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Geometric Bounds for Steklov Eigenvalues on Graphs

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Abstract

We give a thorough introduction to the Steklov problem on finite weighted graphs. On finite graphs, this problem reduces to studying the eigenvalues of a particular matrix defined on a subset of the vertices of the graph. We consider two versions of the Steklov problem, one of which is a 'normalized' version of the other. We prove two novel results that relate the eigenvalues of the Steklov problem to the properties of the underlying graph. The first result consists of upper bounds on the normalized and non-normalized smallest nonzero Steklov eigenvalue, which hold when the underlying graph is planar. The second result is a lower bound on the non-normalized smallest nonzero Steklov eigenvalue which depends on the edge connectivity of the underlying graph.

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Chapter 1

Introduction

This thesis concerns bounds on the eigenvalues of a discrete version of the classical *Steklov problem*, originally posed by V.I. Steklov in the 19th century [Kuz+14]. The classical Steklov problem with spectral parameter σ is posed on a Riemannian manifold M with boundary ∂M as

$$\begin{aligned} \Delta u &= 0, \quad \text{in } M, \\ \frac{\partial u}{\partial n} &= \sigma u, \text{ on } \partial M. \end{aligned} \tag{1.1}$$

Here, Δ denotes the Laplace-Beltrami operator and n denotes the outward-facing unit normal on ∂M. It can be shown that for manifolds M that fulfil reasonable regularity assumptions, the spectrum of the Steklov problem is discrete and non-negative with eigenvalues $0 = \sigma_0 < \sigma_1 \leq \sigma_2 \leq \ldots$, with all eigenvalue multiplicities finite. An alternative perspective on the Steklov problem is to view its eigenvalues as the spectrum of the *Dirichlet-to-Neumann* operator, usually denoted Λ, defined between spaces of 'sufficiently nice' functions f on ∂M. Formally, Λ is defined as

$$\Lambda(f) = \frac{\partial \widehat{f}}{\partial n},$$

where $\widehat{f}$ denotes the *harmonic extension* of f, i.e. the function that agrees with f on ∂M and satisfies $\Delta \widehat{f} = 0$ in M.

As was stated, we will actually be concerned with a *discrete* version of the Steklov problem and Dirichlet-to-Neumann operator which is instead posed on a finite weighted graph G with vertex set $V = \{1, 2, \ldots, n\}$, edge set E, and weights w_{ij} on the edges (i, j) between vertices i and j in E. This discrete Steklov problem concerns functions defined on V. There is a matrix L (in fact, several related matrices), called the *graph Laplacian*, which can be viewed as a discrete analogue of the Laplace operator. The action of L on a function $f : V \to \mathbb{R}$ is

$$(Lf)(i) = \sum_{j:(i,j)\in E} w_{ij}(f(i) - f(j)).$$

One can designate a subset of the vertices of G as the *boundary* B of the graph G, similarly to the way ∂M is the boundary of M. Analogously to the continuous case, for a given function $f : B \to \mathbb{R}$ there is a unique function $u_f : V \to \mathbb{R}$ defined on all of V such that

$$\begin{aligned} (Lu_f)(i) &= 0, \qquad \text{for } i \text{ in } V \setminus B, \\ u_f(i) &= f(i), \text{ for } i \text{ on } B, \end{aligned} \tag{1.2}$$

called the *harmonic extension* of f. The discrete version of the Dirichlet-to-Neumann (DtN) operator is in turn

$$\Lambda_L : f \mapsto (Lu_f)\,|_B,$$

where $|_B$ denotes restriction to B, and the Steklov eigenvalue problem on G with spectral parameter σ is $\Lambda_L f = \sigma f$, for nontrivial f. Sometimes, one instead poses the problem (1.2) using a 'normalized' version of the Laplacian L, which we designate as $\mathcal{L}$. The matrix $\mathcal{L}$ acts on functions f defined on V as

$$\mathcal{L}f(i) = \frac{1}{\sum_{j:(i,j)\in E} w_{ij}} \sum_{j:(i,j)\in E} w_{ij}(f(i) - f(j)).$$

One defines the normalized form of the DtN operator as

$$\Lambda_{\mathcal{L}} : f \mapsto (\mathcal{L}u_f)\,|_B$$

with corresponding Steklov problem $\Lambda_{\mathcal{L}} f = \sigma f$. The eigenvalues σ of the DtN operator (normalized or not) are called *Steklov eigenvalues*. Analogously to their continuous counterpart, one can show that the spectra of Λ_L and $\Lambda_{\mathcal{L}}$ are both real and non-negative. Especially the map Λ_L has a natural physical interpretation in terms of electrical networks (modelled as weighted graphs), where knowledge of Λ_L corresponds to measuring currents in the network at the vertices in B, as we will see in Section 2.4.3. Therefore, understanding the properties of Λ_L is important in the context of discrete versions of for instance the *Calderón problem*, where one investigates to which extent it is possible to reconstruct the whole eletrical network (i.e. its Laplacian matrix) from measuring currents at the boundary. Extensive work on the Calderón problem on graphs has been done by e.g. Curtis, Ingerman, and Morrow [CIM98], Kenyon [Ken11], Kenyon and Wilson [KW17], Colin de Verdière [Col94] and Colin de Verdière, Gitler, and Vertigan [CGV96].

For the Steklov problem on manifolds, an extensive amount of work has been done relating the geometry of the manifold M to especially the smallest nonzero eigenvalue, which we denote σ_1, of the Steklov problem on M. The interested reader is referred to the article [GP17] by Girouard and Polterovich for an in-depth survey of recent results. The discrete Steklov problem seems to be a more recent area of study, but nonetheless some results have been established. In a 2017 paper, Hua, Huang and Wang [HHW17] proved multiple *Cheeger-type* or *isoperimetric* bounds for σ_1. Perrin [Per19; Per20] found lower bounds for σ_1 that depend on the number of boundary vertices and the longest path of minimal length between two boundary vertices, as well as upper bounds for σ_1 on graphs that are the Cayley graph of a group of polynomial growth. There also exist results that relate the continuous case to the discrete case; one example is the paper [CGR18] by Colbois, Girouard, and Raveendran. Therefore, results in the discrete case might in fact also influence the continuous case and vice versa.

In the first part of this thesis, we give the reader a thorough introduction to various aspects of the DtN maps on graphs and hopefully provide some intuition into their physical significance. We also introduce the mathematical machinery needed to establish bounds on Steklov eigenvalues by interpreting them as solutions to optimization problems via the Courant-Fischer Theorem.

In the later parts, we prove two results that relate the Steklov eigenvalues to various aspects of the underlying graph. Both results seem to be novel. The first result is Theorem

3.1, and consists of upper bounds on the normalized and non-normalizzed smallest non-zero Steklov eigenvalues. Theorem 3.1 applies when the underlying graph is planar, and its proof is in the vein of Spielman and Teng [ST07] and Plümer [Plü20]. The second result is Theorem 4.5, which consists of a lower bound on the non-normalized smallest non-zero Steklov eigenvalue, related to an invariant called the *edge connectivity* of the graph. Its proof is partly in the vein of Theorem 2.3 in [Ber+17].

Chapter 2

Notation and preliminary concepts

In this chapter, we fix some notation that will be constantly used throughout the text and define the concepts and quantities of study.

2.1. Knowledge expected from the reader

A reader who has studied mathematics at the master's level will probably not have any major trouble following along in the arguments owing to a lack of background knowledge. The most advanced material that appears are topological concepts familiar from any introductory course in the subject. Experience in graph theory and (undergraduate level) PDE:s will probably give more appreciation for the central objects of study, such as the graph Laplacian, but is hardly required.

2.2. Graph terminology

All of the definitions in this section are standard and can be found in any book on graph theory, for example [Die17]. Unless otherwise stated, graphs in this thesis are finite, undirected and are allowed to have at most one (weighted) edge between two given vertices, but not loops. An (edge weighted) graph will be denoted $G = (V, E, w)$ where V denotes the set of vertices of G, E denotes its set of edges, and $w : E \longrightarrow (0, \infty)$ is the weight function on the edges. Often we will enumerate the n vertices of G by $1, 2, \ldots, n$, in which case w_{ij} is the weight of the edge connecting vertices i and j. Of course, we identify w_{ij} with w_{ji}. We denote the edge itself connecting vertices i and j by e_{ij} or (i, j). The cardinality of a subset S of the edges or vertices of G will be denoted $|S|$. The *vertex measure* on a vertex $i \in V$ is the quantity

$$m(i) := \sum_{j:(i,j)\in E} w_{ij}. \tag{2.1}$$

The *volume* of a subset $S \subset V$ is

$$\mathsf{Vol}(S) := \sum_{i\in S} m(i). \tag{2.2}$$

The *neighborhood* of a vertex i is the set of vertices that are connected to i by an edge. A *subgraph* of a graph G is a graph $F = (V_F, E_F)$ such that $V_F \subset V$ and $E_F \subset E$, with the additional condition that all edges in E_F connect vertices in V_F. A *path* in G between two vertices u, v is a sequence of distinct edges $(u, v_1), (v_1, v_2), \ldots, (v_{k-1}, v_k), (v_k, v)$. Its *path length* is the sum of the weights of the edges in the sequence. A graph is *connected* if there is a path between any two vertices of G. A *cycle* is a path starting and ending at the same vertex. A *tree* is a graph without cycles. A *spanning tree* of a connected graph G is a connected subgraph of G which contains all vertices in V and is also a tree. We will often be concerned with a distinguished subset of the vertices of G which we call the *boundary* of G and denote by B. The geometric flavor of the name *boundary* is oftentimes justified, as will hopefully be made clear later on.

2.3. Laplacians on graphs

We will consider two versions of the Laplacian matrix associated to a graph G in this thesis. If a graph $G = (V, E, w)$ has n vertices, one can identify a function $f : V \to \mathbb{R}$ with the vector in $\mathbb{R}^n$ whose i:th entry is $f(i)$, in which case one can view both of these Laplacians as linear operators (i.e. matrices) on functions f defined on V.

2.3.1. The combinatorial Laplacian

Definition 2.1 (Combinatorial Laplacian)**.** Let G be a graph with n vertices, enumerated as $1, 2, \ldots, n$. The *combinatorial Laplacian* L of G is the $n \times n$ matrix L such that

$$L_{ii} = \sum_{j:(i,j)\in E} w_{ij}, \qquad L_{ij} = -w_{ij}, \text{ if } i \neq j. \tag{2.3}$$

Note that L_{ii} equals $m(i)$, where $m(i)$ is as in (2.1). Directly from the definition, we can note that the action of the combinatorial Laplacian on a function $f \in \mathbb{R}^n$ on the vertices of the graph is

$$(Lf)(i) = \sum_{j:(i,j)\in E} w_{ij}(f(i) - f(j)). \tag{2.4}$$

The expression (2.4) perhaps gives a clearer picture than Definition 2.1 of the fact that at its core, applying the combinatorial Laplacian to a function $f \in \mathbb{R}^n$ amounts to measuring to what extent the value of f at the vertex i differs from the (weighted) average value of f in the neighborhood of i. In particular, if $Lf(i) = 0$ at a vertex i, then $f(i)$ is a weighted average of the function values at its neighboring vertices; we have

$$0 = (Lf)(i) = \sum_{j:(i,j)\in E} w_{ij}(f(i) - f(j)) \quad \Longrightarrow \quad \sum_{j:(i,j)\in E} w_{ij} f(i) = \sum_{j:(i,j)\in E} w_{ij} f(j),$$

which in turn yields

$$f(i) = \frac{\sum_{j:(i,j)\in E} w_{ij} f(j)}{\sum_{j:(i,j)\in E} w_{ij}}. \tag{2.5}$$

This is a discrete analogue to a function on a manifold satisfying Laplace's equation at a point.

Instead of thinking of the combinatorial Laplacian as attached to a graph, one can also view a combinatorial Laplacian as simply a member of a special class of matrices.

Fact 2.2. *An $n \times n$ matrix L is a combinatorial graph Laplacian if and only if the following properties hold:*

1. *L is symmetric.*
2. *The row and column sums of L are both 0.*
3. *All off-diagonal entries of L are non-positive.*

Proof. Use (2.3) to construct a bijection between $n \times n$-matrices satisfying properties 1,2, and 3 and weighted graphs on n vertices. ∎

2.3.2. The normalized Laplacian

Definition 2.3. Let $G = (V, E, w)$ be a graph with vertices enumerated as $1, 2, \ldots, n$. Let L be the combinatorial Laplacian of G, and let D be the diagonal matrix such that $D_{ii} = m(i)$, where $m(i)$ denotes the vertex measure of i as in (2.1). The *normalized Laplacian* of G is the matrix $\mathcal{L} = D^{-1}L$.

From the definition, we see that the action of $\mathcal{L}$ on a function f on the vertices of G is

$$(\mathcal{L}f)(i) = \frac{1}{m(i)} \sum_{j:(i,j)\in E} w_{ij}(f(i) - f(j)). \tag{2.6}$$

Since the calculation in Section 2.3.1 also applies to the normalized Laplacian, applying the normalized Laplacian captures the same notion as the combinatorial Laplacian of measuring to what extent $f(i)$ differs from the weighted average of the function values in the neighborhood of i. However, the measure of to what extent this is the case is 'normalized' by the factor $1/m(i)$.

This 'normalization' phenomenon carries over to spectral properties as well. For instance, it is classical that the eigenvalues of $\mathcal{L}$ are contained in the interval $[0, 2]$, regardless of the underlying graph, while the eigenvalues of the combinatorial Laplacian can only be said to be contained in the graph-dependent interval $[0, 2\max_{i\in V} m(i)]$. Partly for this reason, the eigenvalues of the normalized Laplacian turn out to often relate more closely to other graph invariants than the combinatorial Laplacian when studying general graphs. A lot of results in this direction come from the fact that $\mathcal{L}$ is similar (in the matrix sense of the word) to the *symmetric normalized Laplacian* $\mathbf{L} = D^{-1/2}LD^{-1/2}$, and thus shares its eigenvalues. The symmetric normalized Laplacian $\mathbf{L}$ is more commonly studied than $\mathcal{L}$, but is for various reasons not an appropriate matrix to work with in the context of this thesis. The reader is referred to the excellent text of F. K. Chung [Chu97] for a detailed overview of the spectral properties of the symmetric normalized Laplacian (and, by virtue of similarity, also of the normalized Laplacian). There will be times in this thesis when the references for a result on the eigenvalues of the normalized Laplacian refer to a text which deals with the symmetric normalized Laplacian; however, for the reasons outlined above these results transfer over to the normalized Laplacian as well.

2.3.3. The Laplacian quadratic form

If $f \in \mathbb{R}^n$ is an arbitrary function defined on the vertices of G, the combinatorial Laplacian gives rise to a quadratic form via the usual inner product $(\cdot,\cdot)$ in $\mathbb{R}^n$:

$$\begin{aligned}
(f, Lf) &= \sum_i f(i) \left[\sum_{j:(i,j)\in E} w_{ij}(f(i) - f(j)) \right] \\
&= \sum_i m(i) f(i)^2 - 2 \sum_{(i,j)\in E} w_{ij} f(i) f(j) \\
&= \sum_i \left[\sum_{(i,j)\in E} w_{ij} f(i)^2 \right] - 2 \sum_{(i,j)\in E} w_{ij} f(i) f(j) \\
&= \sum_{(i,j)\in E} w_{ij} \left[f(i)^2 + f(j)^2 \right] - 2 \sum_{(i,j)\in E} w_{ij} f(i) f(j) \\
&= \sum_{(i,j)\in E} w_{ij} (f(i) - f(j))^2.
\end{aligned} \tag{2.7}$$

The quantity $D(f) = \sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2$ is usually referred to as the *Dirichlet energy* or *Dirichlet sum* of the graph, for a given function f. It turns out that the Dirichlet sum is related to the analogue of the Dirichlet problem on graphs, as we will see in Section 2.4.1.

2.3.4. Some spectral properties of Laplacians

As was implied in the discussion regarding the normalized Laplacian in Section 2.3.2, both the combinatorial and normalized Laplacians have real, non-negative eigenvalues. They are also both singular; the all-ones vector $\mathbf{1}$ is an eigenvector of both L and $\mathcal{L}$ with eigenvalue 0. As a first example of the connection between connectivity and the eigenvalues of the Laplacian, one can also show that it holds for both the normalized and combinatorial Laplacian that the multiplicity of the eigenvalue 0 is the number of connected components of G (see Lemma 1.7 in [Chu97] for a proof in the normalized case). In the case of a connected graph, we are therefore guaranteed that the second smallest eigenvalue is nonzero for both Laplacians, and the second smallest eigenvalue is therefore often referred to as the *spectral gap* of each respective Laplacian. As was also mentioned in the discussion regarding the normalized Laplacian, the eigenvalues of the normalized Laplacian are contained in the interval $[0, 2]$ and the eigenvalues of the combinatorial Laplacian are contained in the interval $[0, 2\max_{i\in V} m(i)]$.

2.3.5. Examples of spectral results

The goal of spectral graph theory is to study the eigenvalues and eigenvectors of the different types of Laplacians and other operators on graphs, and how these relate to different properties of the underlying graph, such as its connectivity; we saw some introductory examples in Section 2.3.4. In this section, we aim to show via a few examples that a vast array of striking results in this direction, perhaps more exciting than those in Section 2.3.4, exist. These results are often especially valuable in practical contexts, since the eigenvalues of a graph Laplacian are easily computed algorithmically while determining certain invariants of graphs can often turn out to be computationally intractable (NP-hard).

The first example shows the potential of spectral methods in the context of combinatorics on graphs.

Theorem 2.4 (Kirchhoff Matrix-Tree Theorem). *Let G be a connected graph on n vertices with edge weights all equal to 1. Let L be the combinatorial Laplacian of G, and denote its eigenvalues by $\lambda_0 = 0 < \lambda_1 \leq \ldots \lambda_{n-1}$. Let $t(G)$ denote the number of spanning trees of G. Then*

$$\frac{\prod_{i=1}^{n-1} \lambda_i}{n} = t(G).$$

In the view of the author, this theorem is highly surprising and shows just how varied the applications of Laplacian eigenvalues can be. For a proof of the Matrix-Tree Theorem, we refer to Chapter 9 of [Sta18].

The second example is a theorem that is of great pratical importance, which needs a few definitions. These definitions can all be found in Chapter 2 of [Chu97], along with an extended discussion of the result to come.

Definition 2.5. Let $G = (V, E, w)$ be a graph (with unit weights on the vertices, for simplicity) and $S \subset V$. The set $E(S, V \setminus S)$ denotes the set of edges with one endpoint in S and one endpoint in $V \setminus S$. The *Cheeger constant of* S is the quantity

$$h_G(S) = \frac{|E(S, V \setminus S)|}{\min(\mathsf{Vol}(S), \mathsf{Vol}(V \setminus S))},$$

where $\mathsf{Vol}(S) = \sum_{i \in S} m(i)$ as in (2.2) and $\mathsf{Vol}(V \setminus S)$ is defined analogously. The *Cheeger constant of* G is defined to be

$$h_G = \min_S h_G(S).$$

Remark 2.6. The edges in $E(S, V \setminus S)$ are part of the measures of the vertices in both S and $V \setminus S$, and therefore one sums implicitly over these edges in the expressions of both $\mathsf{Vol}(S)$ and $\mathsf{Vol}(V \setminus S)$. Hence it follows that $h_G \leq 1$.

Intuitively, if the Cheeger constant is large, the graph is sparse, in that its number of edges is roughly linear in the number of vertices, but also highly connected, in the sense that there are no 'bottleneck' sets that need few edges to be removed to be disconnected from the rest of the graph. These properties are highly desirable in practice, for instance when designing something like a power network. It turns out that one can effectively bound the Cheeger constant of a graph via spectral methods, even though it is NP-hard to compute it exactly in general (see [Kai04], Theorem 2).

The theorem below can be found in e.g. Section 2.2 of [Chu97].

Theorem 2.7 (Cheeger inequalities). *Let $G = (V, E, w)$ be a connected unit weighted graph. Let λ_1 denote the smallest nonzero eigenvalue of the normalized Laplacian on G. Then*

$$\frac{h_G^2}{2} \leq \lambda_1 \leq 2h_G.$$

Graphs with 'large' values of λ_1 therefore have a large value of h_G, and a large h_G implies at least a 'rather large' value of λ_1. This makes λ_1 a highly relevant quantity to study when looking for graphs with the desirable properties outlined above. Graphs with 'large' λ_1 are one example of the notion of an *expander graph*, which seemingly appear in many disparate areas of mathematics such as number theory and theoretical computer science. The interested reader is referred to the treatise [HLW06] on expander graphs by Hoory, Linial and Wigderson, where the spectral properties of such graphs are covered in detail.

2.4. The DtN map on graphs

In this section, we introduce the central objects of study in this thesis, which are two related operators acting on the boundary B of a graph G. These operators are called the *combinatorial* and *normalized Dirichlet-to-Neumann (DtN) map*, respectively. We also aim to provide some intuition as to why the DtN maps are natural and interesting objects to study.

2.4.1. Graph boundaries and the Dirichlet problem

Kenyon [Ken11] gives an excellent exposition of the relation between the Dirichlet problem on graphs and the DtN map, which we follow. Classically, the *Dirichlet problem* is formulated on a region U in $\mathbb{R}^n$ and asks for a continuous function that is twice differentiable in the interior of U and takes prescribed values on the boundary of U. If one also asks that this function satisfies the Laplace equation in U, it becomes the following problem:

> *Given f taking values on the boundary of a region U in $\mathbb{R}^n$, is there a unique continuous function u which is twice continuously differentiable in the interior and continuous on the boundary, such that u solves Laplace's equation in the interior of U and $u = f$ on the boundary?*

We will pose a discrete version of the Dirichlet problem on a connected weighted graph G. To do this, we first introduce the discrete analogue of a function that satisfies Laplace's equation.

Definition 2.8 (Harmonic extension)**.** Let $G = (V, E, w)$ be a weighted graph with n vertices and combinatorial Laplacian L. A function $f : V \to \mathbb{R}$ such that $(Lf)(i) = 0$ is said to be *harmonic* at i. If S is a subset of B, a function u is *harmonic in S* if it is harmonic for all i in S.

Let B denote the boundary of G. The discrete Dirichlet problem is the following: Fix a function $f : B \to \mathbb{R}$. We ask for a function $u : V \to \mathbb{R}$ which agrees with f on B and is harmonic on $V \setminus B$:

$$\begin{aligned} (Lu)(i) &= 0, \qquad \text{for } i \text{ in } V \setminus B, \\ u(i) &= f(i), \text{ for } i \text{ in } B. \end{aligned} \tag{2.8}$$

For finite, connected graphs, the discrete Dirichlet problem turns out to always be uniquely solvable. This follows from the discussion in Section 2.4.2, where an explicit expression for the values of u on $V \setminus B$ is obtained following (2.12).

Since we will often refer to the function fulfilling the conditions in (2.8), we give it a proper name.

Definition 2.9 (Harmonic extension)**.** Let G be a graph with boundary B, and let $f : B \to \mathbb{R}$ be a function on the boundary. The function $u_f : V \to \mathbb{R}$ that solves the discrete Dirichlet problem (2.8) on G with boundary conditions given by f is called the *harmonic extension* of f on G.

The following are two classical facts of the harmonic extension which we will occasionally use.

Lemma 2.10. *Suppose we are in the situation of* (2.8) *and* $u_f : V \longrightarrow \mathbb{R}$ *is the harmonic extension of* $f : B \longrightarrow \mathbb{R}$. *Then* u_f *has the following properties.*

1. u_f *takes its extremal values in* B.

2. u_f *is the unique minimizer of the Dirichlet energy* (2.3.3) *among functions that agree with* f *when restricted to* B.

Proof.

1. This follows immediately from noting that $Lu_f = 0$ in $V \setminus B$; by (2.5) this implies that for all i in $V \setminus B$, $u_f(i)$ is the weighted average of its values in the neighborhood of B.

2. See the discussion in Section 3.3 in [Ken11].

■

As an aside, one can ask what happens if we pose the discrete Dirichlet problem on the same graph with the same boundary conditions using the *normalized* Laplacian; that is, we ask for $u : V \longrightarrow \mathbb{R}$ such that

$$\begin{aligned} (\mathcal{L}u)(i) &= 0, \quad \text{for } i \text{ in } V \setminus B, \\ u(i) &= f(i), \text{ for } i \text{ in } B. \end{aligned} \tag{2.9}$$

The function satisfying (2.9) is then in fact precisely the harmonic extension u_f. This follows since $\mathcal{L} = D^{-1}L$, where D is the diagonal matrix such that $D_{ii} = m(i)$, together with the fact that D is invertible if G is connected (or indeed, if there are no vertices in G of measure zero).

With these results in hand, we are ready to define the two maps which will be the central objects of study in this thesis.

Definition 2.11. (Combinatorial Dirichlet-to-Neumann map) Let G be a weighted graph with boundary B. Let $f : B \longrightarrow \mathbb{R}$, and let $u_f : V \longrightarrow \mathbb{R}$ be the harmonic extension of f. The map $\Lambda_L : f \mapsto (Lu_f)\,|_B$ is then the *combinatorial Dirichlet-to-Neumann (DtN) map of* G *w.r.t* B.

Similarly to how the normalized Laplacian relates to the combinatorial Laplacian, we introduce a 'normalized' version of the combinatorial DtN map.

Definition 2.12. (Normalized Dirichlet-to-Neumann map) Let G be a weighted graph with boundary B. Let $f : B \longrightarrow \mathbb{R}$, and let u_f be the harmonic extension of f. The map $\Lambda_{\mathcal{L}} : f \mapsto (\mathcal{L}u_f)\,|_B$ is then the *normalized Dirichlet-to-Neumann (DtN) map of* G *w.r.t* B.

The name *Dirichlet-to-Neumann map* has a natural explanation as follows. In the Dirichlet problem (2.8), we set explicit conditions on the function u solving it, by asking that u agrees with some given function f on the boundary of G. Conditions of this form are usually called *Dirichlet conditions*. Instead of (2.8), we can pose the following problem on G: Given a function $g : B \longrightarrow \mathbb{R}$, we ask for $u : V \longrightarrow \mathbb{R}$ such that

$$\begin{aligned} (Lu)(i) &= 0, \quad \text{for } i \text{ in } V \setminus B, \\ (Lu)(i) &= g(i), \text{ for } i \text{ in } B. \end{aligned} \tag{2.10}$$

Here, unlike in (2.8) we instead pose conditions on Lu on the boundary of G. Such conditions are called *Neumann conditions*. Now, take g to be the function $Lu_f\mid_B: B \longrightarrow \mathbb{R}$, where f is the boundary conditions on G in (2.8) and u_f is the harmonic extension of f. Then, the problems (2.8) and (2.10) will have the same solution u_f. Hence, the (combinatorial) Dirichlet-to-Neumann map can be interpreted as mapping the *Dirichlet* conditions in (2.8) *to* the *Neumann* conditions in (2.10) that would yield the same solution u_f as (2.8). Of course, the exact same argument can be made for the normalized DtN map, in which the Dirichlet problem setting is instead given by (2.9) and the problem (2.10) is posed using the normalized Laplacian.

2.4.2. Matrix expressions of DtN maps

It is sometimes helpful to think of both DtN maps as matrices. If the vertices of a (connected) graph $G = (V, E, w)$ with boundary B are indexed as $1, 2, \ldots, n$, we identify a function $g : V \longrightarrow \mathbb{R}$ with the vector in $\mathbb{R}^n$ whose i:th entry is $g(i)$. Then we can find an expression for the matrix representation of Λ_L in terms of the matrix representation of the combinatorial Laplacian L of G. We show the necessary calculation only for the combinatorial DtN map, since the calculation for the normalized DtN map is very similar.

Index the vertices of G so that the vertices of B come first, and define $f : B \longrightarrow \mathbb{R}$. Then we can write the combinatorial Laplacian L (which is symmetric by definition) as a block matrix

$$L = \begin{bmatrix} P & Q \\ Q^t & R \end{bmatrix}, \tag{2.11}$$

where P acts on the boundary B and R acts on the interior $I = V \setminus B$. Write u_I for the harmonic extension of f restricted to I. Then, we have the following matrix equation for the action of Λ_L on f:

$$Lu_f = \begin{bmatrix} P & Q \\ Q^t & R \end{bmatrix} \begin{bmatrix} f \\ u_I \end{bmatrix} = \begin{bmatrix} \Lambda_L f \\ \mathbf{0} \end{bmatrix}. \tag{2.12}$$

In other words, we have the system

$$\begin{aligned} Pf + Qu_I &= \Lambda_L f \\ Q^t f + Ru_I &= \mathbf{0}. \end{aligned}$$

Hence $u_I = -R^{-1}Q^t f$ (where we know R is invertible, see Theorem 2.17 below). We then plug this expression into the other equation to get

$$Pf - QR^{-1}Q^t f = \Lambda_L f.$$

Then we finally arrive at the expression

$$\Lambda_L = P - QR^{-1}Q^t. \tag{2.13}$$

Algebraically, Λ_L is the *Schur complement* of the Laplacian L w.r.t. R. We elaborate on this concept in Section 2.5. The Schur complement has myriad applications in multiple areas of mathematics, and the interested reader is referred to the treatise [Zha05]. One can pose the analogous matrix equation for the normalized Laplacian as

$$\mathcal{L}u_f = D^{-1}Lu_f = D^{-1}\begin{bmatrix} P & Q \\ Q^t & R \end{bmatrix}\begin{bmatrix} f \\ u_I \end{bmatrix} = \begin{bmatrix} \Lambda_{\mathcal{L}} f \\ \mathbf{0} \end{bmatrix}$$

whence one finds that

$$\Lambda_{\mathcal{L}} = D_B^{-1}(P - QR^{-1}Q^t), \tag{2.14}$$

where D_B is the $|B| \times |B|$-diagonal matrix such that $D_{ii} = m(i)$. Note that the vertices of G are indexed so that the boundary vertices come first, so D_B is the diagonal matrix whose entries are the vertex measures of the boundary vertices in G.

Example 2.13 (DtN maps of the star graph)**.** Consider the star graph S_n on n vertices with unit edge weights and the measure 1 vertices designated as boundary vertices, as in Figure 2.1.

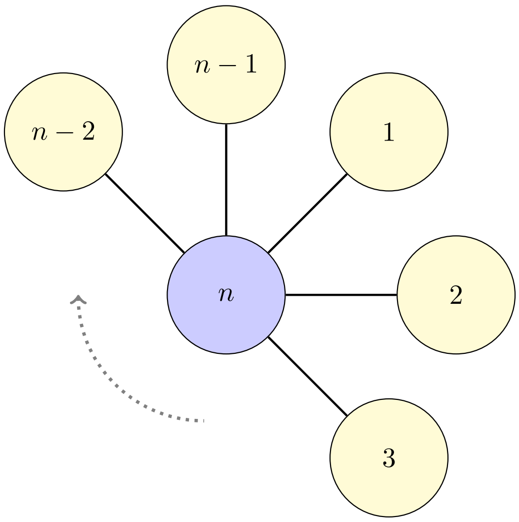


Figure 2.1: The star graph S_n on n vertices.

With the enumeration in Figure 2.1, the combinatorial Laplacian L of S_n becomes

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 & -1 \\ 0 & 1 & 0 & 0 & \dots & 0 & -1 \\ 0 & 0 & 1 & 0 & \dots & 0 & -1 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & \dots & 0 & 1 & -1 \\ -1 & -1 & -1 & -1 & \dots & -1 & n-1 \end{bmatrix}.$$

If we partition L as in (2.11), i.e.

$$L = \begin{bmatrix} P & Q \\ Q^t & R \end{bmatrix},$$

where P acts on the boundary and R acts on the interior, we get

$$P = I_{n-1}; \qquad Q^t = [-1 - 1, \dots, -1]; \qquad R = [n-1],$$

where I_{n-1} denotes the $(n-1)\times(n-1)$ identity matrix. Therefore, the Schur complement formula (2.13) yields that the combinatorial DtN map Λ_L of S_n with regard to the degree 1 vertices is given by

$$\Lambda_L = I_{n-1} - \frac{1}{n-1}QQ^t = I_{n-1} - \frac{1}{n-1}\mathcal{I},$$

where $\mathcal{I}$ is the $(n-1)\times(n-1)$ matrix with all entries equal to 1. Hence

$$\Lambda_L = \frac{1}{n-1}\begin{bmatrix} n-2 & -1 & -1 & -1 & \dots & -1 & -1 \\ -1 & n-2 & -1 & -1 & \dots & -1 & -1 \\ -1 & -1 & n-2 & -1 & \dots & -1 & -1 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ -1 & -1 & \dots & -1 & n-2 & -1 & -1 \\ -1 & -1 & -1 & \dots & -1 & n-2 & -1 \\ -1 & -1 & -1 & -1 & \dots & -1 & n-2 \end{bmatrix}.$$

By virtue of the normalized Schur complement formula (2.14), the combinatorial and normalized DtN maps of S_n coincide since all of the boundary vertices have measure 1. Note that Λ_L also defines a combinatorial Laplacian, namely the combinatorial Laplacian of the complete graph on $n-1$ vertices with edge weights all equal to $1/(n-1)$. This is not a coincidence; by Theorem 2.17, the combinatorial DtN map of a graph *always* defines the combinatorial Laplacian of a graph G_Λ whose vertices are the boundary vertices in G.

2.4.3. DtN map intuition: Electrical networks

An oftentimes helpful tool to better understand weighted graphs and especially the combinatorial Laplacian and combinatorial DtN map on them is the terminology and concepts employed in the study of electrical networks. We think of the weighted graph $G=(V,E,w)$ as an electrical network whose edge weights define *conductances* between vertices. The conductance between two vertices is defined as the reciprocal of the perhaps more familiar *resistance* between those same vertices. A function f defined on (a subset of) the vertices of G is thought of as a *voltage* or *potential* on the network. A voltage induces a current I through the network. At the edge (i,j), the current I_{ij} is given by Ohm's law as

$$I_{ij} = U_{ij}/R_{ij}$$

where U_{ij} is the potential difference between the vertices i,j connected by the edge (i,j), i.e. $U_{ij}=f(i)-f(j)$ up to direction of the current, and R_{ij} is the resistance in the edge (i,j). If we fix the potential at a subset B of the vertices in the network, the familiar Kirchhoff's law states that the net current through a vertex in $V\setminus B$ is zero, or in other words that the amount of current flowing into the vertex is equal to the amount of current flowing out of the vertex. This net current at the vertex i is, by Ohm's law,

$$I_{\text{net}}(i) = \sum_{j:(i,j)\in E}(f(i)-f(j))/R_{ij} = \sum_{j:(i,j)\in E} w_{ij}(f(i)-f(j)) = (Lf)(i).$$

Hence, if $I_{\text{net}}=0$ at every vertex in $V\setminus B$, then $Lf(i)=0$ at every such vertex and the potential satisfying Ohm's law and Kirchhoff's law is precisely the harmonic extension of f as in Definition 2.9. Therefore, the combinatorial DtN map $\Lambda_L : f \mapsto (Lu_f)\,|_B$ can be thought of as mapping the potential $f(i)$ at the boundary vertex i to the *net current* exiting i in the network with fixed potential f at the vertices in B that obeys Ohm's law in the rest of the network. In fact, more is true. In matrix form as in (2.13), Λ_L can actually be shown to itself be the Laplacian matrix of an electrical network whose vertices are those in B, and whose conductances are related to the 'effective' resistances in the original network G. In electrical networks terms, the network whose Laplacian is the combinatorial DtN map of G w.r.t. B is called the *Kron reduction* of G w.r.t. B, and has been extensively studied, see e.g. [DB13]. We will summarize some important properties related to this interpretation of the combinatorial DtN map in Section 2.6.

2.5. The Schur complement

The formula (2.13) expresses the combinatorial DtN map of a graph in terms of submatrices of its combinatorial Laplacian. The precise form of the formula is called the *Schur complement* of the combinatorial Laplacian. In this section, we introduce the Schur complement rigorously and describe how it can be interpreted.

2.5.1. Definition and motivation

At its core, the Schur complement is just an abstract algebraic operation on a matrix. At first glance, it might seem a bit artificial, but the Schur complement has a natural interpretation as a way to decouple a linear equation system consisting of one homogeneous part and one inhomogeneous part, as suggested by the derivation of the Schur complement formula (2.13). We first present the formal definition of the Schur complement and then elaborate on this interpretation.

Definition 2.14 (Schur complement)**.** Let A be an $n \times n$ matrix with entries in $\mathbb{C}$, and suppose A is block partitioned as

$$A = \begin{bmatrix} P & C \\ B & R \end{bmatrix}, \tag{2.15}$$

where P is an $r \times r$ principal submatrix and R is an $(n-r) \times (n-r)$ principal submatrix. Suppose in addition that P is invertible. Then the matrix

$$S_A(P) = R - BP^{-1}C$$

is the *Schur complement* of A w.r.t. P. We can also define a Schur complement of A w.r.t. R if R is invertible; in that case, the matrix

$$S_A(R) = P - CR^{-1}B$$

is the Schur complement of A w.r.t. R.

Remark 2.15. More generally, one can define the Schur complement of a matrix A w.r.t. a subset of its rows and columns, for instance as in Section 2.1 in [DB13]. The notation required to do this is however a bit too cumbersome to make it worthwile for our purposes.

Now, suppose A is a matrix partitioned as in (2.15), and suppose we have a matrix equation

$$\begin{bmatrix} P & C \\ B & R \end{bmatrix} \begin{bmatrix} f_P \\ f_R \end{bmatrix} = \begin{bmatrix} g \\ \mathbf{0} \end{bmatrix}, \tag{2.16}$$

reminiscent of (2.12). Again, as with (2.12) this matrix equation can be thought of as consisting of two coupled subsystems

$$\begin{aligned} Pf_P + Cf_R &= g, \\ Bf_P + Rf_R &= \mathbf{0}, \end{aligned} \tag{2.17}$$

with the matrices C and B representing the coupling terms between the two systems. We want to find a single expression for the inhomogeneous part of (2.17) which is equivalent to the coupled system (2.17), thus decoupling (2.17). If we assume R is invertible, we can solve for f_R to get $f_R = R^{-1}Bf_P$. If we plug this expression for f_R into the inhomogeneous part of (2.17), we end up as in (2.12) with the equivalent matrix equation

$$(P - CR^{-1}B)f_P = g,$$

where the matrix $P - CR^{-1}B$ is precisely the Schur complement of A w.r.t. R.

2.5.2. Spectral bounds on Schur complements

As an example of why one can often expect to be able to estimate the eigenvalues of the combinatorial DtN map of a graph G when the same is possible for its combinatorial Laplacian, we provide a theorem akin to the Cauchy Interlacing Theorem for the combinatorial DtN map of a graph, namely Theorem 2.16. The proof of Theorem 2.16 makes extensive use of the fact that the combinatorial DtN map is the Schur complement of the combinatorial Laplacian w.r.t. the boundary of G. The same result, albeit with a different proof method, can be found in Theorem 3.5 in [DB13].

Theorem 2.16 (DtN Interlacing Theorem)**.** *Let G be a graph with n vertices, combinatorial Laplacian L and boundary B with $|B| = b$. Let Λ_L be the combinatorial DtN matrix of G w.r.t B. Order the eigenvalues of L and Λ_L as $\lambda_0(L) \leq \lambda_1(L) \leq \ldots \leq \lambda_{n-1}(L)$ and $\sigma_0(\Lambda_L) \leq \sigma_1(\Lambda_L) \leq \ldots \leq \sigma_{b-1}(\Lambda_L)$, respectively. Then*

$$\lambda_i(L) \leq \sigma_i(\Lambda_L) \leq \lambda_{i+n-b}(L), \quad i = 0, 1, 2, \ldots, b-1. \tag{2.18}$$

Proof. See Appendix A. ∎

2.6. Properties of the DtN map

An excellent survey of the properties of and areas of use for the combinatorial DtN map Λ_L (in matrix form, i.e. as in (2.13)) and its associated reduction process on weighted graphs is provided by Dörfler and Bullo in [DB13]. The authors use the electrical network terminology outlined in the previous section and refer to the combinatorial DtN matrix as the *Kron reduction* of the combinatorial Laplacian of the network (with regard to a subset B of the vertices of the underlying graph). We refer here to some of the most important properties of the DtN matrix.

The theorem below is a combination of parts of Lemmas 2.1 and 3.4 in [DB13].

Theorem 2.17 (Structural properties of the combinatorial DtN map)**.** *Let L be the combinatorial Laplacian of a connected graph $G = (V, E, w)$. Let B be the boundary of G, and let Λ_L be the combinatorial DtN matrix of G w.r.t. B. Then Λ_L has the following properties:*

1. Well-defined: *The Schur complement formula (2.13) for Λ_L is well-defined when G is connected, in the sense that the matrix R in the Schur complement formula (2.13) is always invertible and the resulting matrix is unique up to relabelling of the vertices.*

2. Closure under Schur complement: *Λ_L is itself the Laplacian matrix of a graph G_Λ whose vertex set is B. Explicitly, this means that Λ_L takes the form of a $b \times b$ matrix with the properties in Fact 2.2.*

3. Connectedness: *Two vertices i, j in G_Λ have an edge between them if and only if there is a path between them in G whose edges are in the set*

$$S = \{(i, j)\} \cup \{(k, l) \in E : k, l = i \text{ or } j \text{ or } k, l \in V \setminus B\}.$$

In particular, G_Λ is connected if G is.

Remark 2.18. This of course implies that Λ_L has all the properties of a Laplacian matrix as outlined in Section 2.3. For instance, we will frequently use that Λ_L is symmetric and positive-semidefinite, and that the kernel of Λ_L is spanned by the all-ones vector if G is connected.

We will not prove these properties except for the fact that R as in (2.13) is always invertible. This cute argument comes from a previous version of [GR21], though it is probably not originally from there.

Proof that R as in (2.13) is invertible. Denote the number of vertices of G by n and the number of boundary vertices in B by b. Enumerate the vertices of G so the the boundary vertices come first and write

$$L = \begin{bmatrix} P & Q \\ Q^t & R \end{bmatrix},$$

where P acts on the boundary B and R acts on the interior $V \setminus B$. Suppose that the kernel of R is non-trivial so that $Rf = \mathbf{0}$ for some f in $\mathbb{R}^{n-b}$. Let

$$\widehat{f} = \begin{bmatrix} \mathbf{0}_b \\ f \end{bmatrix}$$

where $\mathbf{0}_b$ is the all-zeroes vector with b entries. But then $L\widehat{f} = \mathbf{0}$, contradicting that the kernel of L is spanned by the all-ones vector. Hence R is invertible as we wanted. ∎

The properties in Theorem 2.17 suggest that there is another viewpoint of going from the combinatorial Laplacian of to its DtN matrix w.r.t. a subset of the vertices, namely as a *graph reduction process* (i.e. the *Kron reduction* as mentioned in Section 2.4.3) via taking Schur complements. Indeed, as can be seen in Theorem 2.17 as well as in the rest of [DB13], many properties of the original graph G are retained in the graph G_Λ whose Laplacian is the combinatorial DtN matrix of G and whose vertices are the boundary vertices of G. As we saw in Section 2.5.1, Kron reduction provides a way to 'focus in' on a particular subset of the vertices that for some reason or another is of interest. We will not expand further on this topic in this thesis, but highly recommend [DB13] for a detailed account.

2.7. Graph operators and the Courant-Fischer Theorem

The celebrated Courant-Fischer Theorem is an abstract result regarding symmetric matrices that nonetheless yields quite a bit of intuition into eigenvalues of matrices by presenting them as solutions to optimization problems - a *variational characterization* of each respective eigenvalue. We first present the theorem in its entirety and later show what it entails in the special case of studying the eigenvalues of the operators on graphs that we have introduced.

Definition 2.19 (Rayleigh quotient)**.** Let M be a symmetric $n \times n$ matrix with entries in $\mathbb{R}$. The *Rayleigh quotient* of a vector f in $\mathbb{R}^n$ w.r.t. M is

$$R_M(f) := \frac{(f, Mf)}{(f,f)}, \tag{2.19}$$

where $(\cdot,\cdot)$ denotes the usual inner product in $\mathbb{R}^n$. Sometimes, we will write the Rayleigh quotient of M as simply $R(f)$ if there is no risk of confusing which matrix M is being studied.

Remark 2.20. Note that the Rayleigh quotient $R_M(v)$ of an eigenvector v of M is its corresponding eigenvalue λ_v:

$$R_M(v) = \frac{(v, Mv)}{(v,v)} = \frac{\lambda_v(v,v)}{(v,v)} = \lambda_v.$$

Essentially, the Courant-Fischer Theorem states that for appropriately chosen, quite natural restrictions on f, the eigenvalues of M are extremal values of the Rayleigh quotient. In the rest of this section, we will write $S \subseteq \mathbb{R}^n$ to denote a subspace of $\mathbb{R}^n$ and write $f \perp S$ if f is a vector such that $(f,s) = 0$ for all s in S.

The following formulation of the Courant-Fischer Theorem can be found in e.g. [But08], where it is Theorem 32.

Theorem 2.21 (Courant-Fischer)**.** *Let M be a symmetric $n \times n$ matrix with entries in $\mathbb{R}$ and eigenvalues $\lambda_0 \leq \lambda_1 \leq \ldots \leq \lambda_{n-1}$. Then it holds that*

$$\lambda_k = \min_{\substack{S \subseteq \mathbb{R}^n \\ \dim(S) = n-k-1}} \max_{\substack{f \perp S \\ f \neq \mathbf{0}}} R_M(f) = \max_{\substack{S \subseteq \mathbb{R}^n \\ \dim(S) = k}} \min_{\substack{f \perp S \\ f \neq \mathbf{0}}} R_M(f). \tag{2.20}$$

In particular, $\lambda_0 \leq R_M(f) \leq \lambda_{n-1}$ for all f in $\mathbb{R}^n$. The Courant-Fischer Theorem leads to quite explicit expressions for especially the smallest non-zero eigenvalue of the combinatorial and normalized Laplacian and DtN map, as we will see in Corollaries 2.22 and 2.23. Analogous results as those in Corollaries 2.22 and 2.23 hold for the other eigenvalues of each respective operator, but we will focus on estimates of the smallest non-zero eigenvalue of the DtN maps in this thesis. Therefore, we only state Corollaries 2.22 and 2.23 for the smallest non-zero eigenvalue of the operators we study.

Corollary 2.22 (Variational characterizations of the spectral gaps of Laplacians)**.** *Let $G = (V, E, w)$ be a connected graph with n vertices enumerated as $1, 2, \ldots, n$, combinatorial Laplacian L, and normalized Laplacian $\mathcal{L}$. Let $\lambda_1(L)$ and $\lambda_1(\mathcal{L})$ denote the spectral gap of each respective Laplacian. Then*

$$\lambda_1(L) = \min_{\substack{f \in \mathbb{R}^n \\ f \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i=1}^n f(i)^2} \mid \sum_{i=1}^n f(i) = 0 \right\}, \tag{2.21}$$

$$\lambda_1(\mathcal{L}) = \min_{\substack{f \in \mathbb{R}^n \\ f \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i=1}^n m(i) f(i)^2} \mid \sum_{i=1}^n m(i) f(i) = 0 \right\}. \tag{2.22}$$

Proof. The case for L: Since G is connected, the eigenspace of the eigenvalue 0 of L is spanned by the all-ones vector, denoted $\mathbf{1}$. Moreover, L is positive-semidefinite. Hence, for λ_1 the S in the second equation in (2.20) is the space spanned by the all-ones vector. By plugging into the Rayleigh quotient, we get the equation for $\lambda_1(L)$ as

$$\lambda_1(L) = \min_{\substack{f \subseteq \mathbb{R}^n \\ f \neq \mathbf{0}, f \perp \mathbf{1}}} R_L(f) = \min_{\substack{f \subseteq \mathbb{R}^n \\ f \neq \mathbf{0}, f \perp \mathbf{1}}} \frac{(f, Lf)}{(f, f)}.$$

It follows from (2.7) that

$$(f, Lf) = \sum_{(i,j) \in E} w_{ij}(f(i) - f(j))^2.$$

Moreover, the condition $f \perp \mathbf{1}$ means precisely that $\sum_{i=1}^n f(i) = 0$. Therefore, the expression becomes

$$\lambda_1(L) = \min_{\substack{f \in \mathbb{R}^n \\ f \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i=1}^n f(i)^2} \mid \sum_{i=1}^n f(i) = 0 \right\}$$

which is what was sought.

The case for $\mathcal{L}$: We cannot actually use the Courant-Fischer Theorem directly on $\mathcal{L}$ since it is not necessarily a symmetric matrix. Recall however that $\mathcal{L} = D^{-1}L$, where D is the diagonal matrix such that $D_{ii} = m(i)$. Moreover, note that D is invertible if G is connected. Hence $\mathcal{L}$ is similar to the symmetric matrix $\mathbf{L}$ defined as $\mathbf{L} = D^{-1/2}LD^{-1/2}$ and thus has the same eigenvalues as $\mathbf{L}$. We recognize $\mathbf{L}$ as the symmetric normalized Laplacian mentioned in Section 2.3.2. Once again G is connected, so the eigenspace 0 of $\mathbf{L}$ is spanned by the vector $D^{1/2}\mathbf{1}$ since

$$\mathbf{L}D^{1/2}\mathbf{1} = D^{-1/2}LD^{-1/2}D^{1/2}\mathbf{1} = D^{-1/2}L\mathbf{1} = \mathbf{0}.$$

By plugging into the Rayleigh quotient, we get the equation for $\lambda_1(\mathbf{L})$ as

$$\begin{aligned}
\lambda_1(\mathbf{L}) &= \min_{\substack{f \subseteq \mathbb{R}^n \\ f \neq \mathbf{0}, f \perp D^{1/2}\mathbf{1}}} R_M(f) \\
&= \min_{\substack{f \subseteq \mathbb{R}^n \\ f \neq \mathbf{0}, f \perp D^{1/2}\mathbf{1}}} \frac{(f, \mathbf{L}f)}{(f, f)} \\
&= \min_{\substack{f \subseteq \mathbb{R}^n \\ f \neq \mathbf{0}, f \perp D^{1/2}\mathbf{1}}} \frac{(f, D^{-1/2}LD^{-1/2}f)}{(f, f)} \\
&= \min_{\substack{f \subseteq \mathbb{R}^n \\ f \neq \mathbf{0}, f \perp D^{1/2}\mathbf{1}}} \frac{(D^{-1/2}f, LD^{-1/2}f)}{(f, f)}.
\end{aligned}$$

The change of variables $D^{-1/2}f \mapsto g$ (which we can perform since the matrix $D^{1/2}$ is invertible because G is connected) yields

$$\lambda_1(\mathbf{L}) = \min_{\substack{g \subseteq \mathbb{R}^n \\ g \neq \mathbf{0}, D^{1/2}g \perp D^{1/2}\mathbf{1}}} \frac{(g, Lg)}{(D^{1/2}g, D^{1/2}g)}.$$

Again, (2.7) implies that

$$(g, Lg) = \sum_{(i,j)\in E} w_{ij}(g(i) - g(j))^2.$$

Moreover, the condition $D^{1/2}g \perp D^{1/2}\mathbf{1}$ means precisely that $\sum_{i=1}^n m(i)g(i) = 0$. Therefore, our final expression is

$$\lambda_1(\mathbf{L}) = \min_{\substack{g\in\mathbb{R}^n \\ g\neq\mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(g(i) - g(j))^2}{\sum_{i=1}^n m(i)g(i)^2} \mid \sum_{i=1}^n m(i)g(i) = 0 \right\},$$

which is what we wanted. ■

The statement and proof of Corollary 2.22 served mostly as a warm-up for the proof of Corollary 2.23, which uses similar techniques but is slightly more technical.

Corollary 2.23 (Variational characterization of the spectral gaps of DtN maps)**.** *Let $G = (V, E, w)$ be a connected graph with n vertices, enumerated as $1, 2, \ldots, n$. Let B be the boundary of G, and let L denote the combinatorial Laplacian of G. Denote the combinatorial DtN map of G by Λ_L and the normalized DtN map of G by $\Lambda_{\mathcal{L}}$. Let σ_1 denote the spectral gap of each respective DtN map. Then*

$$\sigma_1(\Lambda_L) = \min_{\substack{f\in\mathbb{R}^n \\ f|_B\neq\mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} f(i)^2} \mid \sum_{i\in B} f(i) = 0 \right\}, \tag{2.23}$$

$$\sigma_1(\Lambda_{\mathcal{L}}) = \min_{\substack{f\in\mathbb{R}^n \\ f|_B\neq\mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} m(i)f(i)^2} \mid \sum_{i\in B} m(i)f(i) = 0 \right\}. \tag{2.24}$$

Proof. Write b for the number of boundary vertices in G. We introduce the following notation: For two vectors x and y in $\mathbb{R}^n$ with inner product $(x, y) := (x, y)_V$, we write $(x, y)_B$ to denote the inner product $(x\,|_B, y\,|_B)$ on the boundary B of G. We write $(x, y)_{V\setminus B}$ to denote the inner product $(x\,|_{V\setminus B}, y\,|_{V\setminus B})_{V\setminus B}$ on the interior $V \setminus B$ of G. With this notation, note that

$$(x, y)_V = (x, y)_B + (x, y)_{V\setminus B}.$$

We will use this notation when it is easy to confuse the inner product in $\mathbb{R}^n$ with the inner product in $\mathbb{R}^b$.

The case for Λ_L: By Theorem 2.17, the combinatorial DtN map of G w.r.t. B is again the Laplacian of a connected graph. Therefore, the kernel of Λ_L is spanned by the all-ones vector in $\mathbb{R}^b$, which we denote by $\mathbf{1}$. Take f to be a vector in $\mathbb{R}^b$. Since the combinatorial DtN matrix is a Laplacian and therefore symmetric, we can apply the Courant-Fischer Theorem. Since Λ_L is positive-semidefinite, again by virtue of being a combinatorial Laplacian, the Courant-Fischer Theorem yields that

$$\sigma_1(\Lambda_L) = \max_{\substack{S\subseteq\mathbb{R}^b \\ \dim(S)=1}} \min_{\substack{f\perp S \\ f\neq\mathbf{0}}} R_{\Lambda_L}(f) = \min_{\substack{f\perp\mathbf{1} \\ f\neq\mathbf{0}}} R_{\Lambda_L}(f).$$

The Rayleigh quotient is

$$R_{\Lambda_L}(f) = \frac{(f, \Lambda_L f)}{(f, f)} = \frac{(f, (Lu_f)\,|_B)}{(f, f)},$$

where u_f is the harmonic extension of f to all of $\mathbb{R}^n$. By definition, we have that $Lu_f = 0$ on $V \setminus B$ and that $u_f = f$ on B. Hence, with notation as above we get

$$0 = (u_f, Lu_f)_{V\setminus B} = (u_f, Lu_f)_V - (f, Lu_f)_B.$$

Now (2.7) implies that

$$(u_f, Lu_f)_V = \sum_{(i,j)\in E} w_{ij}(u_f(i) - u_f(j))^2.$$

Therefore, we arrive at the expression

$$(f, Lu_f)_B = \sum_{(i,j)\in E} w_{ij}(u_f(i) - u_f(j))^2. \tag{2.25}$$

From now on we write $(\cdot,\cdot)_B = (\cdot,\cdot)$. Using (2.25), the Rayleigh quotient becomes

$$R_{\Lambda_L}(f) = \frac{(f, \Lambda_L f)}{(f,f)} = \frac{\sum_{(i,j)\in E} w_{ij}(u_f(i) - u_f(j))^2}{\sum_{i\in B} f(i)^2}.$$

Hence, the expression for $\sigma_1(\Lambda_L)$ becomes

$$\lambda_1(\Lambda_L) = \min_{\substack{f\in\mathbb{R}^b \\ f\neq \mathbf{0}, f\perp \mathbf{1}}} \frac{\sum_{(i,j)\in E} w_{ij}(u_f(i) - u_f(j))^2}{\sum_{i\in B} f(i)^2}. \tag{2.26}$$

However, among functions g in $\mathbb{R}^n$ such that $g\mid_B = f$, the harmonic extension u_f of f to $\mathbb{R}^n$ is the unique minimizer of the Dirichlet energy (see Lemma 2.10), which happens to be the numerator in (2.26). This fact lets us write

$$\sigma_1(\Lambda_L) = \min_{\substack{f\in\mathbb{R}^b \\ f\neq \mathbf{0}, f\perp \mathbf{1}}} \left\{ \frac{\min_{\substack{g\in\mathbb{R}^n \\ g|_B = f}} \left\{\sum_{(i,j)\in E} w_{ij}(g(i) - g(j))^2\right\}}{\sum_{i\in B} f(i)^2} \right\},$$

but this is just a reformulation of the expression

$$\sigma_1(\Lambda_L) = \min_{\substack{f\in\mathbb{R}^n \\ f|_B\neq \mathbf{0}, f|_B\perp \mathbf{1}}} \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} f(i)^2}.$$

Finally, we note that the condition $f\mid_B \perp \mathbf{1}$ means precisely that $\sum_{i\in B} f(i) = 0$. This leads to the final expression

$$\sigma_1(\Lambda_L) = \min_{\substack{f\in\mathbb{R}^n \\ f\neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} f(i)^2} \mid \sum_{i\in B} f(i) = 0 \right\},$$

which is what was sought.

The case for $\Lambda_{\mathcal{L}}$: As was the case for the normalized Laplacian, $\Lambda_{\mathcal{L}}$ is not necessarily a symmetric matrix, so we cannot use the Courant-Fischer theorem directly. However, we can use the Schur complement formula (2.14) to note that

$$\Lambda_{\mathcal{L}} = D_B^{-1}(P - QR^{-1}Q^t) = D_B^{-1}\Lambda_L, \tag{2.27}$$

where D_B is the $b \times b$-diagonal matrix whose entries are the vertex measures $m(i)$ of the boundary vertices of G. Note that if G is connected, the matrix D_B is invertible. The expression (2.27) shows that $\Lambda_{\mathcal{L}}$ is similar to, and thus shares its eigenvalues with, $M := D_B^{-1/2}\Lambda_L D_B^{-1/2}$, which is a symmetric matrix since Λ_L is a combinatorial Laplacian. Moreover, since Λ_L is the combinatorial Laplacian of a connected graph, its only eigenvector with eigenvalue 0 consists of the all-ones vector $\mathbf{1}$. This implies that the kernel of M is spanned by $D_B^{1/2}\mathbf{1}$. We now find a variational characterization of the first nonzero eigenvalue of M and thus of $\Lambda_{\mathcal{L}}$. Since Λ_L is a combinatorial Laplacian and therefore positive-semidefinite, M can also be easily seen to be positive-semidefinite. Therefore, the Courant-Fischer Theorem applied to M yields

$$\sigma_1(M) = \max_{\substack{S\subseteq\mathbb{R}^b \\ \dim(S)=1}} \min_{\substack{f\perp S \\ f\neq\mathbf{0}}} R_M(f) = \min_{\substack{f\perp D_B^{1/2}\mathbf{1} \\ f\neq\mathbf{0}}} R_M(f).$$

The Rayleigh quotient of M is

$$R_M(g) = \frac{(g, Mg)}{(g,g)} = \frac{(g, D_B^{-1/2}\Lambda_L D_B^{-1/2} g)}{(g,g)},$$

so expression for $\sigma_1(M)$ becomes

$$\sigma_1(M) = \min_{\substack{g\in\mathbb{R}^b \\ f\neq\mathbf{0}, g\perp D_B^{1/2}\mathbf{1}}} \frac{(g, D_B^{-1/2}\Lambda_L D_B^{-1/2} g)}{(g,g)}.$$

We make a change of variables in $\mathbb{R}^b$ via $D_B^{-1/2} f \mapsto g$ (which we can perform since G is connected, which implies that $D_B^{1/2}$ is invertible). This gives

$$\begin{aligned}\sigma_1(M) &= \min_{\substack{f\in\mathbb{R}^b \\ f\neq\mathbf{0}, D_B^{1/2} f\perp D_B^{1/2}\mathbf{1}}} \frac{(f, \Lambda_L f)}{(D_B^{1/2} f, D_B^{1/2} f)} \\ &= \min_{\substack{f\in R^b \\ f\neq\mathbf{0}, D_B^{1/2} f\perp D_B^{1/2}\mathbf{1}}} \frac{(f, (Lu_f)\mid_B)}{(D_B^{1/2} f, D_B^{1/2} f)}.\end{aligned}$$

Using the same 'Green's formula' (2.25) as in the combinatorial case this becomes

$$\sigma_1(M) = \min_{\substack{f\in\mathbb{R}^b \\ f\neq\mathbf{0}, D_B^{1/2} f\perp D_B^{1/2}\mathbf{1}}} \frac{\sum_{(i,j)\in E} w_{ij}(u_f(i) - u_f(j))^2}{\sum_{i\in B} m(i) f(i)^2}.$$

By the same arguments as in the combinatorial case, this reduces to

$$\sigma_1(M) = \min_{\substack{f\in\mathbb{R}^n \\ f|_B\neq\mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} m(i) f(i)^2} \mid \sum_{i\in B} m(i) f(i) = 0 \right\},$$

as sought.

■

The variational characterizations (2.21), (2.22) of the spectral gaps of the combinatorial and normalized Laplacian are very similar to their respective DtN counterparts (2.23) and (2.24), and indeed, adapting methods used to optimize the expressions in Corollary 2.22 to the expressions in Corollary 2.23 is the major theme in the novel results in this thesis.

2.8. The DtN map on quantum graphs

An approach to the study of network-like objects which is one additional step in the continuous direction is to study (operators on) *metric graphs*, where one thinks of the edges (i, j) of a graph as one-dimensional *intervals* with lengths $L_{ij} \in \mathbb{R}$, whence the graph itself takes the form of a one-dimensional simplicial complex. A metric graph together with a differential operator is usually called a *quantum graph*, and their study is an active field of research; we refer the interested reader to [BK13] for a thorough overview of the field. In some situations, one can show that the analogue of a DtN map on a quantum graph can be directly studied via its discrete counterpart, and so the study of the DtN map on discrete graphs can in fact also be an avenue to new insights into its counterpart on quantum graphs. We will exhibit such a case in this section.

All definitions in this section are standard and can be found, albeit slightly reformulated, in Chapter 1 of [BK13].

2.8.1. Introductory concepts and definitions

Definition 2.24 ((Finite) Metric graph)**.** A finite graph $G = (V, E)$ is a *finite metric graph* if:

1. Each edge (i, j) is identified with an interval $[0, L_{ij}]$. We refer to L_{ij} as the *length* of the edge (i, j). If (i, j) and (i, k) are edges in E, the points corresponding to i in the intervals L_{ij} and L_{ik} are identified. There are situations where infinite edge lengths are natural to consider, but we will limit ourselves to finite edge lengths here.

2. In an edge (i, j) there are two coordinates x_i and x_j taking values in $[0, L_{ij}]$, measuring the distance of a point in (i, j) from the vertices i and j, respectively. Note that $x_i = L_{i,j} - x_j$.

Often one also considers metric graphs with infinitely many vertices but with finite vertex degrees, but we limit ourselves to finitely many vertices as well here. A metric graph can be identified with the one-dimensional simplicial complex which is the union of all the edges and in which we identify all edge ends that correspond to the same vertex. A metric graph can also be readily transformed into a metric space. To do this, we also need to define a path on a metric graph.

Definition 2.25 (Path in a metric graph)**.** Suppose x and y are contained in the edges $(i, j), (k, l)$ respectively and there is a sequence $(i, j), (j, v_1), \ldots, (v_m, k), (k, l)$ of edges in G. The *path* defined by this sequence is the union of the edges $(j, v_1), (v_1, v_2), \ldots, (v_m, k)$ and the subintervals $[0, x] \subset (i, j)$ (w.r.t. the coordinate x_j) and $[0, y] \subset (k, l)$ (w.r.t. the coordinate x_k). The *length* of this path is the sum of the edge lengths of the edges $(j, v_1), (v_1, v_2), \ldots, (v_m, k)$ together with the coordinate values of x and y w.r.t. the coordinates x_j and x_k respectively.

Definition 2.26 (Metric on a metric graph)**.** The metric ρ between two points x, y in a metric graph Γ is the function that maps (x, y) to the length of the shortest path between x and y in Γ.

When studying operators on graphs, one naturally needs a function space on which these operators are defined. The function spaces on quantum graphs that one usually works with are covered by the following two definitions.

Definition 2.27 (Function space (of a metric graph))**.** The *function space* $L_2(\Gamma)$ of a metric graph $\Gamma = (V, E)$ is the space of functions that are in $L_2((i, j))$ when restricted to each edge (i, j) in E.

Definition 2.28 (Sobolev space (of a metric graph))**.** The *Sobolev space* $H^1(\Gamma)$ of a metric graph $\Gamma = (V, E)$ consists of continuous functions on Γ (with the metric as in Definition 2.26 on Γ) that are in the Sobolev spaces $H^1((i, j))$ when restricted to each edge e in E. As remarked in the discussion following Definition 1.3.6 in [BK13], the Sobolev space $H^k(\Gamma)$ is unable to be defined in this way since unlike in the case $k = 1$ there is no natural condition at the vertices. Therefore, one usually just defines

$$\widetilde{H}^k(\Gamma) = \bigoplus_{(i,j)\in E} H^k((i, j)),$$

and varies the vertex conditions towards what is reasonable for the problem at hand.

By continuity, functions in $H^1(\Gamma)$ take on the same value at a vertex i for every edge adjacent to i. By associating a differential operator on a metric graph Γ, it turns into what is called a *quantum graph*. We will consider the operator $-d^2$ defined by the negative second derivative acting on each edge as $f \mapsto -\frac{d^2}{dx^2} f$, where x is a coordinate defined on the edge as in Definition 2.24. Note that the second derivative operator is symmetric w.r.t. the direction of the coordinate in each edge.

We also want to impose conditions on functions defined on Γ. Define

$$\partial f(i) := \sum_{j:(i,j)\in E} \frac{d}{dx_i} f\mid_{(i,j)} (i). \tag{2.28}$$

Note that the direction of each derivative in $\partial f(i)$ is *away* from the vertex i. The most common conditions, and indeed those we will consider, are usually called the *standard* or *continuity-Kirchhoff* conditions:

$$\text{Standard conditions on } f: \begin{cases} f \text{ is continuous on } \Gamma, \text{ and} \\ \text{at each vertex } i, \text{ it holds that } \partial f(i) = 0. \end{cases} \tag{2.29}$$

2.8.2. The DtN map on quantum graphs

The discussion in this section is lifted from Section 3 in [KL20]. In the analogue of the Dirichlet problem setting (2.8) on a quantum graph, we can define a DtN map. More precisely, let $\Gamma = (V, E)$ be a quantum graph with the negative second derivative operator. Let B be a subset of its vertices with $|B| = b$, and let $g \in \mathbb{R}^b$ be a function assigning values to the vertices in B. The Dirichlet-like problem to consider is finding (the unique, for reasons we do not need to elaborate on here) f in $H^1(\Gamma)$ such that

$$\begin{aligned} -\frac{d^2 f}{dx^2} &= 0, \text{ in the interior of each edge,} \\ f\mid_B &= g, \\ \partial f(i) &= 0, \text{ at every vertex } i \text{ in } V \setminus B. \end{aligned} \tag{2.30}$$

Note that we impose continuity-Kirchhoff conditions in the interior $V \setminus B$. In the context of the problem (2.30) on quantum graphs, the conditions $f\mid_B = g$ for some given g, i.e.

explicit conditions on f itself, are usually called *Dirichlet conditions*, just as for the discrete problem (2.8). Similarly to how the problem (2.8) relates to (2.10), one can instead pose a related problem with a different kind of boundary conditions:

$$\begin{aligned} -\frac{d^2 f}{dx^2} &= 0, && \text{in the interior of each edge,} \\ \partial f(i) &= g(i), && \text{for all vertices } i \text{ on } B, \\ \partial f(i) &= 0, && \text{at every vertex } i \text{ in } V \setminus B. \end{aligned} \tag{2.31}$$

Conditions of the form

$$\partial f(i) = g(i), \text{ for all vertices } i \text{ on } B,$$

i.e. conditions on the *derivatives* of a prospective solution to the problem (2.31), are instead called *Neumann conditions*. The *DtN (Dirichlet-to-Neumann) map* M is then the operator that maps given Dirichlet conditions g in $\mathbb{R}^b$ on (2.30) to the Neumann conditions that when posed on (2.31) would yield the same solution f as the the problem (2.30). With some enumeration of the vertices, we can identify M with a $b \times b$ matrix just as in the discrete case. We will show that in fact M is the combinatorial DtN map of the weighted graph $G = (V, E, w)$ with boundary B, where w is the weight function that puts the weight $w_{ij} = \frac{1}{L_{ij}}$ on the edge (i, j). We denote the combinatorial Laplacian of G by L_G.

Gernandt and Rohleder [GR21] give a brief discussion on why this is the case, which we follow. Enumerate the vertices of Γ by $1, \ldots, n$ so that the boundary vertices come first. We are looking for the matrix M such that

$$M \begin{bmatrix} f(1) \\ f(2) \\ \vdots \\ f(b) \end{bmatrix} = \begin{bmatrix} \partial f(1) \\ \partial f(2) \\ \vdots \\ \partial f(b) \end{bmatrix}$$

whenever f is a solution of (2.30) with boundary conditions given by a function g in $\mathbb{R}^b$. Such a function f is linear on every edge; indeed, take an arbitrary vertex i in V. Then the function f such that

$$f\mid_{(i,j)}(x_i) = \frac{x_i}{L_{ij}} g(i) + \frac{L_{ij} - x_i}{L_{ij}} g(j)$$

solves (2.30), so by uniqueness f is necessarily linear. Moreover

$$\frac{d}{dx_i} f\mid_{(i,j)}(i) = \frac{1}{L_{ij}}(f(i) - f(j)) = w_{ij}(f(i) - f(j)).$$

By restricting to the vertices, we get by the continuity-Kirchhoff conditions that for any vertex i in $V \setminus B$, it holds that

$$0 = \sum_{j:(i,j)\in E} \frac{d}{dx_i} f\mid_{(i,j)}(i) = \sum_{j:(i,j)\in E} w_{ij}(f(i) - f(j)) = L_G f(i).$$

Hence, $f\mid_V$ is the (discrete) harmonic extension of g on G in the sense of (2.8). Therefore the matrix M such that

$$(Mf\mid_B)(i) = \sum_{j:(i,j)\in E} \frac{d}{dx_i} f\mid_{(i,j)}(i) = L_G f\mid_V(i) = \Lambda_{L_G} f\mid_V(i),$$

whenever i is a vertex in B, is precisely the matrix that maps $f(i)$ to $(L_G u_f)\mid_B(i) = \Lambda_{L_G} f\mid_B(i)$, where u_f is the harmonic extension of $f\mid_B$ to V. This coincides with the definition of the combinatorial DtN matrix Λ_{L_G} on G w.r.t. B.

Remark 2.29. It is not so surprising that this connection exists if we again consider both the metric graph Γ and discrete graph G as electrical networks, similarly to in Section 2.4.3; the edge lengths L_{ij} have natural interpretations as resistances in the network, so the corresponding discrete conductances are the inverses $1/L_{ij}$. The continuity-Kirchhoff conditions on the interior vertices of Γ (which can be interpreted as demanding that Kirchhoff's current law is satisfied in the interior of Γ) forces f to be harmonic on the vertices, whereby the connection follows.

Chapter 3

Planar graphs with 'balanced' boundary

3.1. The result

In this section, we prove Theorem 3.1 which gives upper bounds on the spectral gaps of the combinatorial and normalized DtN maps of a planar graph G with boundary B. We use a topologically-inclined technique pioneered in Theorem 3.3 in Spielman and Teng [ST07] and generalized in Theorem 3.5 in Plümer [Plü20].

Theorem 3.1. *Let $G = (V, E, w)$ be a planar weighted graph with boundary B. Suppose the number of boundary vertices in G, denoted b, is at least 5. Then the spectral gap $\sigma_1(\Lambda_L)$ of the combinatorial DtN map on G w.r.t. B satisfies*

$$\sigma_1(\Lambda_L) \leq \frac{8 \max_{i \in V} m(i)}{b}. \tag{3.1}$$

If, in addition, the boundary vertices of G satisfy

$$2(m(i) + m(j)) < \sum_{k \in B} m(k), \tag{3.2}$$

for all vertices i, j in B such that (i, j) is in E or $i = j$, the spectral gap $\sigma_1(\Lambda_{\mathcal{L}})$ of the normalized DtN map on G w.r.t. B satisfies

$$\sigma_1(\Lambda_{\mathcal{L}}) \leq \frac{8 \max_{i \in V} m(i)}{\mathrm{Vol}(B)}. \tag{3.3}$$

Remark 3.2. If the boundary of G consists of all of V, the combinatorial DtN map on G is just the combinatorial Laplacian on G. Then, the bound (3.3) specializes to Theorem 3.9 in [Plü20]. If we in addition set all of the edge weights in G to 1, the bound (3.1) specializes to Theorem 3.3 in [ST07].

Remark 3.3. The constraint that the number of boundary vertices is at least 5 comes from the proof of Theorem 3.7, which in turn is integral to the proof of Theorem 3.1. These constraints could potentially be relaxed in special cases, such as when there are no edges between boundary vertices, but are needed in general for the proof of Theorem 3.7 to be valid.

Remark 3.4. A natural question to ask is whether the bounds (3.1) and (3.3) are tight for any graphs whose Steklov eigenvalues are able to be computed explicitly with relative ease. The author has so far not been able to find any such example. We can at least note that the bound (3.1) is better than some trivial bounds; by Theorem 2.16, all of the eigenvalues of the combinatorial DtN map Λ_L of a graph $G = (V, E, w)$ can be bounded by the largest eigenvalue of the combinatorial Laplacian L of G. Furthermore, it is classical that the largest eigenvalue of the combinatorial Laplacian of G can be bounded from above by $2 \max_{i \in V} m(i)$. Therefore, the bound (3.1) improves this (trivial) estimate of $\sigma_1(\Lambda_L)$ whenever there are more than four boundary vertices, which we in any case demand in Theorem 3.1.

We will need to establish quite a bit of background to prove Theorem 3.1. We follow a similar approach as in Section 3 in [ST07]. We start by recalling the variational characterizations of the spectral gaps $\sigma_1(\Lambda_{\mathcal{L}})$ and $\sigma_1(\Lambda_{\mathcal{L}})$ of the combinatorial and normalized DtN maps as in (2.23) and (2.24).

$$\sigma_1(\Lambda_L) = \min_{\substack{f:V\to\mathbb{R}^n \\ f|_B \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} f(i)^2} \mid \sum_{i\in B} f(i) = 0 \right\},$$

$$\sigma_1(\Lambda_{\mathcal{L}}) = \min_{\substack{f:V\to\mathbb{R}^n \\ f|_B \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} m(i) f(i)^2} \mid \sum_{i\in B} m(i) f(i) = 0 \right\}.$$

It will be more instructive to think of the variable f in (2.23) and (2.24) as a vector in $\mathbb{R}^n$ rather than a function on the vertices of G. To emphasize this, we identify f with the vector $v = v_f$ in $\mathbb{R}^n$ whose i:th entry is $f(i)$, and write $f(i)$ as v_i. With this notation, the variational characterizations (2.23) and (2.24) become

$$\sigma_1(\Lambda_L) = \min_{\substack{v\in\mathbb{R}^n \\ v|_B \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(v_i - v_j)^2}{\sum_{i\in B} v_i^2} \mid \sum_{i\in B} v_i = 0 \right\}, \tag{3.4}$$

$$\sigma_1(\Lambda_{\mathcal{L}}) = \min_{\substack{v\in\mathbb{R}^n \\ v|_B \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(v_i - v_j)^2}{\sum_{i\in B} m(i) v_i^2} \mid \sum_{i\in B} m(i) v_i = 0 \right\}. \tag{3.5}$$

Now we establish equivalent expressions for $\sigma_1(\Lambda_L)$ and $\sigma_1(\Lambda_{\mathcal{L}})$ whose input parameters are collections of n vectors in $\mathbb{R}^l$, for an arbitrary integer l, instead of a collection of n real numbers (i.e. the entries of v) as in (3.4) and (3.5). This will help us use topological techniques to construct test functions for (3.4) and (3.5). These equivalent expressions are established in Lemma 3.5, which is analogous to Lemma 3.1 in [ST07].

Lemma 3.5 (Embedding lemma). *Let $G = (V, E, w)$ be a connected weighted graph on n vertices with boundary B. Let l be an arbitrary integer. Then the spectral gaps $\sigma_1(\Lambda_L)$ and $\sigma_1(\Lambda_{\mathcal{L}})$ of the combinatorial and normalized DtN maps Λ_L and $\Lambda_{\mathcal{L}}$ on G can be written as*

$$\sigma_1(\Lambda_L) = \min_{\mathbf{v}_1,\dots,\mathbf{v}_n\in\mathbb{R}^l} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B}\|\mathbf{v}_i\|^2} \mid \sum_{i\in B} \mathbf{v}_i = \mathbf{0}, \{\mathbf{v}_i\}_{i\in B} \textit{ not all } \mathbf{0} \right\}, \tag{3.6}$$

$$\sigma_1(\Lambda_{\mathcal{L}}) = \min_{\mathbf{v}_1,\dots,\mathbf{v}_n\in\mathbb{R}^l} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} \mid \sum_{i\in B} m(i)\mathbf{v}_i = \mathbf{0}, \{\mathbf{v}_i\}_{i\in B} \textit{ not all } \mathbf{0} \right\}. \tag{3.7}$$

Proof. We prove Lemma 3.5 for $\Lambda_{\mathcal{L}}$; the proof method is entirely analogous for Λ_L. Recall from (3.5) that

$$\sigma_1(\Lambda_{\mathcal{L}}) = \min_{\substack{v\in\mathbb{R}^n \\ v|_B \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(v_i - v_j)^2}{\sum_{i\in B} m(i) v_i^2} \mid \sum_{i\in B} m(i) v_i = \mathbf{0} \right\}.$$

Consider a collection $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of vectors in $\mathbb{R}^l$ such that $\sum_{i \in B} m(i)\mathbf{v}_i = \mathbf{0}$. Further we assume that not all of the vectors in the set $\{\mathbf{v}_i\}_{i \in B}$ are the zero vector. Let the k:th entry of the i:th vector be denoted by $v_{i,k}$. Then we can write

$$\begin{aligned}
\frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} &= \frac{\sum_{(i,j)\in E}\sum_{k=1}^{l} w_{ij}(v_{i,k}-v_{j,k})^2}{\sum_{i\in B}\sum_{k=1}^{l} m(i)v_{i,k}^2} \\
&= \frac{\sum_{k=1}^{l}\sum_{(i,j)\in E} w_{ij}(v_{i,k}-v_{j,k})^2}{\sum_{k=1}^{l}\sum_{i\in B} m(i)v_{i,k}^2}.
\end{aligned}$$

However, for each k it holds by assumption that $\sum_{i\in B} m(i)v_{i,k} = 0$. By (3.5) it follows that for each k individually, we have

$$\frac{\sum_{(i,j)\in E} w_{ij}(v_{i,k}-v_{j,k})^2}{\sum_{i\in B} m(i)v_{i,k}^2} \geq \sigma_1(\Lambda_{\mathcal{L}}).$$

By the well-known fact that $\sum_i x_i / \sum_i y_i \geq \min_i x_i/y_i$ for $x_i, y_i > 0$ we then have that

$$\begin{aligned}
\frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} &= \frac{\sum_{k=1}^{l}\sum_{(i,j)\in E} w_{ij}(v_{i,k}-v_{j,k})^2}{\sum_{k=1}^{l}\sum_{i\in B} m(i)v_{i,k}^2} \\
&\geq \min_k \left\{\frac{\sum_{(i,j)\in E} w_{ij}(v_{i,k}-v_{j,k})^2}{\sum_{i\in B} m(i)v_{i,k}^2}\right\} \\
&\geq \sigma_1(\Lambda_{\mathcal{L}}).
\end{aligned} \tag{3.8}$$

What remains is to show that the inequality is not strict, so that if we minimize the left-hand side of (3.8) among collections $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of vectors in $\mathbb{R}^l$ such that $\sum_{i\in B} m(i)\mathbf{v}_i = \mathbf{0}$, we get $\sigma_1(\Lambda_{\mathcal{L}})$. We can see that this is the case as follows: We further restrict the $\mathbf{v}_i$ to be scalar multiples of the all-ones vector $\mathbf{1}$ in $\mathbb{R}^l$, so that $\mathbf{v}_i = c_i\mathbf{1}$, for a collection of n real numbers $c_1, \ldots, c_n$. Then the left-hand side of (3.8) reduces to

$$\frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} = \frac{\sum_{(i,j)\in E} w_{ij}(c_i - c_j)^2}{\sum_{i\in B} m(i)c_i^2}. \tag{3.9}$$

The right-hand side in (3.9) is the same expression as in (3.5), so minimizing over the c_i yields $\sigma_1(\Lambda_{\mathcal{L}})$. However, this minimum cannot be smaller in magnitude than if we minimize the left-hand side of (3.9) over collections $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of vectors in $\mathbb{R}^l$ such that $\sum_{i\in B} m(i)\mathbf{v}_i = \mathbf{0}$, since when we minimize over the c_i we have really only placed additional constraints on the $\mathbf{v}_i$. It follows that

$$\sigma_1(\Lambda_{\mathcal{L}}) \geq \min_{\mathbf{v}_1,\ldots,\mathbf{v}_n\in\mathbb{R}^l}\left\{\frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} \mid \sum_{i\in B} m(i)\mathbf{v}_i = \mathbf{0}, \{\mathbf{v}_i\}_{i\in B} \text{ not all } \mathbf{0}\right\} \geq \sigma_1(\Lambda_{\mathcal{L}}),$$

and we are done. ■

In the rest of the proof of Theorem 3.1, the expressions (3.6) and (3.7) will be used to bound $\sigma_1(\Lambda_L)$ and $\sigma_1(\Lambda_{\mathcal{L}})$ from above by placing a collection of vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ in $\mathbb{R}^3$ in such a way that we can simultaneously control both the numerator and denominator of the Rayleigh quotients in (3.6) and (3.7) while fulfilling the respective constraints of (3.6) and (3.7) on the vectors. The elegant way in which this is done in [ST07], and which we essentially follow, is to embed the graph G on the unit sphere and then put $\mathbf{v}_i$ at the coordinate corresponding to the vertex i in the embedded graph. If we place the vectors in this way, we can think of the quantity $\sum_{i \in B} m(i)\mathbf{v}_i$ as the 'center of mass' of the vectors belonging to boundary vertices, where the vector $\mathbf{v}_i$ has 'mass' $m(i)$. Analogously, we can also think of the quantity $\sum_{i \in B} \mathbf{v}_i$ as the center of mass of the vectors belonging to the boundary vertices, but with the masses of the $\mathbf{v}_i$ all equal to 1. This lets us think of the conditions in (3.6) and (3.7) as demanding that the center of mass of the $\mathbf{v}_i$ should be at the origin in $\mathbb{R}^3$.

By embedding G on the unit sphere and placing $\mathbf{v}_i$ at the i:th vertex of G, the planarity of G will let us use the surface area of the unit sphere to bound the numerators of the Rayleigh quotients in (3.6) and (3.7). Moreover, if none of the "masses" of the $\mathbf{v}_i$ are much larger than the rest of the masses combined as we require via the condition (3.2), it should always be possible to "warp" the embedding of G so that the center of mass of the vectors corresponding to boundary vertices is at the origin. We prove that this is the case in Theorem 3.7.

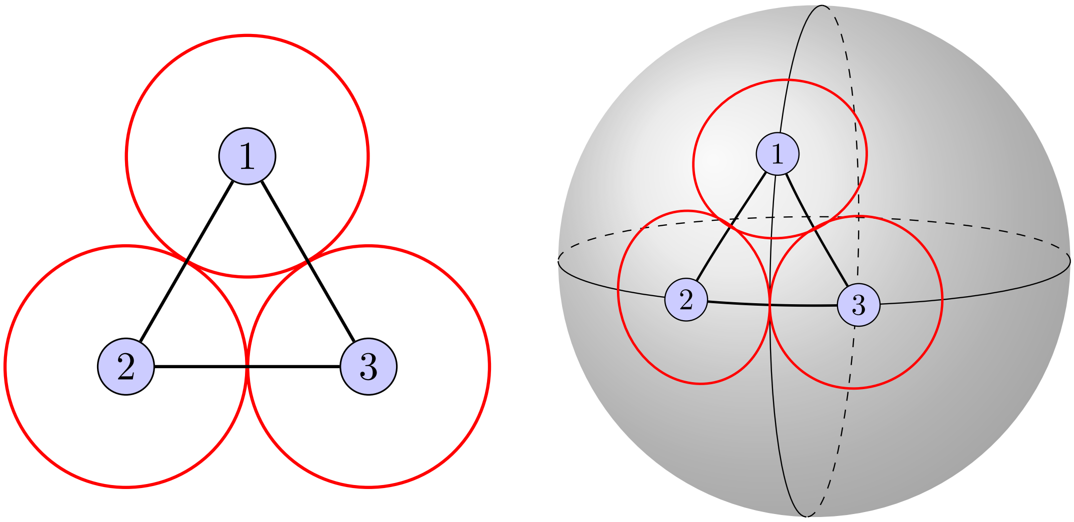
The theorem that lets us bound the numerators the Rayleigh quotients in (3.6) and (3.7) with our arrangement of the $\mathbf{v}_i$ is the classical *Koebe-Andreev-Thurston Theorem* or *Circle Packing Theorem*. A proof and discussion of this and related results can be found in Chapter 13 of [Thu02].

Theorem 3.6 (Circle Packing Theorem). *Let $G = (V, E)$ be a planar graph with vertex set $V = \{1, 2, \ldots, n\}$ and edge set E. Then there is a set of disks $\mathcal{D} = \{D_1, \ldots, D_n\}$ in the plane with disjoint interiors such that D_i and D_j have a single point in common if and only if (i, j) is in E. In fact, a graph is planar if and only if there is such a set of disks.*

In accordance with [ST07], we call an embedding of G as in Theorem 3.6 a *kissing disk embedding* of G in the plane and denote it by $\mathcal{D}_G = \{D_i\}_{i \in V}$. An example of a kissing disk embedding of the complete graph on three vertices can be found in Figure 3.1a. We say that this embedding is *univalent* to emphasize that the disks have disjoint interiors and share at most one point with each other.

The way that we embed G on the unit sphere is to take a kissing disk embedding $\mathcal{D}_G = \{D_i\}_{i \in V}$ of G in the plane and map it to S^2 via stereographic projection. The image of each kissing disk D_i is then what Spielman and Teng call a *cap*, i.e. the intersection of a half-space with the unit sphere. The boundary of each cap will then be a circle on S^2. The image of all of $\mathcal{D}_G$ will then be a collection of caps $\{C_i\}_{i \in V}$ such that the caps C_i and C_j share a single point if and only if (i, j) is an edge in G. Spielman and Teng call such a collection of caps a *kissing cap embedding* of G on the unit sphere. An example of a kissing cap embedding of the complete graph on three vertices can be seen in Figure 3.1b.

We denote a kissing cap embedding of G by $C_G = \{C_i\}_{i \in V}$, where C_i is the cap corresponding to the vertex i. Since the boundary of each cap C_i is a circle, we can unambiguously define the *center* of the cap C_i as the point in C_i equidistant to all boundary points of C_i. We denote the center of the cap C_i by $p(C_i)$ and denote the (Euclidean) distance from $p(C_i)$ to the boundary of C_i by r_i. We call r_i the *radius* of C_i.



(a) A kissing disk embedding of the graph K_3 in the plane.

(b) A kissing cap embedding of K_3 on the unit sphere.

Figure 3.1: Examples of kissing disk and kissing cap embeddings of K_3.

We will show in Theorem 3.7 that with our assumptions on the boundary of G, there exist kissing cap embeddings C_G, C'_G of G such that

$$\sum_{i\in B} m(i)p(C_i) = \mathbf{0}, \qquad \sum_{i\in B} p(C'_i) = \mathbf{0}, \tag{3.10}$$

These kissing cap embeddings will be used to bound $\sigma_1(\Lambda_{\mathcal{L}})$ and $\sigma_1(\Lambda_L)$, respectively.

Formally, the statement of Theorem 3.7 is as follows:

Theorem 3.7 (Kissing cap embedding lemma). *Let $G = (V, E, w)$ be a planar graph with boundary B. Suppose $|B| > 4$. Let $C_G = \{C_i\}_{i\in V}$ be a univalent kissing cap embedding of G on S^2 and let $\mu : V \longrightarrow (0, \infty)$ be a function on V such that*

$$2(\mu(i) + \mu(j)) < \sum_{k\in B} \mu(k), \tag{3.11}$$

for all $i, j \in B$ such that $(i, j) \in E$ or $i = j$. Then there exists a homeomorphism $f : S^2 \longrightarrow S^2$ that maps caps to caps, such that the univalent image kissing cap embedding $\widetilde{C} = (f(C_i))_{i\in B}$ satisfies

$$\sum_{i\in B} \mu(i)p(f(C_i)) = 0, \tag{3.12}$$

where $p(f(C_i))$ denotes the center of the cap $f(C_i)$.

Remark 3.8. The existence of the kissing cap embedding C_G as in (3.10) follows from Theorem 3.7 by choosing the function μ to be the usual vertex measure m as in (2.1). The existence of the kissing cap embedding C'_G as in (3.10) follows from Theorem 3.7 by choosing μ to be identically 1 for all the vertices in G, whereby the condition (3.11) always holds if the number of boundary vertices is greater than 4.

We postpone the proof of Theorem 3.7 to Section 3.2, since it is quite technical. If we take Theorem 3.7 as given for the moment, we have all the tools needed to prove Theorem 3.1.

Proof of Theorem 3.1. The case for $\Lambda_{\mathcal{L}}$: Recall the variational characterization (3.7) of $\sigma_1(\Lambda_{\mathcal{L}})$:

$$\sigma_1(\Lambda_{\mathcal{L}}) = \min_{\mathbf{v}_1,\dots,\mathbf{v}_n\in\mathbb{R}^l} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} \mid \sum_{i\in B} m(i)\mathbf{v}_i = \mathbf{0}, \{\mathbf{v}_i\}_{i\in B} \text{ not all } \mathbf{0} \right\}.$$

We set $l = 3$ in the expression (3.7). We want to bound $\sigma_1(\Lambda_{\mathcal{L}})$ from above by configuring a collection $\mathbf{v}_1, \dots, \mathbf{v}_n$ of vectors in $\mathbb{R}^3$ so that $\sum_{i\in B} m(i)\mathbf{v}_i = \mathbf{0}$, and then input the $\mathbf{v}_i$ into the Rayleigh quotient

$$R_{\Lambda_{\mathcal{L}}}(\mathbf{v}_1, \dots, \mathbf{v}_n) = \frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2}$$

as in (3.7). If the condition (3.2) is satisfied, Theorem 3.7 yields that there is a kissing cap embedding $C_G = \{C_i\}_{i\in V}$ of G such that $\sum_{i\in B} m(i)p(C_i) = \mathbf{0}$. Hence, if we place the vector $\mathbf{v}_i$ on the center $p(C_i)$ of C_i, the condition

$$\sum_{i\in B} m(i)\mathbf{v}_i = \mathbf{0}$$

is satisfied. Moreover, all of the vector lengths are 1 since they are placed on the unit sphere. Denote the radius of the i:th cap by r_i. If cap i is adjacent to cap j, then the squared vector norm $\|\mathbf{v}_i - \mathbf{v}_j\|^2$ will have length at most $(r_i + r_j)^2$ (see Figure 3.2). By Young's inequality, $(r_i + r_j)^2 \le 2(r_i^2 + r_j^2)$. Then we can write

$$\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2 \le 2\max_{i\in V} m(i) \sum_{i=1}^{n} r_i^2.$$

The interiors of the caps are non-overlapping since C_G is a kissing cap embedding. Moreover, it is well-known that the area of the cap C_i is πr_i^2. Therefore, it follows that

$$\sum_{i=1}^{n} \pi r_i^2 \le \{\text{combined area of caps}\} \le 4\pi,$$

since the area of all of S^2 is 4π. With this configuration of the $\mathbf{v}_i$, it follows by (3.7) in Lemma 3.5 that

$$\begin{aligned}
\sigma_1(\Lambda_{\mathcal{L}}) &\le \frac{\sum_{(i,j)\in E} w_{ij}\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} \\
&\le \frac{2\max_{i\in V} m(i) \sum_{i=1}^{n} r_i^2}{\sum_{i\in B} m(i)\|\mathbf{v}_i\|^2} \\
&= \frac{2\max_{i\in V} m(i) \sum_{i=1}^{n} r_i^2}{\sum_{i\in B} m(i)} \\
&\le \frac{8\max_{i\in V} m(i)}{\mathrm{Vol}_G(B)},
\end{aligned}$$

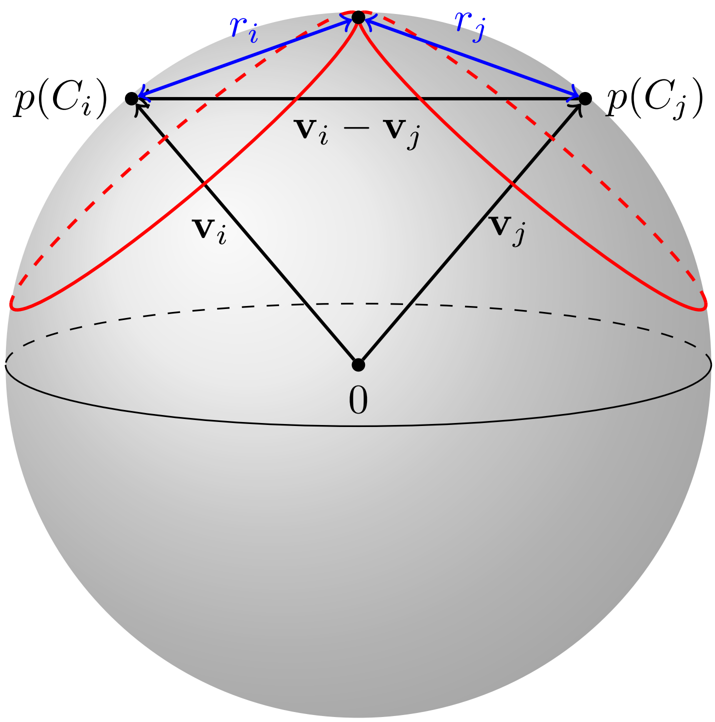


Figure 3.2: A geometric explanation of why $\|\mathbf{v}_i - \mathbf{v}_j\|^2 \leq (r_i + r_j)^2$.

as was sought.

The case for Λ_L: The proof strategy is exactly the same as for $\Lambda_{\mathcal{L}}$. Recall the variational characterization (3.6) of $\sigma_1(\Lambda_{\mathcal{L}})$:

$$\sigma_1(\Lambda_L) = \min_{\mathbf{v}_1,\dots,\mathbf{v}_n \in \mathbb{R}^l} \left\{ \frac{\sum_{(i,j)\in E} w_{ij} \|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} \|\mathbf{v}_i\|^2} \mid \sum_{i\in B} \mathbf{v}_i = \mathbf{0}, \{\mathbf{v}_i\}_{i\in B} \text{ not all } \mathbf{0} \right\}.$$

Here, the Rayleigh quotient is instead

$$R_{\Lambda_L}(\mathbf{v}_1, \dots, \mathbf{v}_n) = \frac{\sum_{(i,j)\in E} w_{ij} \|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} \|\mathbf{v}_i\|^2}.$$

By Theorem 3.7, there is a kissing cap embedding $C'_G = \{C'_i\}_{i\in V}$ of G such that $\sum_{i\in B} p(C'_i) = \mathbf{0}$. Similarly to how the case for $\Lambda_{\mathcal{L}}$ was carried out, we place $\mathbf{v}_i$ at $p(C'_i)$. Then the condition $\sum_{i\in B} \mathbf{v}_i = \mathbf{0}$ is satisfied, and it follows by (3.6) in Lemma 3.5 together with the same arguments as in the case for $\Lambda_{\mathcal{L}}$ that

$$\begin{aligned}
\sigma_1(\Lambda_L) &\leq \frac{\sum_{(i,j)\in E} w_{ij} \|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sum_{i\in B} \|\mathbf{v}_i\|^2} \\
&\leq \frac{2 \max_{i\in V} m(i) \sum_{i=1}^n r_i^2}{\sum_{i\in B} \|\mathbf{v}_i\|^2} \\
&= \frac{2 \max_{i\in V} m(i) \sum_{i=1}^n r_i^2}{b} \\
&\leq \frac{8 \max_{i\in V} m(i)}{b},
\end{aligned}$$

as we wanted. ∎

3.2. Proof of Theorem 3.7

The proof of Theorem 3.7 is quite technical. Most of the work is done already by Plümer in [Plü20] and we follow him very closely in what is to come. We introduce the following notation: Let β be a point on S^2, and let H_β denote the affine hyperplane in $\mathbb{R}^3$ tangential to S^2 at β, i.e.

$$H_\beta = \{y \in \mathbb{R}^3 \mid (y - \beta, \beta) = 0\}.$$

Here, we use $(\cdot, \cdot)$ to denote the usual inner product in $\mathbb{R}^3$. Let $\pi_\beta : H_\beta \to S^2 \setminus \{-\beta\}$ be stereographic projection of H_β onto S^2 w.r.t. β, i.e.

$$\pi_\beta(y) = \frac{4}{\|\beta + y\|^2}(\beta + y) - \beta.$$

The inverse of π_β is

$$\pi_\beta^{-1}(z) = \frac{1}{1 + (z, \beta)}(\beta + z) - \beta$$

where $z \in S^2 \setminus \{-\beta\}$. The standard extension $\pi_\beta(\infty) = -\beta$ extends stereographic projection to a homeomorphism $\pi_\beta : H_\beta \cup \infty \to S^2$. Crucially, stereographic projection (and its inverse) is *circle-preserving* in the following sense as recounted by Plümer:

1. If C defines a circle in H_β, then $\pi_\beta(C)$ is a circle in S^2.
2. If T is a circle in S^2 and $-\beta \notin T$, then $\pi_\beta^{-1}(T)$ is a circle in H_β.
3. If R is a circle in S^2 and $-\beta \in R$, then $\pi_\beta^{-1}(R) \setminus \infty$ is a straight line in H_β.
4. If U is a straight line in H_β, then $\pi_\beta(U) \cup \{-\beta\}$ is a circle in S^2.

A proof of this fact can be found in [DS32], §36. We will also need the notion of a dilation on H_β with centre β and dilation factor λ. We write this map as

$$D_\beta^\lambda : H_\beta \to H_\beta$$
$$D_\beta^\lambda(y) = \beta + \lambda(y - \beta).$$

Dilation also extends to a homeomorphism $D_\beta^\lambda \cup \{\infty\} \to D_\beta^\lambda \cup \{\infty\}$ if we put $D_\beta^\lambda(\infty) = \infty$. Clearly, dilation maps circles to circles and straight lines to straight lines. The procedure we will consider is to take a kissing cap embedding of G on S^2, inverse project it onto H_β for some β in S^2, dilate it on H_β by a factor $\lambda \neq 0$, and finally stereographically project the dilated embedding onto S^2 again. Mathematically, this procedure is executed by the map

$$g_\beta^\lambda := \pi_\beta \circ D_\beta^\lambda \circ \pi_\beta^{-1} : S^2 \to S^2.$$

(The actual map we will use for the inverse projection-dilation-projection procedure can be seen in (3.13), and is a modified version of g_β^λ in which we choose the parameters in a specific way.) By the properties of stereographic projection and dilation outlined above, the map g_β^λ is a homeomorphism that maps circles to circles in S^2. Moreover, it is not hard to see that the map that assigns parameters to g_β^λ, i.e.

$$(0, \infty) \times S^2 \times S^2 \to S^2;$$
$$(\lambda, \beta, z) \mapsto g_\beta^\lambda(z),$$

is continuous. Next, we extend the parameter-assigning map to another map

$$\begin{aligned}[0,\infty)\times S^2\times S^2 &\longrightarrow S^2;\\ (\lambda,\beta,z) &\mapsto g_\beta^\lambda(z)\end{aligned}$$

by designating the limit map $g_\beta^0 : S^2 \longrightarrow S^2$ as

$$g_\beta^0(z) = \begin{cases} -\beta, & z = -\beta \\ \beta, & \text{otherwise} \end{cases}$$

noting that this extension yields continuity of g_β^λ on the relatively open subset $([0,\infty)\times S^2\times S^2)\setminus(0,\beta,-\beta)$. From this one can immediately deduce the following lemma by the definition of continuity:

Lemma 3.9. *Let $K, L \subset S^2$ be compact and such that $z \neq -\beta$ for all points of the form (β, z) in $K\times L$. Let $\varepsilon > 0$. Then there exists some $\delta = \delta(\varepsilon)$ in the interval $(0,1)$ such that*

$$\|g_\beta^\lambda(z) - \beta\| < \varepsilon,$$

for all (λ,β,z) in $[0,\delta]\times K\times L$.

Noting that g_β^λ is circle-preserving, we see that if C is a cap in S^2, then so is $g_\beta^\lambda(C)$, so we can unambigously speak about the center $p(g_\beta^\lambda(C))$ of the cap $g_\beta^\lambda(C)$. By Lemma 3.9 applied to the set $C\times\{\beta\}$ it follows that $p(g_\beta^\lambda(C)) \longrightarrow \beta$ as $\lambda \longrightarrow 0$ for all $\beta \in S^2$ with $-\beta \notin C$. This motivates the extension

$$p(g_\beta^0(C)) := \begin{cases} \beta, & \text{if } \beta \text{ is not in } C, \\ -\beta, & \text{otherwise.} \end{cases}$$

This extension yields continuity of the map $[0,\infty)\times S^2 \longrightarrow S^2; (\lambda,\beta)\mapsto p(g_\beta^\lambda(C))$ on the set $([0,\infty\times S^2)\setminus(\{0\}\times -C)$. Now take a point α in the closed unit ball $\bar{B}^3$ in $\mathbb{R}^3$, and define

$$f_\alpha := \begin{cases} g_{\alpha/\|\alpha\|}^{1-\|\alpha\|}, & \text{if } \alpha \neq 0, \\ \text{The identity map } \mathsf{Id}_{S^2}, & \text{if } \alpha = 0. \end{cases} \tag{3.13}$$

By our previous digression on g_α^λ, it follows that the map $R_C : \alpha \mapsto p(f_\alpha(C))$ is continuous on $B^3 \setminus \{-C\}$. Moreover, if α lies on S^2 we have

$$p(f_\alpha(C)) = \begin{cases} \alpha, & \text{if } \alpha \text{ is not in } C \\ -\alpha, & \text{otherwise.} \end{cases} \tag{3.14}$$

The map f_α is the projection-dilation-projection homeomomorphism that we will use to configure the centers of the caps so that their center of mass is situated at the origin; more formally, we want to find some α in $\bar{B}^3$ such that the map $\Phi : \bar{B}^3 \longrightarrow \mathbb{R}^3$, where

$$\Phi(\alpha) := \sum_{i\in B} \mu(i)p(f_\alpha(C_i)), \tag{3.15}$$

evaluates to $\mathbf{0}$. We will not explicitly construct such a point α; rather, we will prove that must exist using the following easy corollary of Brouwer's fixed point theorem:

Lemma 3.10. *Let $\rho : \bar{B}^3 \to \mathbb{R}^3$ be a continuous map, and assume that for any $\alpha \in S^2$, the image $\rho(\alpha)$ lies on the ray initiated at the origin and passing through α. Then there exists some $\gamma \in \bar{B}^3$ such that $\rho(\gamma) = 0$.*

Proof. If there is no such γ, the map $-\frac{\rho}{\|\rho\|} : \bar{B}^3 \to \bar{B}^3$ is a well-defined, continuous map, but this map has no fixed points; every point in B^3 is mapped to a point on S^2, and the image $\rho(\alpha)$ of every point $\alpha \in S^2$ lies on the ray from the origin to α and is therefore mapped to $-\alpha \neq \alpha$ by the map $\rho/\|\rho\|$. This contradicts Brouwer's fixed point theorem, which states precisely that every continous map $\bar{B}^3 \to \bar{B}^3$ has a fixed point. ■

The final technical frontier which prevents us from simply applying Lemma 3.10 to (3.15) (which is easily seen to fulfill the ray condition by the univalence of the kissing cap embedding $\widetilde{C} = \{f_\alpha(C_i)\}_{i \in V}$ together with the condition (3.11)) is that our map Φ is in fact discontinous on $-C_i$ for each i in B. The way out of this predicament is a final technical lemma which will let us apply a 'smoothing' transitioning process to f_α, when α (which we recall is a point in $\bar{B}^3$) is close to one the caps C_i. This is Lemma 3.8 in [Plü20], and its rather short proof is omitted here since it is not especially illuminating.

Lemma 3.11. *Define the system*

$$V_C = \left\{ U \subset V : \bigcap_{i \in U} C_i \neq 0 \right\}.$$

(By univalence, V_C consists of one-element subsets of V and two-element subsets $\{i, j\} \subset V$ with $C_i \cap C_j \neq 0$). Let ε be in the interval $(0, 1)$. Let $B_\varepsilon(\gamma) \subset \mathbb{R}^3$ denote the open ball of radius ε with center γ. Let $V_\alpha^1(\varepsilon)$ denote the set $\{i \in V : f_\alpha(C_i) \subset B_\varepsilon(\alpha/\|\alpha\|)\}$, i.e. the set of vertices in V whose corresponding caps are contained in the open ball of radius ε around the point $\alpha/\|\alpha\|$. Let $V_\alpha^2(\varepsilon)$ denote the set $V \setminus V_\alpha^1(\varepsilon)$. Then there is some $\delta = \delta(\varepsilon)$ in $(0, 1)$ such that for any α in B^3 with $1 - \delta < \|\alpha\| < 1$ we have that $(V \setminus V_\alpha^1(\varepsilon))$ is contained in V_C.

Proof of Theorem 3.7. Let $C_G = \{C_i\}_{i \in V}$ be a kissing cap embedding of G. Suppose (3.11) is fulfilled by the measure $\mu : V \to \mathbb{R}$ defined on V. Let ε be in $(0, 1)$, and choose $\delta = \delta(\varepsilon)$ in $(0, 1)$ so that the result of Lemma 3.11 holds. Let α be a point in B^3. Define a maximum distance function

$$\mathrm{dist}(\alpha, C_i) := \max_{z \in C_i} \|\alpha - z\|,$$

Define a continuous function $h_i : B^3 \to [0, 1]$ by

$$h_i(\alpha) = \begin{cases} \frac{2 - \mathrm{dist}(\alpha, C_i)}{\delta}, & \text{if } \mathrm{dist}(\alpha, C_i) \geq 2 - \delta, \\ 1, & \text{otherwise.} \end{cases}$$

The triangle inequality implies that

$$\mathrm{dist}(\alpha, C_i) \leq 1 + \|\alpha\|, \tag{3.16}$$

for any nonzero α, and equality holds in (3.16) if and only if the point $-\alpha/\|\alpha\|$ is in C_i. Hence $h_i(\alpha)$ evaluates to 0 if and only if the point $-\alpha$ is in C_i, and it follows that h_i vanishes on the discontinous points of the map $R_{C_i} : \alpha \mapsto p(f_\alpha(C_i))$, which are precisely the points in $-C_i$ as we remarked earlier. Hence we can 'smoothen' the maps R_{C_i} by instead defining $R'_{C_i} : \alpha \mapsto h_i(\alpha)p(f_\alpha(C_i))$. The map R'_{C_i} then defines a continuous map on B^3 for any $i \in V$. Then the map

$$\Phi(\alpha) = \sum_{i \in B} \mu(i) h_i(\alpha) p(f_\alpha(C_i))$$

is a sum of continuous functions and hence also continuous. Moreover it follows by (3.14) that if α is a point on S^2, the map Φ evaluates to

$$\Phi(\alpha) = \sum_{i \in B, -\alpha \notin C_i} \mu(i) h_i(\alpha) \alpha$$

which is on the ray starting at 0 and intersecting α. By Lemma 3.10 we conclude that there is some α in B^3 such that

$$0 = \Phi(\alpha) = \sum_{i \in B} \mu(i) h_i(\alpha) p(f_\alpha(C_i)).$$

Now we just need to show that this α can be chosen to satisfy $\|\alpha\| \leq 1 - \delta(\varepsilon)$ for ε sufficiently small. This will yield

$$\operatorname{dist}(\alpha, C_i) \leq 1 + \|\alpha\| < 2 - \delta, \text{ for all } i\ B, \tag{3.17}$$

making all of the h_i belonging to vertices i in B evaluate to 1 and yielding

$$0 = \sum_{i \in B} \mu(i) p(f_\alpha(C_i)),$$

which is our desired result.

Suppose for the sake of contradiction that $1 - \delta < \|\alpha\| < 1$ holds. We recall some definitions from Lemma 3.11. We defined

$$V_C = \left\{ U \subset V : \bigcap_{i \in U} C_i \neq 0 \right\}$$

and remarked that each subset contained in V_C consists of at most two vertices in V. Moreover, we defined $V^1_\alpha(\varepsilon)$ as the set $\{i \in V : f_\alpha(C_i) \subset B_\varepsilon(\alpha/\|\alpha\|)\}$, i.e. the set of vertices in V whose corresponding caps are contained in the open ball of radius ε around the point $\alpha/\|\alpha\|$. Lemma 3.11 then implies that for our choice of α, the set $V^2_\alpha(\varepsilon) = (V \setminus V^1_\alpha(\varepsilon))$ is contained in V_C, and thus consists of at most two vertices in V.

By definition, we have that $\operatorname{dist}(\alpha, f_\alpha(C_i)) \leq \operatorname{dist}(\alpha, f_\alpha(C_j))$ if i is in $V^1_\alpha(\varepsilon)$ and j is in $V^2_\alpha(\varepsilon)$. This actually implies that $\operatorname{dist}(\alpha, C_i) \leq \operatorname{dist}(\alpha, C_j)$, since f_α is just a dilation on the hyperplane tangential to S^2 at $\alpha/\|\alpha\|$, and therefore $h_i(\alpha) \geq h_j(\alpha)$ if i is in $V^1_\alpha(\varepsilon)$ and j is in $V^2_\alpha(\varepsilon)$. We define D_α as $\min_{v \in V^1_\alpha(\varepsilon)} h_i(\alpha)$. Note that $D_\alpha > 0$, since none of the $h_i(\alpha)$ are 0 if $\|\alpha\| < 1$ by virtue of the inequality (3.16), and we assumed that $1 - \delta < \|\alpha\| < 1$. Then, if i is in $V^1_\alpha(\varepsilon)$ and j is in $V^2_\alpha(\varepsilon)$ we get

$$h_i(\alpha) \geq D_\alpha \geq h_j(\alpha).$$

By definition, we have for i in $V^1_\alpha(\varepsilon)$ that

$$\left\| \frac{\alpha}{\|\alpha\|} - p(f_\alpha(C_i)) \right\| \leq \varepsilon.$$

We write $V_\alpha^1(\varepsilon)$ as V_α^1 and $V_\alpha^2(\varepsilon)$ as V_α^2 in the calculations to come. At this point, it is convenient to also intruduce the following notation: For a subset W of V, we write $\mu(W) = \sum_{i\in W}\mu(i)$. We now have the results and notation needed for estimating the norm of $\Phi(\alpha)$. We do this by splitting the norm of $\Phi(\alpha)$ into two terms as

$$\begin{aligned}
\|\Phi(\alpha)\| &= \left\|\sum_{i\in B}\mu(i)h_i(\alpha)p(f_\alpha(C_i))\right\| \\
&= \left\|\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)p(f_\alpha(C_i)) + \sum_{i\in V_\alpha^2\cap B}\mu(i)h_i(\alpha)p(f_\alpha(C_i))\right\| \\
&\geq \left\|\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)p(f_\alpha(C_i))\right\| - \left\|\sum_{i\in V_\alpha^2\cap B}\mu(i)h_i(\alpha)p(f_\alpha(C_i))\right\|.
\end{aligned}$$

To start with, we have

$$\begin{aligned}
&\left\|\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)p(f_\alpha(C_i))\right\| \\
&\qquad= \left\|\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)\frac{\alpha}{\|\alpha\|} - \sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)\left(\frac{\alpha}{\|\alpha\|} - p(f_\alpha(C_i))\right)\right\| \\
&\qquad\geq \left\|\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)\frac{\alpha}{\|\alpha\|}\right\| - \left\|\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)\left(\frac{\alpha}{\|\alpha\|} - p(f_\alpha(C_i))\right)\right\| \\
&\qquad= \sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha) - \left\|\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha)\left(\frac{\alpha}{\|\alpha\|} - p(f_\alpha(C_i))\right)\right\| \\
&\qquad\geq (1-\varepsilon)\sum_{i\in V_\alpha^1\cap B}\mu(i)h_i(\alpha) \\
&\qquad\geq D_\alpha(1-\varepsilon)\sum_{i\in V_\alpha^1\cap B}\mu(i) \\
&\qquad= D_\alpha(1-\varepsilon)\mu(V_\alpha^1\cap B).
\end{aligned}$$

Simultaneously,

$$\left\|\sum_{i\in V_\alpha^2\cap B}\mu(i)h_i(\alpha)p(f_\alpha(C_v))\right\| \leq D_\alpha\sum_{i\in V_\alpha^2\cap B}\mu(i) = D_\alpha\mu(V_\alpha^2\cap B).$$

With these results, we can estimate the norm of $\Phi(\alpha)$ as

$$\begin{aligned}\|\Phi(\alpha)\| &= \left\| \sum_{i\in B} \mu(i) h_i(\alpha) p(f_\alpha(C_i)) \right\| \\ &= \left\| \sum_{i\in V_\alpha^1 \cap B} \mu(i) h_i(\alpha) p(f_\alpha(C_i)) + \sum_{i\in V_\alpha^2 \cap B} \mu(i) h_i(\alpha) p(f_\alpha(C_i)) \right\| \\ &\geq \left\| \sum_{i\in V_\alpha^1 \cap B} \mu(i) h_i(\alpha) p(f_\alpha(C_i)) \right\| - \left\| \sum_{i\in V_\alpha^2 \cap B} \mu(i) h_i(\alpha) p(f_\alpha(C_i)) \right\| \\ &\geq D_\alpha((1-\varepsilon)\mu(V_\alpha^1 \cap B) - \mu(V_\alpha^2 \cap B)) \\ &\geq D_\alpha(\mu(B) - 2\mu(V_\alpha^2 \cap B) - \varepsilon\mu(B)).\end{aligned} \tag{3.18}$$

We now choose ε, which we only assumed was contained in $(0, 1)$, to be

$$\varepsilon := \min_{U\in V_C} \frac{\mu(B) - 2\mu(U \cap B)}{2\mu(B)} > 0,$$

where we know that $\varepsilon > 0$ by the condition (3.11). Since V_α^2 is contained in V_C, it follows by combining the estimate (3.18) with our choice of ε that

$$\|\Phi(\alpha)\| \geq \frac{D_\alpha \varepsilon \mu(B)}{2} > 0,$$

but this contradicts that $\Phi(\alpha) = 0$. Therefore, $\|\alpha\| \leq 1 - \delta$, whence Theorem 3.7 follows from the remarks surrounding (3.17).

∎

Chapter 4

The DtN map and edge connectivity

A natural measure of the connectivity of a graph is its *edge connectivity*. The edge connectivity is most commonly defined on graphs where one thinks of all edges as having weight 1. We call such a graph $G = (V, E)$ a *combinatorial graph* in this chapter. For combinatorial graphs, the edge connectivity is defined as follows.

Definition 4.1. Let $G = (V, E)$ be a connected combinatorial graph. The *edge connectivity* η of G is the minimal number of edges required to be removed to disconnect the graph.

It seems reasonable to expect a relation between the edge connectivity of a graph G and the spectral gap of the various Laplacians that can be associated to a graph, considering the close links between Laplacian spectral gaps and other measures of connectivity such as the Cheeger constant. Indeed, in Theorem 2.3 in [Ber+17], stated as Theorem 4.2 below, the authors achieve precisely this. They provide a variational proof and generalization of a result originally due to Fiedler (cf. [Fie73]) :

Theorem 4.2. *Let $G = (V, E)$ be a finite, connected combinatorial graph with n vertices, edge connectivity η, and combinatorial Laplacian L. Then the spectral gap $\lambda_1(L)$ of L satisfies*

$$\eta + 1 \geq \lambda_1(L) \geq 2\eta \left[1 - \cos\left(\frac{\pi}{n}\right)\right]. \tag{4.1}$$

The proof of Theorem 4.2 uses the variational characterization (2.21) of $\lambda_1(L)$. We can use the variational characterization (2.23) of the spectral gap $\sigma_1(\Lambda_L)$ of the combinatorial DtN map Λ_L of G to adapt the technique employed to prove the lower bound in (4.1) to prove a similar lower bound for $\sigma_1(\Lambda_L)$. This lower bound is the result we will prove in Theorem 4.5.

As we have seen, in the context of DtN maps it is considerably more natural to study weighted graphs. Hence, we would like to consider some kind of weighted version of edge connectivity. We define it as the following quantity:

Definition 4.3 (Weighted edge connectivity)**.** Let $G = (V, E, w)$ be a finite, connected weighted graph. The *weighted edge connectivity* of G is the minimal amount of total edge weight that needs to be removed to disconnect the graph.

Remark 4.4. If the weights on the edges of G in Definition 4.3 are all equal to 1, the weighted edge connectivity of G coincides with its usual edge connectivity.

With these definitions and remarks in hand, we are ready to prove Theorem 4.5.

Theorem 4.5. *Let $G = (V, E, w)$, be a connected weighted graph with boundary B. Denote the number of vertices in G by n and the number of boundary vertices in G by b. Suppose $b > 1$, and suppose G has weighted edge connectivity v. Then the spectral gap $\sigma_1(\Lambda_L)$ of the combinatorial DtN map Λ_L of G w.r.t. B satisfies*

$$\sigma_1(\Lambda_L) \geq \frac{2v}{n-b+1}\left[1-\cos\left(\frac{\pi}{b}\right)\right]. \tag{4.2}$$

Example 4.6. The example of the path graph P_n with edge weights all equal to 1 and with the end vertices designated as boundary vertices is one case where the bound (4.2) is tight. Let σ_1 denote the spectral gap of the combinatorial DtN map of P_n. As remarked by Perrin in the end of the proof of Theorem 1 in [Per19], it is not hard to see that $\sigma_1 = 2/(n-1)$. Meanwhile, the weighted edge connectivity of P_n is 1 and the number of boundary vertices is 2, so the bound (4.2) yields $\sigma_1 \geq 2/(n-1)$. This matches Perrin's bound in Theorem 1 in [Per19], which is also optimal for the unit weighted path graph.

Example 4.7. For the star graph S_n on n vertices with unit edge weights and with the measure 1 vertices designated as boundary vertices as in Example 2.13, the bound (4.2) is asymptotically significantly worse than Perrin's bound in Theorem 1 in [Per19], as n approaches infinity. From Example 2.13, we can use the well-known result that the spectral gap of the combinatorial Laplacian of a complete graph on b vertices is $b-1$ to conclude that the spectral gap σ_1 of the combinatorial DtN map of the star graph as above is

$$\sigma_1(S_n) = \frac{n-2}{n-1} \sim 1, \text{ for large } n.$$

Meanwhile, Theorem 1 in [Per19] estimates

$$\sigma_1(S_n) \geq \frac{n-1}{2(n-2)^2} \sim \frac{1}{2n}, \text{ for large } n,$$

and (4.2) estimates

$$\sigma_1(S_n) \geq 1-\cos\left(\frac{\pi}{n-1}\right) \sim \frac{\pi^2}{2n^2}, \text{ for large } n.$$

Remark 4.8. If the boundary of G consists of all of V, the combinatorial DtN map on G is just the combinatorial Laplacian on G. Hence, if we in addition set all of the edge weights in G to 1, the bound (4.2) specializes to the previously known lower bound in Theorem 4.2.

Remark 4.9. The method we use in the proof of Theorem 4.5 can not be used to prove analogous results for the normalized DtN map - at least not directly. This is due to the fact that a large portion of the proof of Theorem 4.5 consists of changing the edge weights of G and the other graphs that appear in suitable ways, while still maintaining control over the Rayleigh quotient that appears in the variational characterization of $\sigma_1(\Lambda_L)$ in (2.23). This is possible since the edge weights of the graph in question only appear in the numerator of the Rayleigh quotient in (2.23). The situation is different in the corresponding variational characterization of the spectral gap of the *normalized* DtN map as found in (2.24). There, the edge weights of the graph in question appear in both the numerator and denominator of the Rayleigh quotient, as well as in the condition on which set of functions we minimize the Rayleigh quotient over. This makes it more difficult in the case of the normalized DtN map to retain control over the Rayleigh quotient while modifying the graph one is working with.

Proof of Theorem 4.5.

Step 1: *Bound the spectral gap of Λ_L from below via the Rayleigh quotient of a path graph.*

Recall the variational characterization of the spectral gap of the combinatorial DtN map Λ_L of G as in (2.23):

$$\sigma_1(\Lambda_L) = \min_{\substack{f \in \mathbb{R}^n \\ f|_B \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i\in B} f(i)^2} \mid \sum_{i\in B} f(i) = 0 \right\}.$$

As can be seen in the proof of Corollary 2.23 which in turn yields (2.23), the expression (2.23) is equivalent to

$$\sigma_1(\Lambda_L) = \min_{\substack{f \in \mathbb{R}^b \\ f \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(u_f(i) - u_f(j))^2}{\sum_{i\in B} f(i)^2} \mid \sum_{i\in B} f(i) = 0 \right\}, \tag{4.3}$$

where u_f is the harmonic extension of f to all of V as in Definition 2.9. We designate the Rayleigh quotient associated to (2.23) as

$$R_G(f) = \frac{\sum_{(i,j)\in E} w_{ij}\,(f(i) - f(j))^2}{\sum_{i\in B} f(i)}. \tag{4.4}$$

Let f^0 be a function in $\mathbb{R}^b$ such that $\sum_{i\in B} f^0(i) = 0$ and such that the harmonic extension u_{f^0} of f^0 minimizes (4.4), i.e.

$$R_G(u_{f^0}) = \sigma_1(\Lambda_L).$$

We put a labelling $\{v_i\}_{i=1}^n$ on the vertices in G by designating

$$u_{f^0}(v_1) \leq u_{f^0}(v_2) \leq \ldots \leq u_{f^0}(v_n). \tag{4.5}$$

With this labelling, we write the weight of the edge (v_i, v_j) as w_{v_i,v_j}. By Lemma 2.10, the harmonic function u_{f^0} takes its exremal values on the boundary B, so we can assume that v_1 and v_n are boundary vertices. The proof idea is now the same as in [Ber+17]; we want to replace edges between the vertices labelled as v_i and v_j repsectively with a sequence of edges between $(v_i, v_{i+1}), (v_{i+1}, v_{i+2}), \ldots, (v_{j-1}, v_j)$. If there is already an edge between two vertices in the sequence, we add the weight of the edge (v_i, v_j) to that edge. We illustrate an example of this procedure in Figure 4.1.

The weighted edge connectivity ν of G does not decrease when we perform the procedure in the previous paragraph on G, since whenever we remove an edge (v_i, v_j) with weight w_{v_i,v_j}, we add the weight w_{v_i,v_j} to the edges in the sequence

$$C = (v_i, v_{i+1}), (v_{i+1}, v_{i+2}), \ldots, (v_{j-1}, v_j).$$

Therefore, if the edge (v_i, v_j) was one of the edges in a set S of edges that disconnects G when removed, and whose total edge weight is ν, two cases arise:

1. If none of the edges in C were in S before we performed the procedure in the preceding paragraph, then at least one of them needs to replace (v_i, v_j) in S to disconnect G after the procedure, in which case the sum of the edge weights of the edges in S is at least ν.

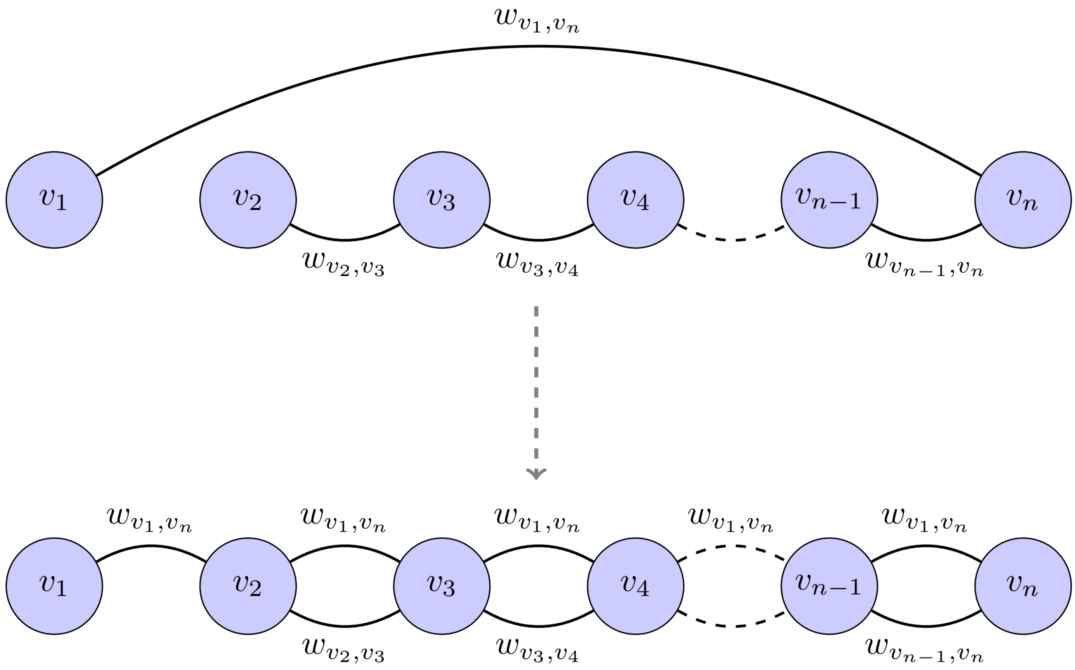


Figure 4.1: An example of the graph altering procedure employed in [Ber+17]; the edge (v_1, v_n) with edge weight w_{v_1,v_n} is replaced by a sequence of edges $(v_1, v_2), (v_2, v_3), \ldots, (v_{n-1}, v_n)$, all with edge weight w_{v_1,v_n}. This figure was inspired by Figure 1 in [Ber+17].

2. If one or more of the edges in C were in S before we performed the procedure, the edge w_{v_i,v_j} is added to the weight of that edge, so the sum of the edge weights of the edges in S after we perform the procedure is at least v.

We denote the graph that is formed by performing this procedure on all edges in G by $\widetilde{G}$, and designate the boundary of $\widetilde{G}$ to be the set of vertices corresponding to boundary vertices in G For this reason, we denote the boundary of $\widetilde{G}$ by B as well. With this choice of boundary, we have that $\sum_{i\in B} f^0(i) = 0$ in $\widetilde{G}$, and we can associate a Rayleigh quotient to $\widetilde{G}$ which we denote $R_{\widetilde{G}}$. We now proceed to show that $R_{\widetilde{G}}(u_{f^0}) \leq R_G(u_{f^0})$.

For easier reading in the paragraph to come, we define

$$w_{v_i,v_j}(u_{f^0}(v_i) - u_{f^0}(v_j))^2 := S(v_i, v_j), \qquad w_{v_i,v_j}\sum_{l=1}^{j-1}\Big(u_{f^0}(v_{l+1}) - u_{f^0}(v_l)\Big)^2 := T(v_i, v_j).$$

The numerator in $R_G(u_{f^0})$ consists of a sum of terms of the form $S(v_i, v_j)$, summing over each pair v_i, v_j such that (v_i, v_j) is an edge in E. The effect of the procedure outlined in the previous paragraph on the numerator in $R_G(u_{f^0})$ is that each term $S(v_i, v_j)$ in the numerator of $R_G(u_{f^0})$ is replaced by the corresponding term $T(v_i, v_j)$. Therefore, the numerator in $R_{\widetilde{G}}(u_{f^0})$ consists of a sum of terms of the form $T(v_i, v_j)$, summing over each pair v_i, v_j such that (v_i, v_j) is an edge in our original graph G. Hence, to show that $R_G(u_{f^0}) \leq R_{\widetilde{G}}(u_{f^0})$ amounts to showing that $T(v_i, v_j) \leq S(v_i, v_j)$ for each pair (v_i, v_j) that constitutes an edge in G. In more explicit terms, we want to prove that

$$\sum_{l=i}^{j-1} \left(u_{f^0}(v_{l+1}) - u_{f^0}(v_l)\right)^2 \le \left(u_{f^0}(v_j) - u_{f^0}(v_i)\right)^2, \tag{4.6}$$

whenever (v_i, v_j) is an edge in G. It is immediate by Jensen's inequality that $\|x\|_2 \le \|x\|_1$ if x is a finite-dimensional vector. Put

$$x := (u_{f^0}(v_{i+1}) - u_{f^0}(v_i), \ldots, u_{f^0}(v_j) - u_{f^0}(v_{j-1})) \in \mathbb{R}^{j-i}. \tag{4.7}$$

We then have

$$\begin{aligned}\left[\sum_{l=i}^{j-1} |u_{f^0}(v_{l+1}) - u_{f^0}(v_l)|^2\right]^{1/2} &\le \sum_{l=i}^{j-1} |u_{f^0}(v_{l+1}) - u_{f^0}(v_l)| \\ &= \sum_{l=i}^{j-1} (u_{f^0}(v_{l+1}) - u_{f^0}(v_l)) \\ &= u_{f^0}(v_j) - u_{f^0}(v_i),\end{aligned}$$

which is what we wanted. The next step is to note that the graph $\widetilde{G}$ formed by applying the procedure outlined above to G is in fact a *path graph* on n vertices (see Figure 4.2) whose end vertices are v_1 and v_n.

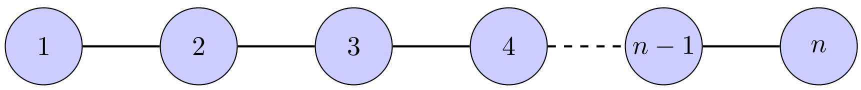


Figure 4.2: The path graph on n vertices.

Moreover, we can note that the weighted edge connectivity of a path graph is precisely the minimum among the edge weights in the graph. Since the weighted edge connectivity does not decrease when we form $\widetilde{G}$ from G, it follows that the minimum among the edge weights of $\widetilde{G}$ is at least ν. Now we can subtract weight from each of the edges in $\widetilde{G}$ so that all edge weights are equal to ν, which only decreases the Rayleigh quotient $R_{\widetilde{G}}(u_{f^0})$. After subtracting weight so that all edge weights are equal to ν, we are left with a path graph on n vertices whose edge weights are all equal to ν and whose boundary vertices are the vertices in the boundary of $\widetilde{G}$. We denote this graph by P. As we remarked, the Rayleigh quotient R_P associated to P fulfills $R_P(f^0) \le R_{\widetilde{G}}(f^0)$.

For clarity, we now introduce the notation $\sigma_1(G)$ to denote the spectral gap of the combinatorial DtN map of G, and analogous notation for the spectral gaps of the combinatorial DtN maps of other graphs that we consider. Collecting our partial results, we so far have the chain of inequalities

$$\sigma_1(P) \le R_P\left(f^0\right) \le R_{\widetilde{G}}\left(f^0\right) \le R_G\left(f^0\right) = \sigma_1(G). \tag{4.8}$$

Step 2: *Get rid of the boundary dependence in $\sigma_1(P)$.*

As we remarked earlier, we know that the end vertices of P are boundary vertices, but which other vertices are boundary vertices will depend on the original graph G as well as the choice of f^0. Therefore, to get a generally applicable result out of (4.8), we need to find a quantity which bounds $\sigma_1(P)$ from below regardless of which non-end vertices in P are boundary vertices.

Enumerate the vertices of P as in Figure 4.2. We identify the boundary of P with that of G and therefore write B for the boundary of P. The Rayleigh quotient of $P = (V_P, E_P)$ is then

$$R_P(g) = \frac{\sum_{(i,j)\in E_P} w_{ij}(g(i) - g(j))^2}{\sum_{i\in B} g(i)^2} = \frac{\nu \sum_{i=1}^{n-1}(g(i) - g(i+1))^2}{\sum_{i\in B} g(i)^2},$$

and by the variational characterization (2.23), $\sigma_1(P)$ is the minimum of $R_P(g)$ among functions g in $\mathbb{R}^n$ such that $\sum_{i\in B} g(i) = 0$. Let $g^0 \in \mathbb{R}^n$ be such a minimizer, so that $R_P(g^0) = \sigma_1(P)$. Denote the indices of the boundary vertices of P by k_j, for $j = 1, 2, \ldots, b$. Note that $k_1 = 1$ and $k_b = n$, since the end vertices of P are boundary vertices. Then the Rayleigh quotient $R_P(g^0)$ can be written as

$$R_P(g^0) = \frac{\nu \sum_{i=1}^{n} \left(g^0(i) - g^0(i+1)\right)^2}{\sum_{i\in B} g^0(i)^2} = \frac{\nu \sum_{j=1}^{b-1} \sum_{i=k_j}^{k_{j+1}-1} \left(g^0(i) - g^0(i+1)\right)^2}{\sum_{i\in B} g^0(i)^2}. \tag{4.9}$$

In the numerator of the right-hand side of (4.9), we have split the sum in the numerator of $R_P(g^0)$ into partial sums with indices from k_j to $k_{j+1} - 1$, where j ranges from 1 to b. We now study these partial sums. Define the vector $A(j)$ as

$$A(j) = \begin{bmatrix} g^0(k_j) - g^0(k_j+1) \\ g^0(k_j+1) - g^0(k_j+2) \\ \vdots \\ g^0(k_{j+1}-1) - g^0(k_{j+1}) \end{bmatrix},$$

and define $B(j)$ as $B(j) = \sum_{i=k_j}^{k_{j+1}-1} \left(g^0(i) - g^0(i+1)\right)^2$. Let $\mathbf{1}$ denote the all-ones vector of length $k_{j+1} - k_j$. Let $(\cdot,\cdot)$ denote the usual inner product in $\mathbb{R}^n$. Then

$$(A(j), \mathbf{1}) = g^0(k_j) - g^0(k_{j+1}).$$

By the Cauchy-Schwarz inequality,

$$(g^0(k_j) - g^0(k_{j+1}))^2 = |(A(j), \mathbf{1})|^2 \leq (A(j), A(j))(\mathbf{1}, \mathbf{1}) = B(j)(k_{j+1} - k_j). \tag{4.10}$$

Now we can use (4.10) to bound $R_P(g^0)$ from below:

$$\begin{aligned} R_P(g^0) &= \frac{\nu \sum_{j=1}^{b-1} \sum_{i=k_j}^{k_{j+1}-1} \left(g^0(i) - g^0(i+1)\right)^2}{\sum_{i\in B} g^0(i)^2} \\ &= \frac{\nu \sum_{j=1}^{b-1} B(j)}{\sum_{i\in B} g^0(i)^2} \\ &\geq \frac{\nu \sum_{j=1}^{b-1} \frac{1}{k_{j+1}-k_j} (g^0(k_j) - g^0(k_{j+1}))^2}{\sum_{i\in B} g^0(i)^2}. \end{aligned} \tag{4.11}$$

The last expression in (4.11) only enumerates over the boundary vertices of P. Now we recall the variational characterization (2.21) of the spectral gap of the combinatorial Laplacian L of a graph with l vertices (we write l instead of n as in (2.21) since n denotes the number of vertices of G here):

$$\lambda_1(L) = \min_{\substack{f \in \mathbb{R}^l \\ f \neq \mathbf{0}}} \left\{ \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i=1}^{l} f(i)^2} \mid \sum_{i=1}^{l} f(i) = 0 \right\}.$$

The Rayleigh quotient associated to (2.21) is

$$R'(f) = \frac{\sum_{(i,j)\in E} w_{ij}(f(i) - f(j))^2}{\sum_{i=1}^{l} f(i)^2}.$$

We recognize the last expression in (4.11) as the Rayleigh quotient associated to the combinatorial Laplacian of a path graph Q on b vertices, where the weight between the vertices i and $i+1$ is $\nu/(k_{i+1} - k_i)$. The largest possible value of the quantity $(k_{i+1} - k_i)$ for any i is $n - b + 1$, which is attained if the boundary vertices of P are arranged as in Figure 4.3. Hence, if we define U as the path graph on b vertices with edge weights

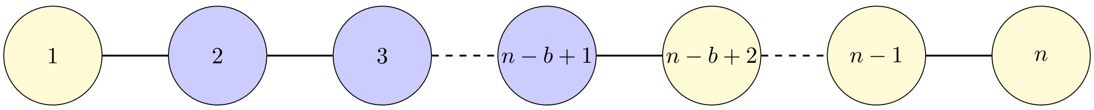


Figure 4.3: The configuration of the boundary of P which maximizes $(k_{i+1} - k_i)$. The $n - b$ interior vertices are blue and the b boundary vertices are yellow.

all equal to $\nu/(n - b + 1)$, we have that $R'_U(g^0 |_B) \leq R'_Q(g^0 |_B)$, and by (2.21) it follows that $\lambda_1(U) \leq R'_U(g^0 |_B)$. The spectral gap of the combinatorial Laplacian on the path graph on b vertices and unit weights on the edges is well-known to be $2\left[1 - \cos\left(\frac{\pi}{b}\right)\right]$, see e.g. Section 6.6 in [Spi19]. Therefore, since all of the edge weights in U are equal to $\nu/(n - b + 1)$, it follows that

$$\lambda_1(U) = \frac{2\nu}{n - b + 1}\left[1 - \cos\left(\frac{\pi}{b}\right)\right].$$

If we summarize our results, we have

$$\frac{2\nu}{n - b + 1}\left[1 - \cos\left(\frac{\pi}{b}\right)\right] = \lambda_1(U) \leq R'_U(g^0 |_B) \leq R'_Q(g^0 |_B) \leq R_P(g^0) = \sigma_1(P). \tag{4.12}$$

If we combine (4.12) and (4.8), we get

$$\sigma_1(G) \geq \frac{2\nu}{n - b + 1}\left[1 - \cos\left(\frac{\pi}{b}\right)\right],$$

as was sought.

■

Chapter 5

Possible future directions

5.1. Higher genus graphs

A natural further direction to consider, suggested by the bound (3.3), is to study more generally how the genus g of a graph, i.e. the minimal genus of a surface on which the graph can be embedded without any edges crossing, affects the spectral gaps of the combinatorial and normalized DtN maps. Similar results have already been achieved in the case of the spectral gap of the Laplacian, for instance by Kelner [Kel04] who generalized the method of Spielman and Teng [ST07] to graphs of genus g, and by Amini and Cohen-Steiner [AC18], who managed to link bounds on the spectral gap of the Laplacian of a graph to that of a carefully constructed Riemannian manifold, so that bounds in the Riemannian manifold case can be applied to the graph case as well. There is also previous work done by Colbois, Girouard and Raveendran [CGR18] which relates the Steklov problem on a Riemannian manifold and a graph, respectively. There seems to be considerable potential in applying (a suitable reformulation of) the methods of Kelner, Amini and Cohen-Steiner to the Steklov problem and to further study the links between the continuous and discrete Steklov problems.

5.2. Circular planar networks

Noting that the combinatorial DtN map is a Laplacian (see Section 2.6), a natural question investigated at length by Curtis, Ingerman and Morrow in [CIM98] is which Laplacians actually arise as the combinatorial DtN maps of graphs with special properties. More specifically, Curtis, Morrow and Ingerman, building on work by Colin de Verdière [Col94] and Colin de Verdière, Gitler, and Vertigan [CGV96] respectively, determine an if and only if condition for a combinatorial Laplacian to be the combinatorial DtN map of a *circular planar network* (CPN), i.e. a planar graph embedded on the disk with boundary vertices on the circle boundary. This property is called *circular minor positivity* and is not necessary to further describe here. The class of graphs with this property has been extensively studied, for instance by Kenyon [Ken11] and Kenyon and Wilson [KW17], and there have been attempts to explicitly reconstruct the CPN from its combinatorial DtN map. The formulas for this reconstruction in [Ken11] and [KW17] unfortunately evade the author's understanding. However, in the right hands they might lead to new bounds on the spectral gap of the Laplacian of graphs G fulfilling circular minor positivity in conjunction with the bound (3.3), if one is able to reconstruct the necessary properties of the CPN whose combinatorial DtN map is the Laplacian of G, since the spectral gap of the DtN map of the CPN is then the spectral gap of the Laplacian of G.

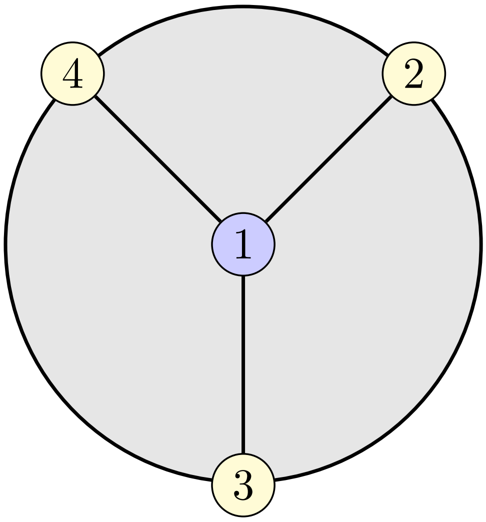


Figure 5.1: An example of a CPN on 4 vertices, with vertices 2, 3, and 4 designated as boundary vertices.

5.3. Semidefinite programming methods

The proof technique and general approach used in the proof of Theorem 3.1 as pioneered by Spielman and Teng [ST07] are seemingly inspired by techniques used in semidefinite programming relaxations in theoretical computer science, cf. for example the classical approximation algorithm for Max − Cut by Goemans and Williamson [GW95]. In general, using semidefinite programming-inspired approaches for constructing test functions for the variational expressions for the spectral gaps of the various Laplacians and DtN matrices associated to a graph seems to be both a powerful and underutilized tool, and in that regard a possibly interesting future area of study.

Appendix A

Proof of Theorem 2.16

In all of this section, we order the eigenvalues of an $n \times n$ matrix A as $\lambda_0(A) \leq \lambda_1(A) \leq \ldots \leq \lambda_{n-1}(A)$. The road to Theorem 2.16 is a bit long and starts with the following theorem, which is Theorem 2.1 in [Zha05].

Theorem A.1 (Schur complement interlacing formula)**.** *Let A be an $n \times n$ Hermitian matrix with entries in $\mathbb{C}$, partitioned as*

$$A = \begin{bmatrix} P & B \\ B^* & D \end{bmatrix}, \tag{A.1}$$

where P is an $r \times r$ principal, invertible, positive semidefinite submatrix. Let $S_A(P)$ denote the Schur complement of A w.r.t. P, and let $0 \oplus S_A(P)$ be the $n \times n$ matrix

$$0 \oplus S_A(P) = \begin{bmatrix} 0 & 0 \\ 0 & S_A(P) \end{bmatrix}.$$

Then

$$\lambda_i(A) \leq \lambda_{i+r}(0 \oplus S_A(P)) \leq \lambda_{i+r}(A), \quad i = 0, \ldots, (n-r) - 1.$$

We need a lemma to prove this theorem.

Lemma A.2. *Let H, A, B be $n \times n$ Hermitian matrices with entries in $\mathbb{C}$, and suppose $H = A + B$. Then*

$$\lambda_i(H) \leq \lambda_{i+k}(A) + \lambda_{n-k-1}(B),$$

for $k = 1, \ldots, (n-i) - 1$, and

$$\lambda_i(H) \geq \lambda_i(A) + \lambda_0(B).$$

Proof. Omitted. The reader is referred to a discussion of this and related results in [Ful98], cf. also Equation 2.0.9 in [Zha05]. ■

Proof of Theorem A.1. We can expand the block matrix formula (A.1) of A as

$$A = \begin{bmatrix} P & B \\ B^* & D \end{bmatrix} = \begin{bmatrix} P & B \\ B^* & B^* P^{-1} B \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & S_A(P) \end{bmatrix} := E + F.$$

Let I_r and I_{n-r} denote the $r \times r$ and $(n-r) \times (n-r)$ identity matrices, respectively. Then we define a matrix Q as

$$Q = \begin{bmatrix} I_r & 0 \\ -B^* P^{-1} & I_{n-r} \end{bmatrix}.$$

With these definitions of the matrices Q and E, the product QEQ^* turns out to be the $n \times n$ matrix whose $r \times r$ principal submatrix in the first r rows and columns consists of P, and with all other entries equal to 0. We denote this matrix by $P \oplus 0$. Since P is positive semidefinite by assumption, so is $P \oplus 0$ and hence also E, since E is similar to $P \oplus 0$ by virtue of the equation $QEQ^* = P \oplus 0$, where $Q^* = Q^{-1}$. Moreover we have

$$\mathsf{rank}(E) = \mathsf{rank}(P) = r < n.$$

Now we use Lemma A.2 to deduce that

$$\lambda_i(A) = \lambda_i(F + E) \leq \lambda_{i+r}(F) + \lambda_{n-r-1}(E) = \lambda_{i+r}(F),$$

where the last equality follows since $\mathsf{rank}(E) = r < n$. (Since we also know that E is singular and positive semidefinite, we get that necessarily $\lambda_{n-r-1}(E) = 0$.) Another application of Lemma A.2 yields

$$\lambda_i(A) = \lambda_i(F + E) \geq \lambda_i(F) + \lambda_0(E) = \lambda_i(F),$$

since by the same reasoning we must have that $\lambda_0(E) = 0$. Noting that $F = 0 \oplus S_A(P)$, we conclude that indeed

$$\lambda_i(A) \leq \lambda_{i+r}(0 \oplus S_A(P)) \leq \lambda_{i+r}(A), \quad i = 0, 1, \ldots, (n-r) - 1.$$

∎

A corollary which follows from Theorem A.1 will give us Theorem 2.16.

Corollary A.3. *Let A be an $n \times n$ Hermitian, positive semidefinite matrix with entries in $\mathbb{C}$, partitioned as*

$$A = \begin{bmatrix} P & B \\ B^* & D \end{bmatrix},$$

where P is an $r \times r$ principal, invertible, positive semidefinite submatrix. Let $S_A(P)$ denote the Schur complement of A w.r.t. P. Then

$$\lambda_i(A) \leq \lambda_i(S_A(P)) \leq \lambda_{i+r}(A), \quad i = 0, \ldots, (n-r) - 1.$$

We need one more lemma to prove this corollary.

Lemma A.4 (Haynsworth additivity formula)**.** *Let A be an $n \times n$ Hermitian matrix, partitioned as in (A.1), with P an $r \times r$ principal submatrix. Define the* inertia *of A as the ordered triple*

$$\mathsf{In}(A) := (p(A), q(A), z(A)) \tag{A.2}$$

where p, q, z is the number of positive, negative, and zero eigenvalues of A, respectively.

Then

$$\mathsf{In}(A) = \mathsf{In}(P) + \mathsf{In}(S_A(P)). \tag{A.3}$$

Proof. Omitted for brevity. For a proof, see Theorem 1.6 in [Zha05]. ∎

Proof of Corollary A.3. If A is positive semidefinite, so is P. By the Haynsworth additivity formula, it is then immediate that $S_A(P)$ is also positive semidefinite. Then it follows that $\lambda_{i+r}(0 \oplus S_A(P)) = \lambda_i(S_A(P))$ for $i = 0, 1, \ldots, n-r-1$, and hence Theorem A.1 implies that

$$\lambda_i(A) \leq \lambda_i(S_A(P)) \leq \lambda_{i+r}(A), \quad i = 0, \ldots, (n-r) - 1.$$

∎

Using Corollary A.3 we can finally associate the eigenvalues of the DtN matrix to its Laplacian matrix.

Theorem 2.16 (DtN Interlacing Theorem). *Let G be a graph with n vertices, combinatorial Laplacian L and boundary B with $|B| = b$. Let Λ_L be the combinatorial DtN matrix of G w.r.t B. Order the eigenvalues of L and Λ_L as $\lambda_0(L) \leq \lambda_1(L) \leq \ldots \leq \lambda_{n-1}(L)$ and $\sigma_0(\Lambda_L) \leq \sigma_1(\Lambda_L) \leq \ldots \leq \sigma_{b-1}(\Lambda_L)$, respectively. Then*

$$\lambda_i(L) \leq \sigma_i(\Lambda_L) \leq \lambda_{i+n-b}(L), \quad i = 0, 1, 2, \ldots, b-1. \tag{2.18}$$

Proof. Partition L in block form as

$$L = \begin{bmatrix} \widehat{L} & B \\ B^t & D \end{bmatrix} \tag{A.4}$$

where D corresponds to the boundary vertices and $\widehat{L}$ to the interior vertices. It is well-known that L is positive-semidefinite. By Theorem 2.17, $\widehat{L}$ as in (A.4) is invertible and by the Schur complement formula (2.13), Λ_L is the Schur complement of L w.r.t $\widehat{L}$. By Corollary A.3 it follows immediately that

$$\lambda_i(L) \leq \sigma_i(\Lambda_L) \leq \lambda_{i+n-b}(L), \quad i = 0, 1, \ldots, b-1. \tag{A.5}$$

■

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