} - \frac{1}{2}\theta^i \\
= &\theta^{i-1}(i - \frac{\theta^{-1} + \theta}{2}) \\
= &\theta^{i-1}(n - \cos(\frac{2\pi i}{m})).
\end{aligned}$$

It is straightforward to check that a similar equality holds for $i = 1$ and $i = m$. Therefore the non zero spectrum of L^n_{down} is $\{n - \cos(2\pi i/m) \mid i = 0, 1, \dots m-1\}$.

Remark The eigenvalues of an orientable n-circuit depend only on its length, thus there are different combinatorial structures which give the same eigenvalues of L^n_{down}. For example, 1, 1.5, 1.5, 2.5, 2.5, 3 are the eigenvalues of L^2_{down} of both simplicial complexes in Fig. 1.1.

An analysis similar to the one above can be carried out for a non-orientable n-circuit of length m. In that case we define p to be

$$p([F_k]) = \begin{cases} [F_{k+1}] \text{ , for } 1 \leq k < m \\ -[F_1] \text{ , for } k = m. \end{cases} \tag{1.100}$$

The remaining calculations are carried out as in Theorem 1.3.9. Thus,

Theorem 1.3.10 *Let Σ be a non-orientable n-circuit of length m. Then the eigenvalues of $L^n_{down}(\Sigma)$ are $n - \sin(2\pi i/m)$ for m even and $n + \cos(2\pi i/m)$ for m odd, where $i = 0, 1, \dots m-1$.*

Proof The characteristic polynomial of the permutation matrix corresponding to the map p from (1.100) is

$$\begin{aligned}
&\det \begin{vmatrix} -\lambda & 1 & 0 & \dots & 0 \\ 0 & -\lambda & 1 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ -1 & 0 & \dots & \dots & -\lambda \end{vmatrix} = \\
=&(-1)^{m+1} \det \begin{vmatrix} 1 & 0 & \dots & 0 \\ -\lambda & 1 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ 0 & \dots & -\lambda & 1 \end{vmatrix} + (-\lambda)^{m+m} \det \begin{vmatrix} -\lambda & 1 & 0 & \dots & 0 \\ 0 & -\lambda & 1 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & \dots & -\lambda \end{vmatrix} \\
=&(-1)^{m+1} + \lambda^m.
\end{aligned}$$

Thus for m odd, the characteristic polynomal of the permutation matrix P is $\lambda^m + 1$. The Eigenvectors of P are $U_\theta = (-1, -\theta, (-\theta)^2, \dots, (-\theta)^{m-1})^T$, where θ is the m-th root of unity. Using Lemma 1.3.3, we can now easily calculate the eigenvalues of L^n_{down}.
Let $E_k := F_{k-1} \cap F_k$ for $2 \leq k \leq m-1$ and let $E_m := F_m \cap F_1$. We have

$$\begin{aligned}
L^n_{down} u_\theta([F_k]) = &\sum_{\substack{E \in S_{n-1}(L): \\ E \in \partial F_k}} \frac{w(F_k)}{w(E)} (-\theta)^{k-1} \\
&+ \frac{w(F_k)}{w(E_k)} \operatorname{sgn}([E_k], \partial[F_k]) \operatorname{sgn}([E_k], \partial F_{k-1}) (-\theta)^{k-2} \\
&+ \frac{w(F_k)}{w(E_{k+1})} \operatorname{sgn}([E_{k+1}], \partial[F_k]) \operatorname{sgn}([E_{k+1}], \partial[F_{k+1}]) (-\theta)^k \\
= &(\frac{2}{2} + n - 1)(-\theta)^{k-1} - \frac{1}{2}(-\theta)^{k-2} - \frac{1}{2}(-\theta)^k \\
= &(-\theta)^{k-1}(n - \frac{(-\theta)^{-1} - \theta}{2}) \\
= &(-\theta)^{k-1}(n - (-\cos(\frac{2\pi k}{m}) + i \sin(\frac{2\pi k}{m}) \\
&- \cos(\frac{2\pi k}{m}) - i \sin(\frac{2\pi k}{m}))/2) \\
= &(-\theta)^{k-1}(n + \cos(\frac{2\pi k}{m}))
\end{aligned}$$

If $k = 1$, then

$$
\begin{aligned}
L^n_{down} u_\theta([F_1]) &= (\frac{2}{2} + n - 1)(-\theta)^m + \frac{1}{2}(-\theta)^{m-1} - \frac{1}{2}(-\theta)^1 \\
&= (-\theta)^m (n - \frac{(-\theta)^{-1} - \theta}{2}) \\
&= (-\theta)^m (n + \cos(2\pi)) \\
&= n + 1.
\end{aligned}
$$

A similar relation holds for $k = m$. For the case when m is even, the proof is analogous to the above proof for m odd. Therefore the non-zero spectrum of $L^n_{down}(\Sigma)$ is

$$
\begin{cases}
\{n - \sin(2\pi i/m) \mid i = 0, 1, \ldots m - 1\} & \text{if } m \text{ is even} \\
\{n + \cos(2\pi i/m) \mid i = 0, 1, \ldots m - 1\} & \text{otherwise.}
\end{cases}
$$

Corollary 1.3.3 *The eigenvalues of $L^n_{down}(\Sigma)$ of an n-path K of length m are $\lambda_k = n - \cos(\pi k/m)$, for $k = 0, \ldots, m - 1$*

Proof Since there are no self-intersections of dimension $(n - 1)$ in an n-path, every path is orientable. From Theorem 1.3.9, follows that in the spectrum of the n-th down Laplacian of an n-circuit of length $2m$, all eigenvalues appear twice, except $(n - 1)$ and $(n + 1)$. In particular, $\lambda_k = n - \cos(k\pi/m) = n - \cos((2m - k)\pi/m) = \lambda_{2m-k}$, for $k \neq 0$ and $k \neq m$. Let $\phi = \exp(ik\pi/m)$, then the eigenvector corresponding to λ_k, $0 \leq k \leq m$ is $u_k = (1, \exp(ik\pi/m, \ldots, \exp(i(2m - 1)k\pi/m)^T$.

The function $v_k = u_k + u_{2m-k}$ is the eigenvector for the eigenvalue λ_k as well

$$
v_k(m) = \mathrm{e}^{i\frac{\pi k}{m}} + \mathrm{e}^{i\frac{\pi(2m-k)}{m}} = \mathrm{e}^{i\frac{\pi k}{m}} + \mathrm{e}^{-i\frac{\pi k}{m}}.
$$

It is now a straightforward calculation to see that the first m entries of v_k, for every $k = 0, 1, \ldots m - 1$, constitute the Eigenvectors of Σ for the eigenvalue $n - \cos(\pi k/m)$.

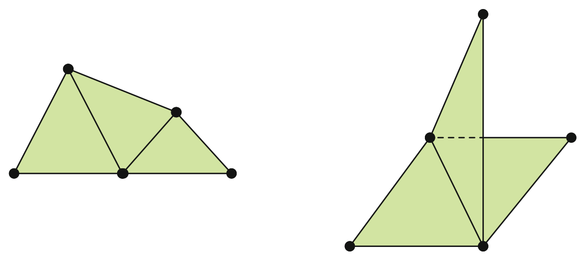
This idea generalizes to paths with self-intersections of dimension $(n - 1)$, but then it is necessary to distinguish among orientable and non-orientable paths. The eigenvalues of a star are described in the following theorem.

Theorem 1.3.11 *Let Σ be an n-star consisting of m, n-simplices. Then the non-zero eigenvalues of $L^n_{down}(\Sigma)$ are n with multiplicity $(m - 1)$ and $(n + 1)$ with multiplicity 1.*

Proof Let F_k, $k \in \{1, \ldots, m\}$, be an n-dimensional face of Σ and let $\bigcap_k F_k = E$. Let $p : B_n(\Sigma, \mathbb{R}) \to B_n(\Sigma, \mathbb{R})$ be a mapping, such that $p([F_k]) = [F_{k+1}]$. Since $F_k \cap F_i = E$, for any two n-faces of K, we can fix the orientations on the F_k such that they induce the same orientation on E. Now it is easy to check that

$$
pL^n_{down} = L^n_{down}p.
$$

Fig. 1.2 Examples of a path and a star



(a) 2-path of length 3

(b) 2-star with 3 rays

Let θ denote an m-th root of unity different from 1 and u the eigenvector of p corresponding to it. Then

$$\begin{aligned}L^n_{down}u_\theta([F_k]) =& \sum_{E,E\in\partial F_k} \frac{w(F_k)}{w(E)}\theta^{k-1} + \sum_{F,F\neq F_k} \frac{w(F)}{w(E)} u_\theta([F])\\ =& n\theta^{k-1} + \frac{1}{m}(1+\theta+\ldots+\theta^{m-1})\\ =& n\theta^{k-1}.\end{aligned}$$

Thus, u_θ is an eigenfunction of $L^n_{down}(\Sigma)$ corresponding to the eigenvalue n. The case when $\theta = 1$ results in the eigenvalue $n+1$ (Fig. 1.2).

1.3.5 Cheeger-Type Inequalities

It is a natural question to ask for Cheeger-type inequalities for the higher Laplacians on simplicial complexes. There are some results for the highest order Laplacian in [41, 42], but not much seems to be known in general.

1.4 Hypergraphs

1.4.1 The Laplacians

We present the Laplace operators on oriented hypergraphs as natural generalizations of those on graphs, following [14, 43–46]. The basic idea underlying the definition of an oriented hypergraph is the following. Assigning an orientation to the edge of a graph means going from one of its vertices, considered as its tail or input, to the other, its head or output. Reversing the orientation means changing the roles of the two vertices and going in the opposite direction. Thus, for an oriented hyperedge, we distinguish now two sets of vertices and move from the tail (input) set to the head (output) set. Here, more generally than for graphs, either of these sets could be empty.[1] Again, we can change the orientation by reversing roles and going in the opposite direction. And since Laplacians should be related to network flows, we treat all the members of the tail set as being parallel to each other, and the same for the head set.

In this section, we consider an oriented hypergraph Γ with vertex set V and hyperedge set H. For a vertex v, we let

$$\deg v := \big|\text{hyperedges containing } v\big| \tag{1.101}$$

and we assume that $\deg v > 0$ for all $v \in V$.

Definition 1.4.1 (Laplace operators) The Laplace operator for functions $f : V \to \mathbb{R}$ on the vertex set V of an oriented hypergraph is

$$\begin{aligned} L^0 f(v) := \; & \frac{\sum_{h_{\text{in}}:v \text{ input}} \left(\sum_{v' \text{ input of } h_{\text{in}}} f(v') - \sum_{w' \text{ output of } h_{\text{in}}} f(w') \right)}{\deg v} \\ & - \frac{\sum_{h_{\text{out}}:v \text{ output}} \left(\sum_{\hat{v} \text{input of } h_{\text{out}}} f(\hat{v}) - \sum_{\hat{w} \text{ output of } h_{\text{out}}} f(\hat{w}) \right)}{\deg v}. \end{aligned} \tag{1.102}$$

The Laplacian for functions $\gamma : H \to \mathbb{R}$ on the hyperedge set H, with $\gamma(h^+) = -\gamma(h^-)$ under a change of orientation, is

$$\begin{aligned} L^1 \gamma(h) := \; & \sum_{v_i \text{ input of } h} \frac{\sum_{h_{\text{in}}:v_i \text{ input}} \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}:v_i \text{ output}} \gamma(h_{\text{out}})}{\deg v_i} \\ & - \sum_{v^j \text{ output of } h} \frac{\sum_{h'_{\text{in}}:v^j \text{ input}} \gamma(h'_{\text{in}}) - \sum_{h'_{\text{out}}:v^j \text{ output}} \gamma(h'_{\text{out}})}{\deg v^j}. \end{aligned} \tag{1.103}$$

When we have a graph, that is, when each hyperedge has a single input and a single output, these two operators reduce to those defined in 1.2 and 1.5,

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

$$L^1 \gamma(e) = \frac{1}{\deg v_0} \cdot \sum_{v_0 \in e' = [v_0, w]} \gamma(e') - \frac{1}{\deg v_1} \cdot \sum_{v_1 \in e'' = [v_1, w]} \gamma(e'') \quad \text{for } e = [v_0, v_1],$$

because the neighbors of v are outputs of the edges for which v is an input and conversely.

And we can generalize all the constructions underlying those operators to the case of oriented hypergraphs. This will then provide us again with powerful tools to analyze the spectra.

[1] But our convention here, which is different from that employed for simplicial complexes is that they should not both be empty.

We start with the *scalar products*.

Definition 1.4.2 For $f, g : V \to \mathbb{R}$, let

$$(f, g)_V := \sum_{v \in V} \deg v \cdot f(v) \cdot g(v). \tag{1.104}$$

For $\omega, \gamma : H \to \mathbb{R}$, let

$$(\omega, \gamma)_H := \sum_{h \in H} \omega(h) \cdot \gamma(h). \tag{1.105}$$

The *boundary* operator is next. It maps functions on vertices to functions on hyperedges that change their sign upon a change of orientation, as always.

Definition 1.4.3 For $f : V \to \mathbb{R}$ and $h \in H$, let

$$\delta f(h) := \sum_{v_i \text{ input of } h} f(v_i) - \sum_{v^j \text{ output of } h} f(v^j). \tag{1.106}$$

We then have

Lemma 1.4.1 *The adjoint of the operator δ w.r.t. the scalar products 1.104, 1.105 is*

$$\delta^*(\gamma)(v) = \frac{\sum_{h_{in}: v \text{ input}} \gamma(h_{in}) - \sum_{h_{out}: v \text{ output}} \gamma(h_{out})}{\deg v}. \tag{1.107}$$

And we then have the analogue of Lemma 1.2.2

Lemma 1.4.2

$$L^0 = \delta^* \delta \tag{1.108}$$

$$L^1 = \delta \delta^* \tag{1.109}$$

and the analogue of Corollary 1.2.1

Corollary 1.4.1 *We have*

$$(f, L^0 f)_V = (\delta f, \delta f)_H = (L^0 f, f)_V \tag{1.110}$$

and

$$(\gamma, L^1 \gamma)_H = (\delta^* \gamma, \delta^* \gamma)_V = (L^1 \gamma, \gamma)_H \tag{1.111}$$

for all f, γ.
In particular, the operators L^0 and L^1 are self-adjoint and nonnegative, and all their eigenvalues are real and nonnegative.
L^0 and L^1 have the same spectrum, except possibly for the multiplicity of the eigenvalue 0.

While the details require a more complicated track keeping of inputs and outputs, the basic ideas of the *proofs* are the same as before, and so, we do not spell out the details here. After all, the point is that we have identified *natural* constructions.

We now consider the matrix formulations of L^0 and L^1. We denote by $v_1, \dots, v_N$ the vertices of Γ and by $h_1, \dots, h_M$ its hyperedges. Given a hyperedge h, we say that two vertices v_i and v_j are *co-oriented in h* if they either are both inputs, or both outputs, for h. Conversely, we say that v_i and v_j are *anti-oriented in h* if they both belong to h but have opposite orientations.

Definition 1.4.4 The *degree matrix* of Γ is the $N \times N$ diagonal matrix

$$D := \mathrm{diag}(\deg v_1, \dots, \deg v_N). \tag{1.112}$$

The *incidence matrix* of Γ is the $N \times M$ matrix $\mathcal{I} := (\mathcal{I}_{ij})_{ij}$, where

$$\mathcal{I}_{ij} := \begin{cases} 1 & \text{if } v_i \text{ is an input of } h_j \\ -1 & \text{if } v_i \text{ is an output of } h_j \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, each row $\mathcal{I}_i$ of $\mathcal{I}$ represents a vertex v_i and each column $\mathcal{I}^j$ of $\mathcal{I}$ represents a hyperedge h_j.

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 $i \neq j$,

$$\begin{aligned} A_{ij} :=& \left|\{\text{hyperedges in which } v_i \text{ and } v_j \text{ are anti-oriented}\}\right| \\ &- \left|\{\text{hyperedges in which } v_i \text{ and } v_j \text{ are co-oriented}\}\right|. \end{aligned}$$

The Laplacians can then be written, in matrix form, as

$$L^0 = \mathrm{Id} - D^{-1}A = D^{-1}\mathcal{I}\mathcal{I}^\top$$

and

$$L^1 = \mathcal{I}^\top D^{-1}\mathcal{I}.$$

In particular, this allows us to simplify (1.102) and 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.

Oriented hypergraphs were introduced by Shi in 1992 [47] as a generalization of signed graphs, that can be seen as oriented hypergraphs for which all hyperedges have size 2. Their corresponding spectral theory has been developed later. The adjacency matrix and the *algebraic Laplacian* $\mathcal{L} := \mathcal{I}\mathcal{I}^\top$ of an oriented hypergraph have been first introduced in [48], whereas the Laplacians L^0 and L^1 have been introduced in [14].

As for graphs, when the hypergraph is *regular*, that is $\deg v \equiv const$, then the spectra of L^0, $\mathcal{L}$ and A differ only by an additive or multiplicative constant. For general hypergraphs, their spectral theory is different. We refer the reader to [48–60] for a vast literature on the adjacency and algebraic Laplacian matrices of oriented hypergraphs. We refer to [14, 17, 34, 43–46, 55, 56, 61, 62] for literature on the hypergraph Laplacians L^0 and L^1, on which we shall focus. We refer to [63, 64] for applications of the latter theory to dynamical systems on hypergraphs.

1.4.2 The Spectrum

Spectra of oriented hypergraphs can exhibit features not found for graphs. In particular, most of the results derived in Sect. 1.2.2 do not generalize to hypergraphs. Let the hypergraph have N vertices. Then L^0 has N real and nonnegative eigenvalues, possibly with multiplicities,

$$0 \leq \lambda_1 \leq \cdots \leq \lambda_N \leq N.$$

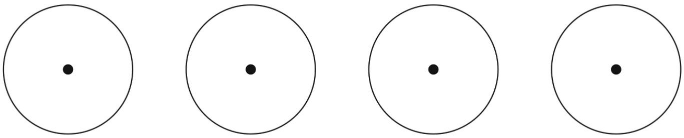
Likewise when we have M hyperedges, L^1 has M eigenvalues, the positive ones agreeing with those of L^0.

These eigenvalues always sum to N, since $L^0 = \mathrm{Id} - D^{-1}A$, therefore the trace of L^0 is N and this implies that also

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

Examples:

1. Consider a hypergraph whose vertices $v_1, \ldots, v_N$ are only contained in *self-loops*, i.e. hyperedges of cardinality 1.

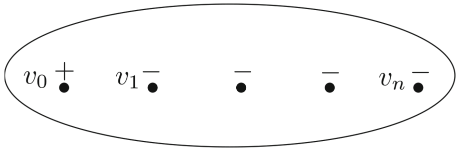


Then, for any function $f : V \to \mathbb{R}$, clearly

$$L^0 f(v_i) = f(v_i).$$

Hence, 1 is the only eigenvalue of L^0. In particular, 0 is not an eigenvalue in this case. This implies that Corollary 1.2.3 does no longer hold for the general case of hypergraphs.

2. Consider a hypergraph with vertices $v_0, v_1, \ldots, v_n$ and a single hyperedge h with v_0 as input and $v_1, \ldots, v_n$ as outputs.



Thus $\deg v = 1$ for all vertices, and

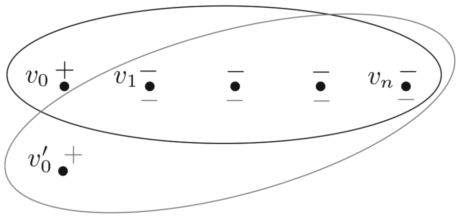
$$L^0 f(v_0) = f(v_0) - \sum_{i=1}^{n} f(v_i)$$

$$L^0 f(v_i) = \sum_{i=1}^{n} f(v_i) - f(v_0) \quad \text{for } i = 1, \ldots, n.$$

For $n = 1$, this is simply the line graph $K_{1,1}$. We let $i = 1, \ldots, n$. Eigenfunctions then are f_0 with $f_0(v_0) = n$, $f_0(v_i) = 1$ with the eigenvalue 0, $f_{i_0}(v_{i_0}) = 1$, $f_{i_0}(v_{j_0}) = -1$ for some pair $1 \leq i_0 < j_0 \leq n$ and $f_0(v_k) = 0$ for all other k, again with eigenvalue 0, and finally $f_{n+1}(v_0) = 1$, $f_{n+1}(v_i) = -1$ with the eigenvalue $n + 1$.

Thus, for $n > 1$, we have several eigenfunctions for the eigenvalue 0, but none of them is constant. This implies that the operator L^0 no longer obeys the maximum principle of Lemma 1.2.3.

3. We next double the vertex v_0, that is, introduce another vertex v_0' and a hyperedge h' with v_0' as input and $v_1, \ldots, v_n$ as outputs.



Then $\deg v_0 = \deg v_0' = 1$, but $\deg v_i = 2$ (as before, $i = 1, \ldots, n$). The previous eigenfunctions extend if we put $f(v_0') = f(v_0)$. We get another eigenfunction f' for the eigenvalue 1 with $f'(v_0) = 1$, $f'(v_0') = -1$, $f'(v_i) = 0$.

In the previous example, the duplication of a vertex produced the eigenvalue 1. This is always the case, as shown in Lemma 1.4.3 below, that generalizes the results on duplication for graphs that we systematically discussed in Sect. 1.2.3.

Definition 1.4.5 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,

$$A_{il} = A_{jl} \quad \text{for each } l = 1, \dots, N.$$

In particular, $A_{ij} = A_{jj} = 0$.

Remark In the case of graphs, Definition 1.4.5 coincides with the classical definition of duplicate vertices that we presented in Sect. 1.2.2.

Lemma 1.4.3 *Let v_i and v_j are duplicates of each other. Let $f : V \to \mathbb{R}$ be such that $f(v_i) = -f(v_j) \neq 0$ and $f = 0$ otherwise. Then, $L^0 f = f$, that is, 1 is an eigenvalue for L^0 and f is a corresponding eigenfunction.*

Proof It is easy to see that, by definition of f,

- $L^0 f(v_i) = f(v_i)$,
- $L^0 f(v_j) = f(v_j)$, and
- For each $l \neq i, j$,

$$\begin{aligned} L^0 f(v_l) &= -\frac{1}{\deg v_l}\big(A_{li} f(v_i) + A_{lj} f(v_j)\big) \\ &= -\frac{1}{\deg v_l}\big(A_{li} f(v_i) - A_{li} f(v_i)\big) \\ &= 0 = f(v_l). \end{aligned}$$

□

Corollary 1.4.2 *If there are n duplicate vertices, 1 is an eigenvalue with multiplicity at least $n - 1$.*

Proof Assume that $v_1, \dots, v_n$ are duplicate vertices. For each $i = 1, \dots, n-1$, 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 1.4.3 the f_i's are eigenfunctions corresponding to the eigenvalue 1. Also, $\dim(\mathrm{span}(f_1, \dots, f_{n-1})) = n - 1$, therefore the multiplicity of 1 is at least $n - 1$.

Similarly to duplicate vertices, we define and discuss *twin vertices*.

Definition 1.4.6 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 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 $A_{ij} < 0$. Also, while duplicate vertices exist for graphs, twin vertices cannot exist for graphs, since in this case each edge has one input and one output.

We now generalize the notions of duplicate vertices and twin vertices by defining *duplicate families of twin vertices*.

Definition 1.4.7 A family $V_1 \sqcup \ldots \sqcup V_l \subset V$ of vertices is an *l-duplicate family of t-twin vertices* if

- For each $a \in \{1, \ldots, l\}$, $|V_a| = t$ and the t vertices in V_a are twins of each other;
- For each $a, b \in \{1, \ldots, l\}$ with $a \neq b$, for each $v_i \in V_a$ and for each $v_j \in V_b$, v_i and v_j are duplicates of each other.

Proposition 1.4.1 *If* Γ *contains an* l*-duplicate family of* t *twins, then*

- t *is an eigenvalue with multiplicity at least* $l - 1$*, and*
- 0 *is an eigenvalue with multiplicity at least* $l(t - 1)$.

Proof In order to show that t is an eigenvalue with multiplicity at least $l - 1$, consider the following $l - 1$ functions. For $a = 2, \ldots, l$, let $f_a : V \to \mathbb{R}$ such that $f_a := 1$ on V_1, $f_a := -1$ on V_a and $f_a := 0$ otherwise. Then,

- For each $v_j \in V_1$,

$$L^0 f_a(v_j) = 1 - \frac{1}{\deg v_j} \sum_{v_k \in V_1 \setminus \{v_j\}} - \deg v_j = 1 + t - 1 = t \cdot f_a(v_j);$$

- For each $v_i \in V_a$,

$$L^0 f_a(v_i) = -1 - \frac{1}{\deg v_i} \sum_{v_k \in V_a \setminus \{v_i\}} \deg v_i = -1 - (t - 1) = t \cdot f_a(v_i);$$

- For each $v_k \in V \setminus V_1 \sqcup V_a$,

$$L^0 f_a(v_k) = -\frac{1}{\deg v_k} \left(\sum_{v_j \in V_1} A_{jk} - \sum_{v_i \in V_a} A_{ik} \right) = 0 = t \cdot f_a(v_k).$$

  Therefore, f_a is an eigenfunction for t. Furthermore, the functions $f_2, \ldots, f_l$ are linearly independent, hence t is an eigenvalue with multiplicity at least $l - 1$.

Similarly, in order to prove that 0 is eigenvalue with multiplicity at least $l(t - 1)$, let $V_a = \{v_1^a, \ldots, v_t^a\}$ and consider the $l(t - 1)$ functions $g_b^a : V \to \mathbb{R}$ defined as follows, for $a = 1, \ldots, l$ and $b = 2, \ldots, t$. Let $g_b^a(v_1^a) := 1$, $g_b^a(v_b^a) := -1$ and $g_b^a := 0$ otherwise. Then, each g_b^a is an eigenfunction for 0. Since, furthermore, these are $l(t - 1)$ linearly independent functions, 0 has multiplicity at least $l(t - 1)$.

1.4.3 Rayleigh Quotients and the Courant-Fischer-Weyl Scheme

The constructions of Sect. 1.2.3 naturally extend to oriented hypergraphs. In particular, all the eigenvalues of L^0 and L^1 can be characterized in terms of minmax values of Rayleigh quotients. For instance, the largest eigenvalue λ_N of L^0 (which is also the largest eigenvalue of L^1 can be characterized in two different ways [14]

$$\lambda_N = \max_f \frac{(\delta f, \delta f)_H}{(f, f)_V}$$
$$= \max_f \frac{\sum_{h \in H} \left(\sum_{v_i \text{ input of } h} f(v_i) - \sum_{v^j \text{ output of } h} f(v^j) \right)^2}{\sum_{v \in V} \deg v f(v)^2}$$

and

$$\lambda_N = \max_\gamma \frac{(\delta^* \gamma, \delta^* \gamma)_V}{(\gamma, \gamma)_H}$$
$$= \max_\gamma \frac{\sum_{v \in V} \frac{1}{\deg v} \cdot \left(\sum_{h_{\text{in}}: v \text{ input}} \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}: v \text{ output}} \gamma(h_{\text{out}}) \right)^2}{\sum_{h \in H} \gamma(h)^2}.$$

As a consequence of these characterizations of λ_N one can prove, for instance, Theorem 1.4.1 below [45], showing a generalization of the following inequalities that hold for graphs,

$$\frac{N}{N-1} \leq \lambda_N \leq 2,$$

that we have seen in Sect. 1.2, to the general case of hypergraphs. Before stating it, we need to define *bipartite hypergraphs*, which naturally generalize bipartite graphs, as well as a few other preliminary definitions. As we shall see, analogously to the graph case, λ_N gives a measure of bipartitness for all oriented hypergraphs.

Definition 1.4.8 A hypergraph Γ is *bipartite* (Fig. 1.3) if one can decompose the vertex set as a disjoint union $V = V_1 \sqcup V_2$ such that, for every hyperedge h of Γ, either h has all its inputs in V_1 and all its outputs in V_2, or vice versa.

Definition 1.4.9 The *cardinality* of a hyperedge h, denoted $|h|$, is the number of vertices in h. A hypergraph is said to be *k-uniform* if all its hyperedges have cardinality k.

Clearly, graphs and signed graphs are 2-uniform hypergraphs.

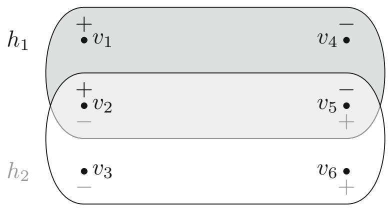


Fig. 1.3 A bipartite hypergraph with $V_1 = \{v_1, v_2, v_3\}$ and $V_2 = \{v_4, v_5, v_6\}$

Definition 1.4.10 A hypergraph $\hat{\Gamma} = (\hat{V}, \hat{H})$ is a *sub-hypergraph* of $\Gamma = (V, H)$, denoted $\hat{\Gamma} \subset \Gamma$, if $\hat{V} \subseteq V$ and

$$\hat{H} = \{h \cap \hat{V} : h \in H\}.$$

Given a sub-hypergraph $\hat{\Gamma} \subset \Gamma$, we let

$$\eta(\hat{\Gamma}) := \frac{\sum_{v \in \hat{V}} \frac{\deg_{\hat{\Gamma}}(v)^2}{\deg v}}{|\hat{H}|},$$

where $\deg_{\hat{\Gamma}}(v)$ denotes the degree of v in $\hat{\Gamma}$ and $|\hat{H}|$ is the number of hyperedges in $\hat{\Gamma}$.

Theorem 1.4.1 *For every connected, oriented hypergraph* Γ*,*

$$\lambda_N \leq \max_{h \in H} |h|, \tag{1.113}$$

with equality if and only if Γ *is bipartite and* $|h|$ *is constant for all* h*, and*

$$\lambda_N \geq \max_{\hat{\Gamma} \subset \Gamma \text{ bipartite}} \eta(\hat{\Gamma}). \tag{1.114}$$

Proof We first prove (1.113). Let $f : V \to \mathbb{R}$ be an eigenfunction for λ_N. Then,

$$\begin{aligned}
\lambda_N &= \frac{\sum_{h \in H} \left(\sum_{v_i \text{ input of } h} f(v_i) - \sum_{v^j \text{ output of } h} f(v^j) \right)^2}{\sum_{v \in V} \deg v f(v)^2} \\
&\leq \frac{\sum_{h \in H} \left(\sum_{v \in h} |f(v)| \right)^2}{\sum_{i \in V} \deg v f(v)^2},
\end{aligned}$$

with equality if and only if f has its nonzero values on a bipartite sub-hypergraph. Now, for each $h \in H$,

$$\begin{aligned}
\left(\sum_{v \in h} |f(v)| \right)^2 &= \sum_{v \in h} f(v)^2 + \sum_{\{v,w\}:\, v \neq w \in h} 2 \cdot |f(v)| \cdot |f(w)| \\
&\leq \sum_{v \in h} f(v)^2 + \sum_{\{v,w\}:\, v \neq w \in h} \left(f(v)^2 + f(w)^2 \right) \\
&= \sum_{v \in h} f(v)^2 + \sum_{v \in h} (|h| - 1) f(v)^2 \\
&= |h| \cdot \sum_{v \in h} f(v)^2,
\end{aligned}$$

with equality if and only if $|f|$ is constant on all $v \in h$. Therefore,

$$\begin{aligned}
\frac{\sum_{h\in H}\left(\sum_{v\in h}|f(v)|\right)^2}{\sum_{i\in V}\deg v f(v)^2} &\le \frac{\sum_{h\in H}\sum_{v\in h}|h|\cdot\sum_{v\in h} f(v)^2}{\sum_{i\in V}\deg v f(v)^2}\\
&= \frac{\sum_{v\in V}\sum_{h\ni v}|h|\cdot f(v)^2}{\sum_{i\in V}\deg v f(v)^2}\\
&\le \left(\max_{h\in H}|h|\right)\cdot\frac{\sum_{v\in V}\deg v f(v)^2}{\sum_{i\in V}\deg v f(v)^2}\\
&= \max_{h\in H}|h|,
\end{aligned}$$

where the first inequality is an equality if and only if $|f|$ is constant (since we assuming that Γ is connected), and the last inequality is an equality if and only if $|h|$ is constant for all h. Putting everything together, we have that

$$\lambda_N \le \max_{h\in H}|h|,$$

with equality if and only if $|h|$ is constant for all $|h|$ while $|f|$ is constant and it is defined on a bipartite sub-hypergraph (that is, $|f|$ is constant and Γ is bipartite). This proves the first claim.

It is left to prove (1.114). Given a bipartite sub-hypergraph $\hat{\Gamma}\subset\Gamma$, let $\gamma': H\to\mathbb{R}$ be 1 on $\hat{H}$ and 0 otherwise. Then, up to changing (without loss of generality) the orientations of the hyperedges,

$$\begin{aligned}
\lambda_N &= \max_{\gamma:H\to\mathbb{R}}\frac{\sum_{v\in V}\frac{1}{\deg v}\cdot\left(\sum_{h_{\text{in}}:v\text{ input}}\gamma(h_{\text{in}})-\sum_{h_{\text{out}}:v\text{ output}}\gamma(h_{\text{out}})\right)^2}{\sum_{h\in H}\gamma(h)^2}\\
&\ge \frac{\sum_{v\in V}\frac{1}{\deg v}\cdot\left(\sum_{h_{\text{in}}:v\text{ input}}\gamma'(h_{\text{in}})-\sum_{h_{\text{out}}:v\text{ output}}\gamma'(h_{\text{out}})\right)^2}{\sum_{h\in H}\gamma'(h)^2}\\
&\ge \frac{\sum_{v\in\hat{V}}\frac{1}{\deg v}\cdot\left(\sum_{h_{\text{in}}:v\text{ input}}\gamma'(h_{\text{in}})-\sum_{h_{\text{out}}:v\text{ output}}\gamma'(h_{\text{out}})\right)^2}{\sum_{h\in H}\gamma'(h)^2}\\
&= \frac{\sum_{v\in\hat{V}}\frac{\deg_{\hat{\Gamma}}(v)^2}{\deg v}}{|\hat{H}|}.
\end{aligned}$$

Since the above inequality is true for all $\hat{\Gamma}$, this proves (1.114).

Observe that, in the graph case, since $|h|=2$ for each (hyper)edge, (1.113) tells us that

$$\lambda_N \le 2,$$

with equality if and only if the graph is bipartite. (1.113) is therefore a generalization of the classical upper bound for λ_N of Corollary 1.2.4 to the case of hypergraphs.

Also, given 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, by (1.114),

$$\lambda_N \geq \eta(\hat{\Gamma}) = 1 + \sum_{w\sim v} \frac{1}{\deg w \cdot \deg v} \geq 1 + \sum_{w\sim v} \frac{1}{(N-1)\cdot \deg v} = 1 + \frac{1}{N-1} = \frac{N}{N-1}.$$

Hence, from (1.114), we can re-infer the fact that $\lambda_N \geq N/(N-1)$ for graphs.

In the following **examples**, we exhibit the sharpness of (1.114):

1. Let $\Gamma = K_N$ be the complete graph on N nodes. 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,

$$\eta(\hat{\Gamma}) = \frac{N}{N-1} = \lambda_N.$$

   Therefore, (1.114) is an equality for K_N.
2. Let $\Gamma = K_N \setminus \{(v_1, v_2)\}$ be the complete graph with an edge (v_1, v_2) removed. We know, from [19], that $\lambda_N = (N+1)/(N-1)$. Let $\hat{\Gamma}$ be the bipartite sub-graph of Γ given by the edges that have either v_1 or v_2 as endpoint. Then,

$$\eta(\hat{\Gamma}) = \frac{N+1}{N-1} = \lambda_N.$$

   Therefore, (1.114) is an equality for $\Gamma = K_N \setminus \{(v_1, v_2)\}$.
3. For a bipartite, k-uniform hypergraph Γ, by Theorem 1.4.1 $\lambda_N = k$. Also,

$$\eta(\Gamma) = \frac{\sum_{v\in V} \deg v}{M} = \frac{\sum_{h\in H} |h|}{M} = \frac{M\cdot k}{M} = k.$$

   Therefore, (1.114) is an equality also in this case.

Theorem 1.4.1 shows that, as in the graph case, the largest eigenvalue λ_N measures how different a hypergraph is from a bipartite one. Proposition 1.4.2 below shows that all bipartite hypergraphs that have the same vertices and hyperedges, independently of the input/output structure, are isospectral with each other. Before stating it, we define the *underlying hypergraph* and the *signless Laplacian* of Γ.

Definition 1.4.11 The *underlying hypergraph* of Γ is the oriented hypergraph obtained from Γ by letting each vertex be an input for all hyperedges in which it is contained. The *signless Laplacian* of Γ is the Laplacian L^0 of its underlying hypergraph.

Remark Assume that Γ is a graph and let Γ_+ be its underlying hypergraph. Then, the adjacency matrices of Γ and Γ_+ are such that $A(\Gamma_+) = -A(\Gamma)$, while the degree matrices of Γ and Γ_+ coincide. Therefore, the Laplacians of Γ and Γ_+ are

$$L^0(\Gamma) = \mathrm{Id} - D(\Gamma)^{-1}A(\Gamma) \quad \text{and} \quad L^0(\Gamma_+) = \mathrm{Id} + D(\Gamma)^{-1}A(\Gamma) = 2 \cdot \mathrm{Id} - L^0(\Gamma),$$

respectively. Hence, λ is an eigenvalue for $L^0(\Gamma)$ if and only if $2 - \lambda$ is an eigenvalue for $L^0(\Gamma_+)$.

Proposition 1.4.2 *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 L^0, 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.

We discuss two **examples,** namely the *hyperflowers*, that generalize star graphs, and the *c-complete hypergraphs*, that generalize complete graphs.

Example 4 Given $t \geq 1$, an oriented hypergraph $\Gamma = (V, H)$ on N nodes and M hyperedges is a *hyperflower with t twins* if (Fig. 1.4):

- The vertex set can be decomposed as $V = C \sqcup P$, where C is the *core* and P is given by tM *peripheral vertices* $v_{11}, \ldots, v_{t1}, \ldots, v_{1M}, \ldots, v_{tM}$;
- Forgetting about the input/output structure, the hyperedges are

$$h = C \sqcup \bigcup_{i=1}^{t} v_{ij} \ \text{ for } j = 1, \ldots, M.$$

If Γ is a bipartite hyperflower, by Proposition 1.4.2 we can assume, when computing the spectrum, that all its vertices are inputs for all the hyperedges in which they are contained. In this case, since all hyperedges have cardinality $N - tM + t$, by Theorem 1.4.1 $\lambda_N = N - tM + t$. Furthermore, by Proposition 1.4.1, t is an eigenvalue with multiplicity at least $M - 1$. We have therefore listed M eigenvalues whose sum is N. Since Γ has, in total, N eigenvalues whose sum is N, this implies that 0 has multiplicity $N - M$. Note that the star graph is a bipartite hyperflower with $t = N - M = 1$. Hence, the above computations show that the star graph has eigenvalues 0 with multiplicity 1, 1 with multiplicity $N - 2$ and 2 with multiplicity 1.

Example 5 Given $c \geq 2$, we say that Γ is a *c-complete hypergraph* if, forgetting about the input/output structure, its hyperedges are all possible $\binom{N}{c}$ hyperedges of

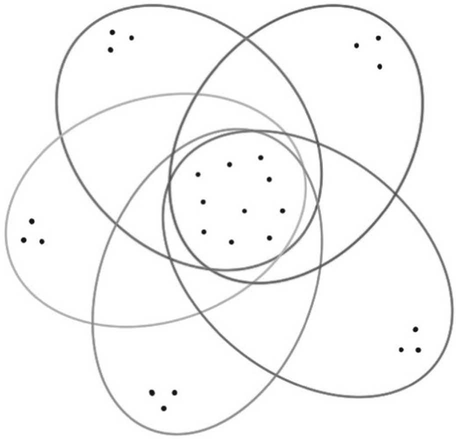


Fig. 1.4 A hyperflower with 3 twins

cardinality c. If Γ is a bipartite, c-complete hypergraph and we are interested in computing its spectrum, we can again assume, without loss of generality, that all vertices are always inputs for the hyperedges in which they are contained. In this case, by Theorem 1.4.1, $\lambda_N = c$. Moreover, observe that each vertex has degree $d := \binom{N-1}{c-1}$, while $a := A_{ij} = -\binom{N-2}{c-2}$ is constant for all $i \neq j$. Therefore, $\frac{a}{d} = -\frac{c-1}{N-1}$ and

$$L^0 f(v) = f(v) - \frac{a}{d}\left(\sum_{w \neq v} f(w)\right) = f(v) + \frac{c-1}{N-1}\left(\sum_{w \neq v} f(w)\right),$$

for all $v \in V$. Now, for each $i = 2, \ldots, N$, let $f_i(v_1) := 1$, $f_i(v_i) := -1$ and $f_i := 0$ otherwise. Then,

- $L^0 f_i(v_1) = 1 - \frac{c-1}{N-1} = \frac{N-c}{N-1} \cdot f_i(v_1)$,
- $L^0 f_i(v_i) = -1 + \frac{c-1}{N-1} = \frac{N-c}{N-1} \cdot f_i(v_i)$, and
- $L^0 f_i(v_j) = 0 = \frac{N-c}{N-1} \cdot f_i(v_j)$ for all $j \neq 1, i$.

Therefore, the f_i's are $N-1$ linearly independent eigenfunctions with eigenvalue $\frac{N-c}{N-1}$. This implies that the spectrum of Γ is given by c with multiplicity 1, and $\frac{N-c}{N-1}$ with multiplicity $N-1$.

In particular, if Γ is the complete graph K_N, we can apply the above computations to the underlying hypergraph of K_N (which is a signed graph) and say that this has eigenvalues 2 with multiplicity 1, and $\frac{N-2}{N-1}$ with multiplicity $N-1$. Since λ is an eigenvalue for the underlying hypergraph if and only if $2-\lambda$ is an eigenvalue for the original hypergraph, this implies that the eigenvalues of K_N are 0 with multiplicity 1 and $\frac{N}{N-1}$ with multiplicity $N-1$, as we already knew from Sect. 1.2.2.

1.4.4 Cheeger-Type Estimates

The Cheeger inequalities

$$\frac{1}{2}h^2 \leq \lambda_2 \leq 2h \tag{1.115}$$

for connected graphs (cf. (1.42)) have been generalized in [44] to the case of connected, k-uniform, bipartite hypergraphs, and it remains an open question whether they can be generalized for all connected oriented hypergraphs. The idea developed in [44] is the following. Given a connected graph Γ, its underlying hypergraph Γ_+ is a signed graph that has the same Cheeger constant as Γ. Moreover, λ is an eigenvalue for $L^0(\Gamma)$ if and only if $2-\lambda$ is an eigenvalue for $L^0(\Gamma_+)$. Therefore, the Cheeger inequalities in (1.115) can be equivalently reformulated in terms of the second largest eigenvalue of $L^0(\Gamma_+)$, as

$$\frac{1}{2}h(\Gamma_+)^2 \leq 2-\lambda_{N-1}(\Gamma_+) \leq 2h(\Gamma_+). \tag{1.116}$$

This equivalent formulation of the Cheeger inequalities in (1.115) can be used in order to prove a generalization for uniform, bipartite hypergraphs. We state the generalized inequalities, but we do not provide the proof here.

Let Γ be a connected, k-uniform, bipartite hypergraph. As for the case of graphs that we discussed in Sect. 1.2.4, given $S \subseteq V$, we let $\overline{S} := V \setminus S$ and

$$\mathrm{vol}(S) := \sum_{v \in S} \deg v.$$

Moreover, for $r \in \{1, \dots, k\}$, we let

$$E_r(S) := \{e \in E : |e \cap S| = r\}.$$

Clearly, for each $r \in \{1, \dots, k\}$, $E_r(S) = E_{k-r}(\overline{S})$. Also,

$$E_k(S) = \{e \in E : e \subseteq S\},$$

$$E_0(S) = \{e \in E : e \subseteq \overline{S}\}$$

and

$$\mathrm{vol}(S) = \sum_{r=1}^{k} r|E_r(S)|.$$

With the above notations, we can define the generalized Cheeger constant, as follows.

Definition 1.4.12 Given $\emptyset \neq S \subsetneq V$, let

$$h(S) := \frac{\sum_{r=1}^{k-1} |E_r(S)| r(k-r)}{\min\{\text{vol}(S), \text{vol}(\overline{S})\}}.$$

The *Cheeger constant* of Γ is

$$h := \min_{\emptyset \neq S \subsetneq V} h(S).$$

Observe that the quantity

$$\sum_{r=1}^{k-1} |E_r(S)| r(k-r)$$

appearing in the numerator of $h(S)$ counts the number of pairwise connections between S and $\overline{S}$. Furthermore, if Γ is a graph, then $k = 2$, $E_1(S)$ is the set of edges between S and $\overline{S}$, and the Cheeger constant defined above coincides with the one introduced by Pólya and Szegö, see (1.40).

The following theorem, proved in [44], generalizes (1.116) which is, on its turn, equivalent to the classical Cheeger inequalities in (1.115).

Theorem 1.4.2 *Let Γ be a connected, k-uniform, bipartite hypergraph. Then,*

$$\frac{1}{2(k-1)} h^2 \leq k - \lambda_{N-1} \leq 2(k-1)h.$$

Similarly, the Cheeger-like constant Q defined, for a graph, as

$$Q := \max_{e=(v,w)\in E} \left(\frac{1}{\deg v} + \frac{1}{\deg w} \right),$$

has been generalized in [45] for any oriented hypergraph, as

$$Q := \max_{h \in H} \left(\sum_{v \in h} \frac{1}{\deg v} \right).$$

The lower bound in Theorem 1.2.4, $Q \leq \lambda_N$, has been proved to hold for all oriented hypergraphs.

1.4.5 Generalizations

An oriented hypergraph can be seen as a classical hypergraph such that, in addition, for each vertex v and each hyperedge h, there exists a coefficient $C(v, h) \in \{-1, 0, +1\}$, where

$$C(v, h) = 0 \iff v \notin h, \tag{1.117}$$

while $C(v, h) = +1$ if and only if v is an input for h, and similarly $C(v, h) = -1$ if and only if v is an output for h. Various generalizations of this constructions have been studied in the context of spectral theory:

- *Chemical hypergraphs* are a generalization of oriented hypergraphs in which (1.117) does not necessarily hold, that is, one can have $C(v, h) = 0$ even if $v \in h$. The idea is that, in this case, v can be seen as *both* an input and an output for h, in which case v is said to be a *catalyst* for h. Chemical hypergraphs and their Laplacians have been introduced in [14], and the corresponding spectral results change based on the definition of generalized vertex degree that one considers. If

$$\deg v := |\{h \in H : C(v, h) \neq 0\}|,$$

then a chemical hypergraph Γ is isospectral to the oriented hypergraph obtained from Γ by removing catalysts from the hyperedges. If

$$\deg v := |\{h \in H : v \in h\}|,$$

by using the definition of Laplacian in (1.13), as in [14], the matrix formulation of L^0 becomes

$$L^0 = \hat{D} - D^{-1}A,$$

where $\hat{D}$ is the diagonal matrix with diagonal entries

$$\hat{D}_{ii} := \frac{\deg v_i - |\{h \in H : v_i \in h \text{ as catalyst}\}|}{\deg v_i}.$$

In this case, most of the results that we stated for oriented hypergraphs still hold. The main difference is that the eigenvalues are generally smaller, since now

$$\sum_{i=1}^{N} \lambda_i = N - \sum_{i=1}^{N} \frac{|\{h \in H : v_i \in h \text{ as catalyst}\}|}{\deg v_i}$$

can be smaller than N.
- *Complex unit hypergraphs* [56] are a generalization of oriented hypergraphs in which the coefficients $C(v, h)$ are from the complex unit circle, and (1.117) still holds. In this case, most of the spectral results for oriented hypergraphs can be generalized. The difference is that, instead of being symmetric operators, the Laplacians are now Hermitian operators and therefore the proofs require slightly different methods.
- *Hypergraphs with real coefficients* [17, 65] are a generalization of oriented hypergraphs in which (1.117) holds and the coefficients $C(v, h)$ are real numbers. In the case when, for all v and h, $C_{v,h} \geq 0$ and $\sum_{h \in H} C_{v,h} = 1$, we can see each coefficient $C_{v,h}$ as the *probability* of the vertex v to belong to the hyperedge h. In the case when the coefficients are integers, we can see each vertex as a chemical

element, each hyperedge as a chemical reaction and each coefficient $C_{v,h}$ as the chemical *stoichiometric coefficient* of the element v in the reaction h. Moreover, in the case when $C(v,h) =: w(h)$ only depends on h, for each hyperedge h and for each vertex v, we can see these hypergraphs as *weighted hypergraphs*.
If $\Gamma = (V, H, \{C(v,h) : v \in V \text{ and } h \in H\})$ is a hypergraph with real coefficients, its vertex degrees are defined by

$$\deg v := \sum_{h \in H} C(v,h)^2,$$

and it is easy to see that this generalizes (1.101). Moreover, the *degree matrix* of Γ is still defined by (1.112), the *incidence matrix* of Γ is defined by $\mathcal{I} := (\mathcal{I}_{ij})_{ij}$, where

$$\mathcal{I}_{ij} := C(v_i, h_j),$$

and the *adjacency matrix* of Γ is $A := (A_{ij})_{ij}$, where $A_{ii} := 0$ for all $i = 1, \dots, N$ and, for $i \neq j$,

$$A_{ij} := -\sum_{h \in H} C(v_i, h) \cdot C(v_j, h).$$

The generalized *Laplacians* are then defined, in matrix form, as

$$L^0 := \mathrm{Id} - D^{-1}A = D^{-1}\mathcal{I}\mathcal{I}^\top \quad \text{and} \quad L^1 := \mathcal{I}^\top D^{-1}\mathcal{I},$$

and most of the properties that we discussed for oriented hypergraphs can be generalized to the more general setting of hypergraphs with real coefficients.

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