Optimizing Extremal Eigenvalues of Weighted Graph Laplacians and Associated Graph Realizations

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Chapter 1

Introduction

Spectral graph theory is a classical field in discrete mathematics that investigates connections between structural properties of graphs and spectral properties of associated matrix representations. A central new tool that allows a fresh look on such connections is semidefinite optimization (SDO). Extremal eigenvalues, i.e., the smallest and largest one, the sum of $k$ largest eigenvalues of symmetric matrices and so on can be considered as functions from the set of symmetric matrices to real numbers. The values of a lot of those functions are optimal values of semidefinite programs. So the theory of SDO can be applied. This involves an associated dual program which offers an interesting interpretation of the underlying eigenvalue problem as a graph realization problem.

In this thesis, we will consider finite simple graphs $G = (N, E)$ with node set $N = \{1, \ldots, n\}$ and nonempty edge set $E \subseteq \{(i, j) : i, j \in N, i \neq j\}$. The edges will be weighted by nonnegative real numbers $w_{ij} \geq 0$ ($ij \in E$).

A graph may be represented via the adjacency matrix. Its spectrum, the corresponding eigenspaces and relations to the underlying graph were investigated extensively, see [3, 13, 56] and the references therein.

We are interested in the spectrum and associated eigenspaces of the Laplacian matrix $L_w$ of an edge weighted graph. It is a symmetric matrix of order $n$ and is defined by

$$[L_w]_{ii} = \sum_{k \in E} w_{ik} \text{ for } i \in N, \quad [L_w]_{ij} = -w_{ij} \text{ for } ij \in E \quad \text{and} \quad [L_w]_{ij} = 0 \text{ otherwise.}$$

The weighted Laplacian is positive semidefinite, which can be seen by the associated quadratic form

$$x^\top L_w x = \sum_{ij \in E} w_{ij} (x_i - x_j)^2.$$  

(1.1)
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and its smallest eigenvalue equals zero with corresponding eigenvector $1$, the vector of all ones. It is often referred to as the trivial eigenvalue and eigenvector.

In this thesis, we will consider nontrivial extremal eigenvalues of the weighted Laplacian: the second smallest and the largest one together with their corresponding eigenspaces. By applying SDO to get associated graph realization problems, we will prove connections of optimal solutions to the eigenspace of the weighted Laplacian and to structural properties of the graph, in particular to its separator structure.

Before we explain the content of the following chapters in more detail we want to emphasize the relevance of the Laplacian and its spectrum by mentioning several applications and corresponding references. The approach of SDO and resulting graph realization problems were already applied in different contexts. So we give some examples and references of related problems. Finally, we summarize the main ideas and results of the remaining chapters of this thesis in connection with related research.

1.1 Applications of the Laplacian

The weighted Laplacian is a generalization of the usual (combinatorial) Laplacian. Choosing each edge weight equal to one, the so weighted Laplacian is just the Laplacian of an unweighted graph. In different contexts the Laplacian is known under different names.

As it plays an important role in the Matrix-Tree-Theorem of Kirchhoff, it is also called Kirchhoff matrix \cite{13, 70, 71}.

In the theory of electrical networks the Laplacian is often called matrix of admittance because any graph may be considered as an electrical network with each edge having unit admittance or conductivity \cite{15, 36}.

Zimm used the Laplacian for his research on polymer dynamics \cite{100}, so Zimm matrix is another synonym \cite{41, 68, 101}.

Indeed, on the excellent spectral graph theory homepage \cite{18}, chemical applications are even said to be one of the origins of spectral graph theory. There are a lot of topological indices, \textit{e. g.}, the Wiener index, quantifying the structure and the branching pattern of a molecule, which are based on the Laplacian spectrum, see, \textit{e. g.}, \cite{45, 54, 71} and the references therein. Note that the Wiener index is closely related to the so called Kirchhoff index of a connected electrical network \cite{96}. Also aspects of energy of a molecule or more general of graphs take the Laplacian spectrum into account \cite{46, 60, 78}.

The importance of the (weighted) Laplacian arises as, \textit{e. g.}, the eigenvectors are closely related to the graph’s structure. They give useful hints for partitioning a graph, \textit{i. e.}, partitioning the node set into disjoint subsets, such that some constraints hold. Examples
are graph bisection, spectral clustering, the maximum cut problem and isoperimetric numbers. Also ordering problems, stable sets and coloring as well as routing problems take the Laplacian spectrum into account. Because there are a lot of excellent surveys on the Laplacian spectrum and its applications [3, 17, 69, 70, 72], we refrain from explaining them in detail.

Further applications of the Laplacian in computer science are given in [14, 31].

While there are a lot of papers, surveys and books on the Laplacian spectrum, [7] pays special attention to the Laplacian eigenvectors and their geometric properties. The theory of discrete nodal domains on graphs, i.e., connected subgraphs on which an eigenvector does not change sign, is described. Note that discrete nodal domains are the counterpart of solutions of Schrödinger equations on manifolds.

1.2 Eigenvalue Problems and Semidefinite Programming

The successful and rapid development of semidefinite programming (SDP) also brought significant progress in the solution of extremal eigenvalue optimization problems. With the use of matrix inequalities (see, e.g., [5]) one gets natural semidefinite formulations of eigenvalue functions of symmetric matrices, in particular of the smallest and the maximum eigenvalue. Results are published, e.g., in [61, 76, 77]. Optimizing such eigenvalue functions, such as maximizing the smallest eigenvalue under some constraints, leads to semidefinite programs.

What connections exist between semidefinite matrices or SDP and graph realization problems?

Symmetric positive semidefinite matrices may be characterized by Gram matrices (see Section 2.1). That means for a symmetric positive semidefinite matrix \( A \in \mathbb{R}^{n \times n} \) there exists a matrix \( U \in \mathbb{R}^{d \times n} \) with appropriate \( d \), such that \( A = U^T U \). Considering each column of \( U \) as a vector in \( \mathbb{R}^d \), \( U = [u_1, \ldots, u_n] \), a matrix entry \( [A]_{ij} \) is just the scalar product of the vectors \( u_i \) and \( u_j \).

As mentioned, the Laplacian is a positive semidefinite matrix. Column and row \( i \) are assigned to node \( i \) of the underlying graph. We also may assign vector \( i \) of a corresponding Gram representation of the Laplacian to node \( i \), by the above considerations, resulting in a realization of the graph in \( \mathbb{R}^d \). In 2005, Fiedler considered this geometric interpretation of the Laplacian and the graph and related it to quadrics [29].

A slightly different approach which has been applied in this thesis, is used to reformulate semidefinite programs as graph realization problems. Semidefinite matrices are the variables of a semidefinite program (see Section 2.2, equation (2.9)) - in this thesis, it will
be the dual program of the eigenvalue optimization problem. We assign the vectors of a
Gram representation of these variables to the graph’s nodes. Then a reformulation of the
program in terms of vectors (of a Gram representation) may be interpreted as a graph
realization problem.

In general, a graph realization problem is just the following: Given a graph we are interested
in positions of the graph’s nodes in $\mathbb{R}^d$, for some $d \in \mathbb{N}$, such that some constraints hold.

One such realization problem is the so called molecule problem [4, 51, 67]: Is there a
realization of a given graph in $\mathbb{R}^d$ having given edge length? Is this realization unique
(up to congruence)? The problem to decide whether there exists a realization of a graph
with given edge length in a real space of any dimension is called Euclidean distance matrix
completion problem (EDM) [4]. These questions and problems are also closely related to
finding a smallest dimension for which a graph is realizable.

An overview of geometric realizations of graphs is provided in [66], containing, beside oth-
ers, unit distance graphs, orthogonal representations, metric embeddings and connections
to graph parameters, like the Colin de Verdière number.

Having a solution to a graph realization problem it may not be unique. But we may favor
some solutions or a special one because of other criteria not considered yet. In this sense,
evaluating the possible realizations and finding a best possible graph realization gives rise
to an optimization problem.

A celebrated problem, in which the mentioned connections are established and exploited,
is the Lovász $\vartheta$-number of a graph. In 1979 Lovász introduced the $\vartheta$-number [65] as an
optimal value of orthogonal graph realizations, i. e., graph realizations in which nonadjacent
nodes have orthogonal positions. In the same paper, he also proved other characterizations
of $\vartheta$, for instance that it equals the minimal maximum eigenvalue of a matrix in a set of
symmetric matrices. A third characterization is given via SDP. Further characterizations
of $\vartheta$ and connections to graph invariants can be found in [33, 59] and the references therein.

Another example is the $\sigma$-function of a graph [11, 33] which is closely related to $\vartheta$. It
is defined in terms of the normalized weighted Laplacian of a graph and may also be
characterized in many different ways. Galtman [33] contrasted those of $\vartheta$ with those of $\sigma$
and pointed out, that the feasible sets of the optimization problems differ only slightly.

The advantage of different characterizations is obvious: each provides the opportunity to
interpret a given problem in different ways. Thus, the problem may suddenly appear in
another, sometimes unexpected, context, not considered yet. Also different problems and
topics may suddenly link up.

In this thesis, we will consider special eigenvalue optimization problems on graphs by
following the described approach. Thus, different characterizations will be developed and
optimal solutions will be analyzed in view of the graph’s structure.
1.3 Outline

Chapter 2: Preliminary Notions and Results

This chapter serves as a short introduction and repetition of basic notions and results of linear algebra (Section 2.1), semidefinite optimization (Section 2.2) and graph theory (Section 2.3), used in this thesis.

Chapter 3: The Second Smallest Eigenvalue of the Laplacian

The smallest eigenvalue of the weighted Laplacian is known to be zero with corresponding eigenvector of all ones. So the first or rather the smallest interesting eigenvalue of the weighted Laplacian is the second smallest one, which will be the focus of this chapter.

A lot of researchers followed this topic from different viewpoints. There are bounds on the second smallest eigenvalue of the unweighted Laplacian [1, 6, 87], also upper bounds on a family of graphs [34] using semidefinite formulations. The effect of node deletion on the second smallest eigenvalue was investigated in [57]. Wang et al. considered a maximization problem [92]: within a family of graphs they wanted to identify a graph with maximal second smallest eigenvalue of the unweighted Laplacian.

Besides these more recent references we want to emphasize Fiedler’s research on the second smallest Laplacian eigenvalue, as it is a starting point of our considerations on this topic. In 1973, Fiedler called the second smallest Laplacian eigenvalue the algebraic connectivity of a graph [23, 25] because he verified upper bounds depending on the degree of the graph’s nodes and connections to the vertex and edge connectivity. In this sense one may view the second smallest eigenvalue of the Laplacian as a measure of connectivity of the graph. Several connections were established between the spectrum of the Laplacian and structural properties of the graph.

In further research, he considered the algebraic connectivity and related eigenvectors of edge weighted graphs, i.e., the second smallest eigenvalue of the weighted Laplacian, in relation to edge cuts and cut vertices [24, 25]. The analysis of trees was very fruitful, which was continued by several other researchers [41, 55, 73, 101].

Fiedler also introduced a maximization problem which, however, differs from Wang’s one. For a given graph $G = (N, E)$ Fiedler considered all nonnegative edge weightings with average value on each edge equal to one. He was interested in weightings maximizing the algebraic connectivity. Another interpretation of this problem is the following: The Laplacian of an unweighted graph is the same as the Laplacian of a weighted graph, having unit weight on each edge. Thus, the total edge weight of a graph, i.e., the sum of all edge weights, is just the number of edges. Fiedler’s problem is the same as redistributing the
edge weights so that the total edge weight is again the number of edges and the second smallest Laplacian eigenvalue becomes maximal, i.e.,

\[
\hat{a}(G) := \max \left\{ \lambda_2(L_w) : \sum_{ij \in E} w_{ij} = |E|, \, w_{ij} \geq 0 \ (ij \in E) \right\}.
\]

Fiedler called the corresponding (optimal) second smallest eigenvalue \( \hat{a}(G) \) the \textit{absolute algebraic connectivity of a graph} \cite{7}. Considerations for trees are published in \cite{7, 9}. For surveys on the second smallest eigenvalue of the Laplacian of a graph with numerous references we recommend \cite{6, 30}.

In honor of Fiedler’s research the eigenvectors corresponding to the second smallest eigenvalue are often called \textit{Fiedler vectors}.

Based on the absolute algebraic connectivity, G"orling et al. \cite{2, 3} considered the problem from a semidefinite point of view. In the first three sections of this chapter, we will summarize their results. In view of the following chapters we need a slightly different representation of the problem than G"orling et al. used in their research, so we will adapt their representation and their results. Nevertheless, most ideas can be found in \cite{2, 3}. We will specifically point out new aspects and results.

The approach of G"orling et al. is to reformulate \( \hat{a}(G) \) by an appropriate matrix inequality, to get an SDP with corresponding dual program. The latter one can be interpreted as graph realization problem: One searches for a graph realization \( u_i \in \mathbb{R}^{|N|} \ (i \in N) \) and a real number \( \xi \in \mathbb{R} \) such that the barycenter is in the origin \[ \sum_{i \in N} u_i = 0, \]

the sum of the squared distances of the nodes to the origin equals one \[ \sum_{i \in N} \|u_i\|^2 = 1, \]

and the edges are as short as possible, i.e., \[ \|u_i - u_j\|^2 \leq \xi \ (ij \in E) \] for minimal \( \xi \).

Indeed, they considered a more general problem. The bound on the length of edges \( \xi \) is the same for all the edges in the above formulation. To get different bounds for different edges they introduced nonnegative edge parameters \( l_{ij} \ (ij \in E) \) and used them to scale the bound for each edge, i.e., \[ \|u_i - u_j\|^2 \leq l_{ij}^2 \xi \ (ij \in E). \] Furthermore, they weighted the graph’s nodes by given positive node parameters. These node and edge parameters also occur in the primal and dual formulations, but nevertheless, they do not change the character of the original problem as an optimization problem of the second smallest eigenvalue of a scaled weighted Laplacian.
Strong duality is a useful tool in SDO. While Göring et al. established strong duality only for the case of positive edge parameters (see [40]), we discuss strong duality and attainment of optimal solutions for nonnegative edge parameters in more detail, resulting in Proposition 3.4.

In the following, optimal solutions of the primal, the dual and the realization problem are analyzed respectively. So, Proposition 3.7 states a direct connection of optimal graph realizations and the eigenspace of the second smallest eigenvalue of an optimal weighted Laplacian. It turns out that projections of an optimal realization onto a one-dimensional subspace, spanned by an arbitrary vector, yield eigenvectors to this eigenvalue.

The original formulation of Göring et al., which is a scaled version of the above one and which is presented in Section 3.2, requires connected graphs as input data. Our formulation may also be applied to nonconnected graphs. In Proposition 3.8, we characterize optimal realizations and prove the existence of one-dimensional optimal realizations of this class of graphs.

Connections to the separator structure of the graph are detected by Theorem 3.10 which is also called Separator-Shadow Theorem. Considering the origin as a light source and the convex hull of a separator of a given realization as a wall or barrier there is shadow behind the wall. The theorem states, that all but one separated components of an optimal realization lie in the shadow of the separator. Interpreting nodes as articulations and edges as bars one can fold the graph, if its structure allows. In this sense, an unfolding property of optimal realizations is given by the theorem. Indeed, by scaling and a reformulation, the graph realization problem turns out to be a maximum variance unfolding problem.

The interpretation of the above graph realization problem as maximum variance unfolding problem was also established by Sun et al. [89]. Furthermore, they observed that the primal problem is closely related to fastest mixing Markov chains, interpreting the edge weights as transition rates between associated nodes.

We have already mentioned in Section 1.2 that low dimensional graph realizations are of interest. Therefore, Göring et al. introduced the rotational dimension of a graph, which turned out to be a minor monotone graph parameter. The rotational dimension is the maximal minimum dimension of an optimal graph realization for all possible node and edge parameters. Note that there are some similarities to the Colin de Verdière number, see [40] for a discussion and further references. Depending on the tree-width of the graph, a bound on the minimal dimension of optimal realizations and thus, the rotational dimension of the graph is given in Theorem 3.14.

While Fiedler already took the symmetry of the graph into account regarding optimal edge weights, it was of no interest for Göring et al. We generalize Fiedler’s result by Proposition 3.17 and apply it to edge transitive graphs (Corollary 3.18).

Section 3.4, which is independent of Göring’s et al. research, concludes the chapter with another new pair of primal and dual semidefinite programs whose optimal solutions are
closely related to the eigenspace of the second smallest eigenvalue of the unweighted Laplacian. The programs arise by choosing special node parameters, i.e., they all equal one, and by replacing the edge parameters by additional variables. So we optimize over the edge weights as well as the bounds on the edge length. In this case projections of an optimal corresponding realization onto a one-dimensional subspace spanned by an arbitrary vector yield eigenvectors to the second smallest eigenvalue of the unweighted Laplacian, i.e., Fiedler vectors. Let us mention that this section is mainly based on the article [50] which is joint work with Christoph Helmberg.

Chapter 4: Minimizing the Maximum Eigenvalue

The previous chapters implied that there are close connections between the (absolute) algebraic connectivity, i.e., the second smallest eigenvalue of the Laplacian, and properties of the graph. Now, it seems quite natural to consider the largest Laplacian eigenvalue, which is also called Laplacian spectral radius. As it is also semidefinite representable using a matrix inequality we may apply the same approach as in the previous chapter.

It seems hopeful to get results which relate this extremal eigenvalue to structural properties of the graph because there are, e.g., a lot of bounds on the maximum Laplacian eigenvalue, depending on several graph invariants, like the number of nodes and number of edges [75], the node degrees [82, 93, 99], the diameter [62], the dominating number [74, 87] and the covering number [86].

Before we are going to summarize the main results of this chapter let us mention some further research on the maximum Laplacian eigenvalue. The effects of little changes of the graph, e.g., adding or subdividing an edge, on the maximum Laplacian eigenvalue are discussed in [43, 44].

An interesting generalization of edge weighted graphs was considered by Das et al. They used positive definite matrices as edge weights. The maximum eigenvalue of a corresponding weighted Laplacian was analyzed in [16].

There are also optimization problems which are related to the Laplacian spectral radius. In [90, 63], the authors identify weighted trees with maximum Laplacian spectral radius within a family of weighted trees, so they consider a maximization problem.

In analogy to his research on the second smallest eigenvalue, Fiedler [27] considered the problem of minimizing the maximum eigenvalue of the weighted Laplacian for nonnegative edge weightings with average value on each edge equal to one. In particular, trees and bipartite graphs are investigated and connections between the latter graph class and doubly stochastic matrices are shown.

The fourth chapter of this thesis contains the author’s results on the maximum Laplacian eigenvalue of a graph. Sections 4.1 to 4.5 is joint work with Frank Göring and Christoph
1.3. OUTLINE

Helmberg and is based on [38]. Section 4.6 is joint work with Christoph Helmberg and is mostly taken from [50].

In some sense the problem of this chapter and the corresponding results are similar to those of the previous chapter but, there is also a dual aspect. The second smallest Laplacian eigenvalue is the smallest nontrivial one and the maximum eigenvalue lies on the opposite end of the Laplacian spectrum. It is for this reason that we call them extremal eigenvalues, even though the zero eigenvalue is the smallest one. Also optimal solutions and some of their interpretations have such a dual character.

In the first section we reformulate a generalization of Fiedler’s optimization problem of minimizing the maximum eigenvalue as a semidefinite program, additionally taking positive node and nonnegative edge parameters into account.

Following the semidefinite approach we get a corresponding Lagrange dual program and an associated graph realization formulation, for which strong duality and attainment of optimal solutions hold (Proposition 4.1). Of course, the realization problem is different from the one in the previous chapter: for a graph \( G = (N, E) \) with node parameters \( s_i > 0 \) (\( i \in N \)) and edge parameters \( l_{ij} \geq 0 \) (\( ij \in E \)) we want to find node positions \( v_i \in \mathbb{R}^{|N|} \) (\( i \in N \)), such that the sum of weighted squared distances of the nodes to the origin equals one

\[
\sum_{i \in N} s_i \|v_i\|^2 = 1,
\]

the edge lengths now are bounded from below by \( l_{ij}^2 \xi \) and \( \xi \) should be as large as possible. Furthermore, we do not require explicitly that the barycenter is in the origin. It turns out, that the origin is the barycenter of optimal realizations anyways (Proposition 4.4).

There is a slight relation to tensegrity theory (see [84]) by the Karush-Kuhn-Tucker conditions. That means, interpreting optimal weights as forces along the edges of the graph, an optimal realization will be in equilibrium, i.e., in each node the forces will cancel out.

Furthermore, maps of optimal realizations onto one-dimensional subspaces turn out to be eigenvectors to the optimal maximum eigenvalue (Proposition 4.2). So in some sense, we have a map of (a part of) the eigenspace, corresponding to the minimal maximum eigenvalue.

In Section 4.2, we analyze optimal realizations and prove some basic structural results. While the edge lengths are bounded from below, that means not all nodes may lie in the origin, they also cannot be arbitrarily far away. More precisely, optimal realizations lie within a closed ball of appropriate dimension (Proposition 4.5). Considering the graph itself, that means choosing the edge parameters to be equal, isolated nodes are the only ones that are embedded in the origin (Theorem 4.7). However, by choosing appropriate edge parameters we may force some nodes to the origin.
One of our main results of this chapter, Theorem 4.8, ensures the existence of a one-dimensional realization for bipartite graphs. In contrast, for a special choice of edge parameters a complete graph is embedded in a regular \((n-1)\)-dimensional simplex, Example 4.9. Subdividing all edges of a complete graph gives rise to a bipartite graph. Thus, a complete graph is a minor of a special bipartite graph. Hence, the importance of the theorem arises from two facts: on the one hand, it proves that a graph parameter in the same vein of the rotational dimension will not be minor monotone and on the other hand, it ensures that there exists a realization of minimal possible dimension for bipartite graphs.

We also identify special optimal primal solutions, that means special optimal edge weights, considering the symmetry of the underlying graph. In particular, the result is applied to edge transitive graphs.

A second important result, called the Sunny-Side Theorem (Theorem 4.13) provides a connection of optimal realizations to the separator structure of the graph. Unfortunately, it is a weaker result than the Separator-Shadow Theorem of the previous chapter. Nevertheless, let once again the origin be a light source, \(e.g\.), the sun and, in this case, the affine hull of a separator of a given realization be a wall. Then there is light in front of the wall and shadow behind it. The theorem states that the barycenters of all the separated components of the graph lie on the sunny side of the wall or separator. Hence, the theorem implies a folding property of optimal realizations, folding occurs along separators. We note that the interpretations of the theorems corresponding to the second smallest eigenvalue and to the maximum eigenvalue, respectively, have again a dual character.

A bound on the minimal dimension of an optimal realization, depending on the tree-width of a graph (Theorem 4.15) is a third significant result. The bounds of Chapter 3 and of this chapter are almost the same. But as the proofs use in one case the unfolding and in the other case the folding property, the similarity is not obvious. Furthermore, we identify a family of graphs for which the bound is tight, \(i.e\.), best possible.

The chapter finishes with two more related semidefinite problems. The first one is a scaled version of minimizing the maximum eigenvalue. One may also observe its dual character as in this case, the variance of the vectors corresponding to a graph realization is minimized. The second problem arises from the scaled one, by additionally optimizing over the edge parameters. Then, optimal realizations may also be seen as maps of eigenvectors to the maximum eigenvalue of the unweighted Laplacian.

**Chapter 5: Minimizing the Difference of Maximum and Second Smallest Eigenvalue**

So far, we have considered relations of the nontrivial extremal eigenvalues of the weighted Laplacian of a graph to corresponding graph realizations as well as to structural properties...
of the graph separately. In Chapter 5, we are interested how these eigenvalues interact. Therefore, we will optimize both eigenvalues at the same time, by minimizing the difference of the maximum and second smallest eigenvalue.

Indeed, sums of Laplacian eigenvalues are also considered in several papers. For example, [32, 47] bound the sum of the $k$ largest Laplacian eigenvalues, [64, 97, 98] investigate the sum of powers of Laplacian eigenvalues and [9, 35] discuss minimizing the effective resistance of an electrical network which is proportional to the sum of the inverses of the positive Laplacian eigenvalues.

The difference of maximum and second smallest eigenvalue of the Laplacian of a graph was investigated in [85]. The authors’ goal was to redistribute edge and node weights such that the nontrivial spectrum of the Laplacian lie within an interval of minimal size. In fact, the authors fixed one of the extremal eigenvalues and then minimized the interval’s size. So in some sense, they optimized the extremal eigenvalues separately.

However, we want to optimize both eigenvalues at the same time, without fixing one of them. The goal is that all the nontrivial eigenvalues are close together. Another motivation is given by the uniform sparsest cut problem that we will point out next.

The uniform sparsest cut problem is a node bipartitioning graph problem, see, e. g., [52]. Let $G = (N, E)$ be a connected graph with given edge weights $w_{ij} \geq 0 \ (ij \in E)$. A bipartition of the node set $N$ is $N = S \cup (N \setminus S)$ for a nonempty, proper subset $S$ of $N$. Let $\bar{S}$ denote $N \setminus S$.

The set of edges leaving $S$ is called an edge cut $E(S, \bar{S}) := \{ij \in E : i \in S, j \in \bar{S}\}$ and its weight is defined by $w(S, \bar{S}) := \sum_{ij \in E(S, \bar{S})} w_{ij}$.

The uniform sparsest cut problem searches for an edge cut or a node partition such that the ratio of the edge cut’s weight to the number of nodes in $S$ times the number of nodes in the complement $\bar{S}$ is minimal, i. e.,

$$\min_{\substack{\mathcal{S} \subseteq N \\ \mathcal{S} \neq \emptyset}} \frac{w(S, \bar{S})}{|S||\bar{S}|}.$$ 

There are upper and lower bounds for the uniform sparsest cut in terms of the eigenvalues of the weighted Laplacian of the graph:

According to the well known Courant-Fischer characterization of eigenvalues of symmetric matrices (Theorem 2.2), the second smallest eigenvalue $\lambda_2(L_w)$ and the largest eigenvalue $\lambda_{\max}(L_w)$ of the weighted Laplacian may be characterized as

$$\lambda_2(L_w) = \min\{x^T L_w x : \|x\| = 1, 1^T x = 0\} \quad \text{and} \quad \lambda_{\max}(L_w) = \max\{x^T L_w x : \|x\| = 1\},$$

respectively.
For any node bipartition $N = S \cup \bar{S}$ using vector $x \in \mathbb{R}^{|N|}$ with $x_i = |S|^{-1}$ for $i \in S$ and $x_i = -|\bar{S}|^{-1}$ for $i \in \bar{S}$ the quadratic form (1.1) of $L_w$ together with the eigenvalue characterizations yield the bounds

$$\frac{1}{|N|} \lambda_2(L_w) \leq \frac{w(S, \bar{S})}{|S||\bar{S}|} \leq \frac{1}{|N|} \lambda_{\max}(L_w)$$

(see also [3]). That means that the value of the uniform sparsest cut lies within an interval bounded by the eigenvalues divided by the number of nodes of the graph.

Minimizing the difference of maximum and second smallest eigenvalue of weighted Laplacians we get nonnegative edge weightings of a graph that minimize the size of the bounding interval.

Like in the previous chapters, we reformulate the eigenvalue problem as a semidefinite pair of primal and dual programs and establish strong duality as well as the attainment of optimal solutions (Proposition 5.1).

The corresponding graph realization problem is in some sense a combination of the single graph realization problems of the previous chapters. That means we are searching for two graph realizations, one corresponding to the second smallest eigenvalue (for a moment we call it the $\lambda_2$-realization) and one corresponding to the maximum eigenvalue (the $\lambda_{\max}$-realization). In both realizations the sum of weighted squared distances of the nodes to the origin equals one and the $\lambda_2$-realization has its barycenter in the origin. Although it is not explicitly required, the origin is also the barycenter of optimal $\lambda_{\max}$-realizations (Proposition 5.8). Both realizations are coupled as the squared edge length of the $\lambda_{\max}$-realization should be greater or equal to the squared edge length of the $\lambda_2$-realization. For each edge this difference should be as large as possible.

As before the maps of optimal realizations onto one-dimensional subspaces turn out to be eigenvectors to the corresponding optimal eigenvalue (Proposition 5.2).

Like in the previous chapters, optimal solutions have some basic structural properties which are established in Section 5.2. So we identify complete graphs to be the only ones having optimal value zero (Theorem 5.4). Considering a graph with corresponding edge weights we may delete edges with zero weight. The so weighted graph may decompose into several connected components. Proposition 5.6 states that there is an optimal edge weighting, such that the maximum eigenvalue of each component with at least two nodes (considering the related submatrices) is identical to the optimal maximum eigenvalue of the whole graph. If the optimal weighted graph is not connected, it turns out that each component of an optimal $\lambda_2$-realization collapses to a single point (Proposition 5.9). Optimal realizations of an arbitrary graph lie within a closed ball of appropriate dimension, see Proposition 5.11.

In particular, we will point out and exploit connections of feasible and optimal solutions of the coupled problem to the single ones. If both, the node and edge parameters are positive
then feasible realizations of the coupled problem are also feasible in the single ones and vice versa, see Theorem 5.14 for a precise statement. While feasibility holds, optimality may be lost. But for an optimal \( \lambda_{\text{max}} \)-realization of the coupled problem we may find appropriate parameters, such that it is optimal for the single problem with the new parameters (Theorem 5.15). An almost analogous result holds for optimal \( \lambda_2 \)-realizations. Unfortunately, we have to exclude some special cases, see Theorem 5.18. Because of the previous two theorems, the Sunny-Side Theorem and the Separator-Shadow Theorem hold for optimal \( \lambda_{\text{max}} \) and (almost all) optimal \( \lambda_2 \)-realizations. Thus, optimal realizations corresponding to the second smallest eigenvalue will have an unfolding character and optimal realizations corresponding to the maximum eigenvalue will have a folding character. The bounds on the dimension of optimal realizations depending on the tree-width of the graph follow, as well.

It may happen that while the graph itself is connected, the resulting weighted graph is not connected. Connected graphs loosing connectedness by an optimal edge weighting are those graphs for which we cannot guarantee that optimal \( \lambda_2 \)-realizations are also optimal in an appropriate single problem. Therefore, it would be interesting to know those graphs. Their characterization does not seem to be easy as, e. g., also \( k \)-edge connected graphs may loose connectedness (Example 5.28). We will start a discussion of this problem at the end of Section 5.3.

Special graph classes like bipartite graphs and graphs having some symmetry, are investigated in Section 5.4, followed by a scaled version of the eigenvalue problem in Section 5.5.

The chapter closes by considering the scaled program and additionally optimizing over the edge parameters in Section 5.6. Again, there are two graph realizations corresponding to the second smallest and the maximum eigenvalue of the unweighted Laplacian. Maps of optimal realizations on one-dimensional subspaces are eigenvectors with respect to these eigenvalues. Optimal solutions of this coupled problem and optimal solutions of the single ones (see sections 3.4 and 4.6) are closely related. By appropriate scaling optimal realizations of the coupled problem are also optimal in the single ones and vice versa, see Theorem 5.46 for a precise statement.

The theory presented in this chapter is joint work with Frank Göring and Christoph Helmberg and is mostly taken verbatim from [37]. However, we have added some examples and further explanations. We would like to emphasize that the result of Section 5.6 concerning the relationship of optimal solutions of the single problems to optimal solutions of the coupled problem, Theorem 5.46, is new.

Chapter 6: Some Open Problems

With an outlook on further research, we present some remaining open problems and related questions on the topic.
CHAPTER 1. INTRODUCTION

Acknowledgment

At this point, I would like to thank all those who have supported me throughout my doctorate study. First of all, I am deeply indebted to Prof. Dr. Christoph Helmberg for his guidance and professional support, helping me to tackle and to finish this dissertation. My gratitude also goes to my colleagues, especially those of the Algorithmic and Discrete Mathematics Group. Thank you for valuable comments, ideas, counterexamples, reading and checking this work. Many thanks to my family and friends for understanding and encouragement. Last, but not least, my sincere thanks to Sebastian for love and patience.
Chapter 2

Preliminary Notions and Results

By combining spectral graph theory and semidefinite optimization, in this thesis we study structural properties of the graph, in particular properties of the graph’s separator structure. This chapter serves to summarize the basic theoretical concepts and results that are used in this thesis. It is divided into the three sections linear algebra, semidefinite optimization and graph theory. The materials in this chapter are standard. Readers who are familiar with these basic results are encouraged to skip ahead to Chapter 3.

In the first section we consider the vector space over real $n \times m$ matrices, introduce an inner product and give spectral properties of symmetric matrices. We recall some characterizations of positive semidefinite matrices and the notation and definitions of hulls, cones and projections. We refer to [53] and [42] for an overview on this topic. A useful lemma about different calculations of distances within a set of vectors completes the section (cf. [38]).

The semidefinite programming section is mainly based on [48, 49] but we also refer to [95]. We present a primal-dual pair of standard programs and give a short introduction to semidefinite duality theory. In this thesis we will use slightly different programs. The conditions that ensure strong duality will fail. Thus we state a weaker condition, based on a result of vector optimization. While the discussion and result seem to be folklore we include them for the sake of completeness.

The third section recalls the basic notions of graph theory from [20] and [12]. More precisely we review the Laplacian, some special subgraphs and certain graph classes, node separators, a graph’s tree-decomposition, the tree-width and minors of a graph as well as connectivity. Finally, we consider the symmetry of a graph via its automorphism group. The latter part is mostly taken from [37].
2.1 Linear Algebra

Symmetric Matrices

Let $A$ be a matrix in $\mathbb{R}^{n \times m}$. The set of all real $n \times m$ matrices is isomorphic to the vector space $\mathbb{R}^{n \cdot m}$. In the vector space of matrices the inner product of matrices $A, B \in \mathbb{R}^{n \times m}$ is

$$\langle A, B \rangle := \text{tr}(B^\top A) = \sum_{ij} [A]_{ij}[B]_{ij}.$$ 

The trace $\text{tr}(\cdot)$ is the sum of the diagonal elements of a square matrix. Because of

$$\text{tr}(C^\top AB) = \text{tr}(BC^\top A)$$

for $A, B, C \in \mathbb{R}^{n \times n}$, the transpose serves as adjoint in this inner product, $\langle AB, C \rangle = \langle A, CB^\top \rangle$. The norm associated with the inner product is called Frobenius norm. It is defined as

$$\|A\|_F := \sqrt{\langle A, A \rangle}.$$ 

If not stated otherwise the vectors are column vectors. For $m = 1$ we prefer $a^\top b$ instead of $\langle a, b \rangle$ for the inner product of $a, b \in \mathbb{R}^n$. The norm of $a \in \mathbb{R}^n$ is then the usual Euclidean norm

$$\|a\| = \left( \sum_{i=1}^{n} [a]_i^2 \right)^{1/2}.$$ 

A matrix $A \in \mathbb{R}^{n \times n}$ is said to be orthogonal if its rows and columns are orthogonal unit vectors, i.e., for $i, j \in \{1, \ldots, n\}$

$$[A]_{ij}^\top [A]_{ij} = [A]_{ij} [A]_{ij}^\top = \begin{cases} 1 & i = j, \\ 0 & i \neq j. \end{cases}$$

We also write $a \perp b$ if the vectors $a, b \in \mathbb{R}^n$ are orthogonal.

If a scalar $\lambda \in \mathbb{C}$ and a vector $x \in \mathbb{C}^n \setminus \{0\}$ satisfy $Ax = \lambda x$, then $\lambda$ is called an eigenvalue of $A$ and $x$ an eigenvector of $A$ associated with $\lambda$. The set of all $\lambda \in \mathbb{C}$ that are eigenvalues of $A$ is called the spectrum of $A$.

A matrix $A \in \mathbb{R}^{n \times n}$ is symmetric if it satisfies $A = A^\top$, i.e., $[A]_{ij} = [A]_{ji}$ ($1 \leq i < j \leq n$). We denote the set of all real symmetric matrices by $\mathcal{S}^n$. It can be interpreted as a vector space in $\mathbb{R}^{\frac{n(n+1)}{2}}$.

The spectrum of a symmetric matrix is closely related to the matrix structure, which is demonstrated by the following theorem.
Theorem 2.1 (Spectral Theorem for Symmetric Matrices) Let $A \in S^n$. Then

1. all the eigenvalues $\lambda_1, \ldots, \lambda_n$ of $A$ are real; and

2. there is an orthogonal matrix $P \in \mathbb{R}^{n \times n}$ such that $A = P \Lambda P^\top$, with diagonal matrix $\Lambda \in \mathbb{R}^{n \times n}$ having the eigenvalues of $A$ on its diagonal.

Proof. See, e.g., Theorem 2.5.6 in [53].

The decomposition of a symmetric matrix $A$ of the previous theorem is also called *eigenvalue decomposition*. A set of orthonormal eigenvectors associated with the eigenvalues of $A$ forms the columns of the matrix $P$ in respective order.

While in general the order of the eigenvalues of $A$ is arbitrary, we arrange them throughout the following in nondecreasing order, $\lambda_{\text{min}} = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n = \lambda_{\text{max}}$.

The eigenvalues are the roots of the characteristic polynomial of $A$. The eigenvalues of a symmetric matrix may also be characterized as optimal solutions of optimization problems. These are based on the orthogonality of the corresponding eigenvectors.

Theorem 2.2 (Courant-Fischer) Let $A \in S^n$ with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ and let $k$ be a given integer with $1 \leq k \leq n$. Then

$$
\min_{w_1, w_2, \ldots, w_{n-k} \in \mathbb{R}^n} \max_{x \perp w_1, w_2, \ldots, w_{n-k}, x \neq 0} \frac{x^\top A x}{x^\top x} = \lambda_k
$$

(2.1)

and

$$
\max_{w_1, w_2, \ldots, w_{k-1} \in \mathbb{R}^n} \min_{x \perp w_1, w_2, \ldots, w_{k-1}, x \neq 0} \frac{x^\top A x}{x^\top x} = \lambda_k.
$$

(2.2)

Proof. See, e.g., Theorem 4.2.11 in [53].

In the special cases $k = n$ and $k = 1$ we may omit the outer optimization of equations (2.1) and (2.2) respectively, as the set over which the optimization takes place is empty. Then Theorem 2.2 is also known as *Rayleigh-Ritz Theorem*.

An application of Theorem 2.2 are lower and upper bounds on the eigenvalues of the sum of matrices. They are composed of the sum of eigenvalues of the individual matrices.
**Theorem 2.3 (Weyl)** Let $A$ and $B$ be real symmetric matrices of the same order and let the eigenvalues $\lambda_i(A)$, $\lambda_i(B)$, and $\lambda_i(A+B)$ be arranged in nondecreasing order $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. For each $k \in \{1, 2, \ldots, n\}$ we have
\[
\lambda_k(A) + \lambda_1(B) \leq \lambda_k(A+B) \leq \lambda_k(A) + \lambda_n(B). \tag{2.3}
\]

**Proof.** See, e.g., Theorem 4.3.7 in [53].

How do the eigenvalues change in dependence on matrix transformation? The next theorem states, that the numbers of eigenvalues that are positive, negative, or zero do not change under a congruence transformation.

**Theorem 2.4 (Sylvester’s Law of Inertia)** Let $A, B \in \mathbb{R}^{n \times n}$ be symmetric matrices. There is a nonsingular matrix $S \in \mathbb{R}^{n \times n}$ such that $A = SBS^\top$ if and only if $A$ and $B$ have the same inertia, that is, the same number of positive, negative, and zero eigenvalues.

**Proof.** See, e.g., Theorem 4.5.8 in [53].

**Positive (Semi-)Definite Matrices**

A symmetric matrix $A \in \mathcal{S}^n$ is positive semidefinite ($A \succeq 0$ or $A \in \mathcal{S}^n_+$) if $x^\top Ax \geq 0$ for all $x \in \mathbb{R}^n$. It is positive definite ($A \succ 0$ or $A \in \mathcal{S}^n_{++}$) if $x^\top Ax > 0$ for all $x \in \mathbb{R}^n \setminus \{0\}$. If $A - B$ is positive semidefinite for symmetric matrices $A$ and $B$, this is denoted by $A \succeq B$. Note that in this sense $\succeq$ is a partial order, often called the Löwner partial order.

From the definition above follows that any principal submatrix of a positive definite (semidefinite) matrix is again positive definite (semidefinite). The next observation follows immediately.

**Observation 2.5** A symmetric block diagonal matrix is positive definite (semidefinite) if and only if all its diagonal blocks are positive definite (semidefinite).

There are several characterizations of positive (semi-) definite matrices. We will bring some to mind. The first one is connected to the matrix’ eigenvalues.

**Theorem 2.6** A symmetric matrix $A \in \mathcal{S}^n$ is positive semidefinite if and only if all of its eigenvalues are nonnegative. It is positive definite if and only if all of its eigenvalues are positive.
2.1. LINEAR ALGEBRA

We give a proof for the case that \( A \) is positive semidefinite. The proof of the other case follows the same argumentation.

**Proof.** Let \( A \in S^n_+ \) and \( \lambda_i \) be an eigenvalue of \( A \) with corresponding eigenvector \( x_i \). Then
\[
0 \leq x_i^\top Ax_i = x_i^\top \lambda_i x_i = \lambda_i \|x_i\|^2,
\]
thus \( \lambda_i \geq 0 \) for all \( i = 1, \ldots, n \).

Let otherwise \( \lambda_i \geq 0 \) for all \( i = 1, \ldots, n \). As \( A \) is symmetric, there exists an eigenvalue decomposition \( A = P \Lambda P^\top \), with \( \Lambda \) being a diagonal matrix having the eigenvalues on the main diagonal and \( P \) being orthogonal. Then
\[
x^\top Ax = x^\top P \Lambda P^\top x = (P^\top x)^\top \Lambda P^\top x = \sum_{i=1}^n \lambda_i \|P^\top x\|^2 \geq 0 \text{ for all } x \in \mathbb{R}^n.
\]

A further characterization of positive semidefinite matrices results from Gram matrices. Given a set of vectors \( \{a_1, \ldots, a_k\} \subset \mathbb{R}^n \) let \( A = [a_1, \ldots, a_k] \in \mathbb{R}^{n \times k} \). The Gram matrix \( G \in \mathbb{R}^{k \times k} \) of \( \{a_1, \ldots, a_k\} \) is defined as \( [G]_{ij} = a_i^\top a_j \) and \( G = A^\top A \) respectively. The rank of \( G \) equals the rank of \( A \), that is the maximum number of linearly independent rows or columns, respectively.

**Theorem 2.7** A matrix \( G \in S^k \) is positive semidefinite if and only if it is a Gram matrix.

**Proof.** Let \( G \) be symmetric positive semidefinite. Let \( P \Lambda P^\top \) be an eigenvalue decomposition of \( G \). Then \( G \) is the Gram matrix of the columns of \( A = \Lambda^{1/2} P^\top \).

On the other hand let \( G \) be the Gram matrix of \( A \in \mathbb{R}^{n \times k} \). Positive semidefinite follows by \( x^\top G x = x^\top A^\top Ax = \|Ax\|^2 \geq 0 \) for all \( x \in \mathbb{R}^k \).

The third characterization is known as Fejer’s Theorem.

**Theorem 2.8 (Fejer’s Theorem)** A symmetric matrix \( A \in \mathbb{R}^{n \times n} \) is positive semidefinite if and only if \( \langle A, B \rangle \geq 0 \) for all positive semidefinite matrices \( B \in \mathbb{R}^{n \times n} \).

**Proof.** See, *e. g.*, Corollary 7.5.4 in [53].

Because of Fejer’s Theorem we already know that the inner product of \( A, B \in S^n_+ \) is nonnegative. In which cases is it zero? The answer is traced back to matrix multiplication.

**Theorem 2.9** For \( A, B \in S^n_+ \) we have \( \langle A, B \rangle \geq 0 \) and \( \langle A, B \rangle = 0 \) if and only if \( AB = 0 \).

**Proof.** Using the eigenvalue decomposition \( A = P \Lambda P^\top = \sum_{i=1}^n \lambda_i [P]\_i [P]^\top \_i \) the inner product reads
\[
\langle A, B \rangle = \langle \sum_{i=1}^n \lambda_i [P]\_i [P]^\top \_i, B \rangle = \sum_{i=1}^n \lambda_i \langle [P]^\top \_i B [P]\_i \rangle \geq 0.
\]
Equality holds if and only if \([P]\_i \) lies in the kernel of \( B \) for \( \lambda_i > 0 \) if and only if \( AB = 0 \).
Hulls, Cones and Projection

A vector $x$ is called a **linear combination** of $x_1, \ldots, x_k \in \mathbb{R}^n$ if, for some $\alpha \in \mathbb{R}^k$,

$$x = \sum_{i=1}^{k} \alpha_i x_i.$$  

It is called

- **conic combination** if in addition $\alpha_i \geq 0$ ($i = 1, \ldots, k$).
- **affine combination** if in addition $\sum_{i=1}^{k} \alpha_i = 1$.
- **convex combination** if in addition $\alpha_i \geq 0$ ($i = 1, \ldots, k$) and $\sum_{i=1}^{k} \alpha_i = 1$.

If neither $\alpha = 0$ nor $x \in \{x_1, \ldots, x_k\}$ we call the linear (conic, affine, convex) combination **proper**. The set of all vectors that are linear combinations of finitely many vectors of a set $A \subseteq \mathbb{R}^n$ is called the **linear hull** and is denoted by $\text{lin}(A)$. The analogous definition gives rise to the **conic**, **affine** and **convex hull** denoted by $\text{cone}(A)$, $\text{aff}(A)$ and $\text{conv}(A)$, respectively.

A subset $A \subseteq \mathbb{R}^n$ is called **linearly independent** if none of its members is a proper linear combination of elements of $A$. The **dimension** of $A$ is the cardinality of the largest linearly independent subset of $A$ and is denoted by $\text{dim}(A)$.

A subset $A \subseteq \mathbb{R}^n$ is called a **convex cone** if it is closed under nonnegative multiplication and addition, i.e., $x, y \in A$ implies $\beta(x + y) \in A$ for all $\beta \geq 0$. The positive semidefinite matrices are an example of a convex cone.

Let $A \subseteq \mathbb{R}^n$, $x \in \mathbb{R}^n$. Then $p_A(x)$ is called **projection of $x$ onto $A$** if $p_A(x) \in A$ and $\|x - p_A(x)\| \leq \|x - a\|$ for all $a \in A$. So if it exists the projection of a vector $x$ onto a subset $A$ is a vector in $A$ with minimal Euclidean distance to $x$. If $A$ is convex the projection is unique, if it exists.

**Miscellaneous**

When calculating distances within a finite subset $\{v_1, \ldots, v_n\} \subset \mathbb{R}^d$, it may make sense to partition the set and consider only the distances to the subsets’ weighted barycenter. This is a well known and often used concept in physics. We state it precisely in the next lemma, allowing the vectors to be additionally weighted by $s_i$ ($i = 1, \ldots, n$) (see also [38]). For this purpose we introduce the notations

$$\bar{s}(A) = \sum_{i \in A} s_i \quad \text{for } A \subseteq \{1, \ldots, n\}$$
for the weight of the barycenter and for $\bar{s}(A) \neq 0$

$$\bar{v}(A) = \frac{1}{\bar{s}(A)} \sum_{i \in A} s_i v_i$$

for the barycenter of the weighted vectors specified by $A$.

**Lemma 2.10** Given $v_i \in \mathbb{R}^d$ and weights $s_i > 0$ for $i \in N$ with finite $N$ partitioned into disjoint sets, i.e., $N = \bigcup_{J \in P} J$ for some finite family $P$, there holds

$$\bar{v}(N) = \frac{1}{\bar{s}(N)} \sum_{J \in P} \bar{s}(J) \bar{v}(J)$$

(2.4)

and

$$\sum_{i \in N} s_i \|v_i - \bar{v}(N)\|^2 =$$

$$= -\bar{s}(N) \|\bar{v}(N)\|^2 + \sum_{i \in N} s_i \|v_i\|^2$$

(2.5)

$$= \frac{1}{2\bar{s}(N)} \sum_{i,j \in N} s_i s_j \|v_i - v_j\|^2$$

(2.6)

$$= \sum_{J \in P} \sum_{j \in J} s_j \|v_j - \bar{v}(J)\|^2 + \sum_{J \in P} \bar{s}(J) \|\bar{v}(J) - \bar{v}(N)\|^2$$

(2.7)

$$= \sum_{J \in P} \left( \sum_{j \in J} s_j \|v_j - \bar{v}(J)\|^2 + \frac{1}{2\bar{s}(N)} \sum_{K \in P} \bar{s}(J) \bar{s}(K) \|\bar{v}(J) - \bar{v}(K)\|^2 \right).$$

(2.8)

**Proof.** Equation (2.4) is verified by direct computation. Equation (2.5) follows by

$$\sum_{i \in N} s_i \|v_i - \bar{v}(N)\|^2 = \sum_{i \in N} s_i \|v_i\|^2 + \sum_{i \in N} s_i \|\bar{v}(N)\|^2 - 2 \sum_{i \in N} s_i v_i^\top \bar{v}(N)$$

$$= \sum_{i \in N} s_i \|v_i\|^2 + \bar{s}(N) \|\bar{v}(N)\|^2 - 2\bar{s}(N) \bar{v}(N)^\top \bar{v}(N)$$

$$= \sum_{i \in N} s_i \|v_i\|^2 - \bar{s}(N) \|\bar{v}(N)\|^2.$$
For (2.6),
\[
\sum_{i \in N} s_i \|v_i - \bar{v}(N)\|^2 = \sum_{i \in N} s_i \|v_i\|^2 - \frac{2}{\bar{s}(N)} \sum_{i,j \in N} s_is_j v_i^\top v_j + \frac{1}{\bar{s}(N)} \sum_{i,j \in N} s_is_j v_i^\top v_j
\]
\[
= \sum_{i \in N} s_i \|v_i\|^2 - \frac{1}{\bar{s}(N)} \sum_{i,j \in N} s_is_j v_i^\top v_j
\]
\[
= \frac{1}{2\bar{s}(N)} \sum_{i,j \in N} (s_is_j \|v_i\|^2 - 2s_is_j v_i^\top v_j + s_is_j \|v_j\|^2)
\]
\[
= \frac{1}{2\bar{s}(N)} \sum_{i,j \in N} s_is_j \|v_i - v_j\|^2.
\]

Next, (2.7) is proved by
\[
\sum_{j \in N} s_j \|v_j - \bar{v}(N)\|^2 = \sum_{J \in P} \sum_{j \in J} s_j \|v_j - \bar{v}(J) + \bar{v}(J) - \bar{v}(N)\|^2
\]
\[
= \sum_{J \in P} \sum_{j \in J} s_j \|v_j - \bar{v}(J)\|^2 + 2 \sum_{J \in P} \sum_{j \in J} s_j (v_j - \bar{v}(J))^\top (\bar{v}(J) - \bar{v}(N))
\]
\[
+ \sum_{J \in P} \bar{s}(J) \|\bar{v}(J) - \bar{v}(N)\|^2
\]
\[
= \sum_{J \in P} \sum_{j \in J} s_j \|v_j - \bar{v}(J)\|^2 + 2 \sum_{J \in P} (\bar{v}(J) - \bar{v}(N))^\top \sum_{j \in J} s_j (v_j - \bar{v}(J))
\]
\[
+ \sum_{J \in P} \bar{s}(J) \|\bar{v}(J) - \bar{v}(N)\|^2.
\]

Finally, (2.8) follows from using (2.4) and (2.6) for the second summand in (2.7).

In the end let us mention that 1 denotes the vector of all ones, 0 denotes the vector of all zeros and the matrix \(I\) denotes the identity matrix of appropriate size. The \(i\)th unit vector of the canonical basis of \(\mathbb{R}^n\) is denoted by \(e_i\). If all components of a vector \(a \in \mathbb{R}^n\) are nonnegative (positive) we write \(a \geq 0\) (\(a > 0\)), \(i.e.,\) it is a componentwise inequality.

For \(J \subseteq \{1, \ldots, m\}\) and a matrix \(A = [a_1, \ldots, a_m] \in \mathbb{R}^{n \times m}\) we denote by \(A_J\) the set \(\{a_j : j \in J\}\). In this section we have denoted the element \(ij\) of a matrix \(A\) by \([A]_{ij}\). If there is no danger of confusion we will often write \(A_{ij}\) instead. Finally, for a vector \(a \in \mathbb{R}^n\) we denote by \(\text{diag}(a)\) the diagonal matrix having \(a\) on its main diagonal, \(i.e.,\) \([\text{diag}(a)]_{ii} = [a]_i\) for \(i = 1, \ldots, n\) and zero otherwise.

### 2.2 Semidefinite Programming

Semidefinite programming deals with the optimization of a linear matrix function over the cone of symmetric positive semidefinite matrices subject to linear matrix constraints. A
primal program in standard form can be written as

\[
\begin{align*}
\text{minimize} & \quad \langle C, X \rangle \\
\text{subject to} & \quad AX = b, \\
& \quad X \succeq 0
\end{align*}
\]  

with given parameter \( b \in \mathbb{R}^m \), \( C \in \mathcal{S}^n \) and linear operator \( A : \mathcal{S}^n \to \mathbb{R}^m \). The operator \( A \) acts on \( X \) via

\[
A = \begin{bmatrix} 
\langle A_1, X \rangle \\
\vdots \\
\langle A_m, X \rangle 
\end{bmatrix}
\]

with \( A_i \in \mathcal{S}^n \) \((i = 1, \ldots, m)\). Let \( A^\top \) denote the adjoint operator of \( A \), i.e., \( \langle AX, y \rangle = \langle X, A^\top y \rangle \) for all \( X \in \mathcal{S}^n \) and \( y \in \mathbb{R}^m \). So \( A^\top y = \sum_{i=1}^m y_i A_i \in \mathcal{S}^n \).

We use a Lagrangian approach to lift the equality constraint of (2.9) into the objective function. Thus the Lagrange function with Lagrange multiplier \( y \in \mathbb{R}^m \) is

\[
\mathcal{L}(X, y) = \langle C, X \rangle + \langle b - AX, y \rangle.
\]

Rewriting (2.9) and exchanging inf and sup we get the inequality (cf. [81], Lemma 36.1)

\[
\inf_{X \succeq 0} \sup_{y \in \mathbb{R}^m} \langle C, X \rangle + \langle b - AX, y \rangle \\
\geq \sup_{y \in \mathbb{R}^m} \inf_{X \succeq 0} \langle C, X \rangle + \langle b - AX, y \rangle \\
= \sup_{y \in \mathbb{R}^m} \inf_{X \succeq 0} \langle b, y \rangle + \langle X, C - A^\top y \rangle.
\]  

(2.10)

The equality of (2.9) and the left-hand side of (2.10) follows as

\[
\sup_{y \in \mathbb{R}^m} \langle C, X \rangle + \langle b - AX, y \rangle < \infty
\]

if and only if \( AX = b \). With an analog argumentation we get the dual program of (2.9) from the right-hand side of (2.10): because of the inner minimization and Fejer’s Theorem (Theorem 2.8)

\[
\inf_{X \succeq 0} \langle b, y \rangle + \langle X, C - A^\top y \rangle > -\infty
\]

if and only if \( C - A^\top y \succeq 0 \). The dual program of (2.9) reads

\[
\begin{align*}
\text{maximize} & \quad \langle b, y \rangle \\
\text{subject to} & \quad A^\top y \preceq C, \\
& \quad y \in \mathbb{R}^m.
\end{align*}
\]

(2.11)

As both programs (2.9) and (2.11) are semidefinite programs (cf. [48]) it is somewhat arbitrary which one is called primal and which is dual. Indeed in the next chapters we will interchange the terms as we call that program the primal one which we consider first.
Comparing the objective values of (2.9) and (2.11), we obtain (using Fejer’s Theorem (Theorem 2.8) for the inequality)

\[ \langle C, X \rangle - \langle b, y \rangle = \langle C, X \rangle - \langle AX, y \rangle \]
\[ = \langle C - A^\top y, X \rangle \geq 0 \] (2.12)

for all feasible \( X \) of (2.9) and feasible \( y \) of (2.11). The inequality is also called weak duality. For optimal solutions it specifies the gap between primal and dual optimal values. In contrast to linear programming, the gap may be strictly positive in semidefinite programming.

So we have to ask for conditions that ensure a zero gap. We call this equivalence of optimal values of the primal and the dual problem strong duality. Note that this definition of strong duality does not imply attainment of optimal solutions.

One condition that ensures strong duality is the existence of a feasible solution lying in the interior of the cone of positive semidefinite matrices, \( i.e., \) the existence of a Slater point.

**Definition 2.11** A point \( X \) is strictly feasible for (2.9) if it is feasible for (2.9) and \( X \succ 0 \).

A point \( y \) is strictly feasible for (2.11) if it is feasible for (2.11) and \( A^\top y \prec C \).

A semidefinite program is strictly feasible if it has a strictly feasible solution.

The following strong duality theorem holds.

**Theorem 2.12 (Strong Duality, [48])** Let

\[ p^* = \inf \{ \langle C, X \rangle : AX = b, X \succeq 0 \} \quad \text{and} \quad d^* = \sup \{ \langle b, y \rangle : A^\top y \preceq C, y \in \mathbb{R}^m \} \]

(i) If (2.9) is strictly feasible with \( p^* \) finite, then \( p^* = d^* \) and it is attained for (2.11).

(ii) If (2.11) is strictly feasible with \( d^* \) finite, then \( p^* = d^* \) and it is attained for (2.9).

(iii) If (2.9) and (2.11) are strictly feasible, then \( p^* = d^* \) is attained for both problems.

In the following we consider a slightly different pair of semidefinite programs and discuss strong duality. While the discussion and results seem to be folklore we include them for the sake of completeness.

We add some affine constraints in the dual program, \( i.e., \) \( A \in \mathbb{R}^{m \times k} \) and \( c \in \mathbb{R}^k \). By the above Lagrangian approach we get the primal-dual pair
2.2. SEMIDEFINITE PROGRAMMING

\[ \begin{align*}
\text{minimize} & \quad \langle C, X \rangle + \langle c, x \rangle \\
\text{subject to} & \quad AX + Ax = b, \\
& \quad X \succeq 0, \ x \geq 0
\end{align*} \tag{2.13} \]

\[ \begin{align*}
\text{maximize} & \quad \langle b, y \rangle \\
\text{subject to} & \quad A^\top y \preceq C, \\
& \quad A^\top y \leq c, \\
& \quad y \in \mathbb{R}^m.
\end{align*} \tag{2.14} \]

Indeed we may rewrite (2.13) and (2.14) as standard semidefinite programs (2.9) and (2.11) using

\[
X \succeq 0, \ x \geq 0 \quad \iff \quad \begin{pmatrix}
X & 0 & \cdots & 0 \\
0 & x_1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & x_k
\end{pmatrix} \succeq 0
\]

(cf. Observation 2.5). Then a feasible solution \((X, x)\) of (2.13) \((y)\) of (2.14)) turns out to be strictly feasible if \(X \succ 0\) and \(x > 0\) \((A^\top y < C\) and \(A^\top y < c\)). If there exists such a strictly feasible solution for (2.13) or (2.14) or for both, Theorem 2.12 ensures strong duality.

Now we assume that the affine constraints specify at least one equation, i.e., there exist some \(i, j \in \{1, \ldots, k\}\) with \([A]_i = -[A]_j\) and \([c]_i = -[c]_j\), thus

\[ [A]_i^\top y \leq [c]_i \quad \text{and} \quad [A]_j^\top y \geq [c]_j. \]

Then, (2.14) is not strictly feasible because there is no \(y \in \mathbb{R}^m\) with \([A]_i^\top y < [c]_i\) and \([A]_j^\top y > [c]_j\). The condition of Theorem 2.12 is too strong. We will prove (see Corollary 2.15), that a weak Slater condition is sufficient, namely a feasible solution that only satisfies the semidefinite constraint strictly.

**Definition 2.13** A point \(y\) is strictly feasible with respect to the semidefinite constraint for (2.14) if it is feasible for (2.14) and satisfies \(A^\top y < C\).

While [81] gives an applicable strong duality result in the case that the affine constraints turn all out to be equations, a result of vector optimization (see e.g. [8]) discusses the general case. For the sake of completeness we will recall it and infer a strong duality theorem for semidefinite programming.

**Theorem 2.14** ([8], Theorem 3.2.14 and Remark 3.2.6) Let \(S \subseteq \mathbb{R}^m\) be a nonempty convex set, \(f : \mathbb{R}^m \to \mathbb{R} \cup \{\pm \infty\}\) a proper and convex function and \(g : \mathbb{R}^m \to \mathbb{R}^k\), \(g(y) = (g_1(y), \ldots, g_k(y))^\top\) a vector function having each component \(g_i, \ i = 1, \ldots, k\), affine such that \(\text{dom} f \cap S \cap g^{-1}(-\mathbb{R}_+^k) \neq \emptyset\). If \(\exists y' \in \text{ri}(\text{dom} f \cap S)\) such that \(g(y') \leq 0\), then for \(\inf_{y \in \mathcal{Y}} f(y)\) with \(\mathcal{Y} = \{y \in S : g(y) \leq 0\}\) and its Lagrange dual \(\sup_{x \geq 0} \inf_{y \in S} \{f(y) + \langle x, g(y) \rangle\}\) strong duality holds and the dual has an optimal solution.
\textbf{Corollary 2.15 (Strong Duality)} Suppose that there exists a strictly feasible solution $\tilde{y}$ with respect to the semidefinite constraint for (2.14) and let
\begin{align*}
p^* &= \inf \{ \langle C, X \rangle + \langle c, x \rangle : AX + Ax = b, X \succeq 0, x \geq 0 \} \\
d^* &= \sup \{ \langle b, y \rangle : A^T y \preceq C, A^T y \leq c, y \in \mathbb{R}^m \}.
\end{align*}
Then $p^* = d^*$ and if $p^*$ is finite it is attained for some feasible $(X, x)$ of (2.13).

\textbf{Proof.} We rewrite the primal and dual program in terms of Theorem 2.14. Let therefore $S = \{ y \in \mathbb{R}^m : A^T y \preceq C \}$, $f(y) = -\langle b, y \rangle$, $g(y) = A^T y - c$ and $\mathcal{Y} = \{ y \in S : g(y) \leq 0 \}$. Note that
\begin{itemize}
    \item $S$ is convex and as $\tilde{y} \in S$ it is not empty,
    \item the affine function $f$ is convex and proper with $\text{dom} f = \mathbb{R}^m$,
    \item by definition all components of $g$ are affine and $\tilde{y} \in g^{-1}(-\mathbb{R}^k_+)$.\end{itemize}
As $\tilde{y} \in \text{ri}(\text{dom} f \cap S)$ and $g(\tilde{y}) \leq 0$ all conditions of Theorem 2.14 are satisfied thus strong duality holds for
\begin{align*}
\inf \{ f(y) : y \in \mathcal{Y} \} \quad \text{and} \quad \sup \inf \{ f(y) + \langle x, g(y) \rangle \}
\end{align*}
and the dual has an optimal solution.

It remains to show that the pair of primal and dual programs from above is equivalent to (2.13) and (2.14).

By construction $\sup \{ \langle b, y \rangle : A^T y \preceq C, A^T y \leq c, y \in \mathbb{R}^m \} = -\inf \{ f(y) : y \in \mathcal{Y} \}$ and
\begin{align*}
\sup \inf \{ f(y) + \langle x, g(y) \rangle \} &= \sup_{x \geq 0} \inf_{y \in S} \{ \langle -c, x \rangle + \inf_{y \in \mathcal{S}} \langle A - b, y \rangle \} \\
&= \sup_{x \geq 0} \{ \langle -c, x \rangle + \inf_{y \in \mathcal{S}} \sup_{X \succeq 0} \langle A - b, y \rangle + \langle A^T y - C, X \rangle \} \\
&\overset{(*)}{=} \sup_{x \geq 0} \{ \langle -c, x \rangle + \sup_{y \in \mathcal{S}} \inf_{X \succeq 0} \langle AX + Ax - b, y \rangle + \langle -C, X \rangle \} \\
&= \sup_{x \geq 0} \{ \langle -c, x \rangle + \langle -C, X \rangle + \inf_{y \in \mathcal{S}} \langle AX + Ax - b, y \rangle \} \\
&= \sup \{ \langle -c, x \rangle - \langle C, X \rangle : AX + Ax = b, X \succeq 0, x \geq 0 \} \\
&= -\inf \{ \langle C, X \rangle + \langle c, x \rangle : AX + Ax = b, X \succeq 0, x \geq 0 \}.
\end{align*}
The third equality $(*)$ follows from Theorem 2.12 because we construct the Lagrangian of a standard semidefinite program for which $\tilde{y}$ is a strictly feasible solution. \hfill \blacksquare
2.3. GRAPH THEORY

Strong duality, i.e., the equality of primal and dual optimal values, induces semidefinite complementarity conditions if primal and dual solutions are attained. Let \((X, x)\) be feasible for (2.13) and \(y\) for (2.14). If they fulfill

\[
\langle X, C - A^\top y \rangle = 0 \quad \text{and} \quad \langle x, c - A^\top y \rangle = 0
\] (2.15)

then they are optimal as the optimal values are the same

\[
0 = \langle X, C - A^\top y \rangle + \langle x, c - A^\top y \rangle = \langle C, X \rangle + \langle c, x \rangle - \langle AX + Ax, y \rangle.
\]

2.3 Graph Theory

Let \(G = (N, E)\) be a finite undirected simple graph, i.e., without loops and multiple edges, with node set \(N = \{1, \ldots, n\}\) and nonempty edge set \(E \subseteq \{(i, j) : i, j \in N, i \neq j\}\). For an edge \((i, j)\) we also write \(ij\) if there is no danger of confusion.

For a subset of nodes \(S \subseteq N\) the induced subgraph is the graph with node set \(S\) and edge set \(\{(i, j) : i, j \in S, ij \in E\}\).

Given nonnegative edge weights \(w_{ij} \geq 0 (ij \in E)\) the weighted Laplacian of \(G\) is the matrix \(L_w(G) \in \mathbb{R}^{n \times n}\) with

\[
[L_w(G)]_{ij} := \begin{cases} 
-w_{ij} & ij \in E, \\
\sum_{k \in E} w_{ik} & i = j, \\
0 & \text{otherwise}.
\end{cases}
\]

We often use another representation of \(L_w(G)\): the fact that two nodes \(i, j \in N, i \neq j\), are adjacent may be represented by an \((n \times n)\)-matrix

\[
E_{ij} := \begin{bmatrix} 
i & j \\
1 & -1 \\
-1 & 1
\end{bmatrix}
\]

having four nonzero entries, i.e., 1 at positions \(ii\) and \(jj\), \(-1\) at positions \(ij\) and \(ji\) and zero otherwise. Thus, the weighted Laplacian reads

\[
L_w(G) = \sum_{ij \in E} w_{ij} E_{ij}.
\]

If \(G\) is clear from the context we simply write \(L_w\).
The Laplacian $L(G)$ of a graph $G$ is just the weighted Laplacian with all weights equal to one. As the matrices $E_{ij}$ are symmetric positive semidefinite and the weights are non-negative the (weighted) Laplacian is symmetric positive semidefinite, too. Its smallest eigenvalue is $\lambda_1 = 0$ with corresponding eigenvector $\mathbf{1}$.

A graph is called \textit{connected} if there exists a path between any two of its nodes. A \textit{component} of a graph $G = (N,E)$ is a maximal connected subgraph. A graph is called $k$-\textit{connected} for $k \in \mathbb{N}$, if $n > k$ and the removal of any node set $X \subseteq N$ with $|X| < k$ does not destroy connectedness. Because of Menger’s theorem, in a $k$-connected graph any pair of nodes is connected by $k$ node disjoint paths.

A \textit{tree} is a connected graph not containing any cycles, \textit{i.e.}, there is no sequence of edges $v_1v_2, v_2v_3, \ldots, v_kv_1$ in the graph. A \textit{spanning tree} $(N,E_T)$ of a connected graph $G = (N,E)$ is a subgraph of $G$ which is a tree, \textit{i.e.}, $E_T \subseteq E$ and $|E_T| = n - 1$.

A (node-) \textit{separator} of a connected graph $G$ is a subset $S \subseteq N$ of nodes, whose removal decomposes the graph into at least two connected components. Often we will not discern every single component arising this way but simply speak of two or more separated sets of nodes.

Important structural graph properties are associated with the tree-decomposition and tree-width.

**Definition 2.16** Let $G = (N,E)$ be a graph, $T$ a tree, and let $N := (N_t)_{t \in T}$ be a family of node sets $N_t \subseteq N$ indexed by the nodes $t$ of $T$. The pair $(T,N)$ is called a \textit{tree-decomposition} of $G$ if it satisfies the following three conditions:

1. $N = \bigcup_{t \in T} N_t$;
2. for every edge $e \in E$ there exists a $t \in T$ such that $e \subseteq N_t$;
3. if $t_2$ is on the $T$-path from $t_1$ to $t_3$, then $N_{t_1} \cap N_{t_3} \subseteq N_{t_2}$.

The width of $(T,N)$ is the number $\max\{|N_t| - 1 : t \in T\}$. The tree-width $\text{tw}(G)$ of $G$ is the least width of any tree-decomposition of $G$.

Note that a tree-decomposition of a complete graph $K_n = (N, \{ij : i,j \in N, i \neq j\})$ is for instance $N = \{N\}$ and $T = (N, \emptyset)$. Its tree-width is $\text{tw}(K_n) = n - 1$. 


2.3. GRAPH THEORY

Considering trees we can choose $N = E$ as each edge forms one set $N_t$. We can choose the edge set of $T$ as the edge set of any spanning tree of the original tree’s line graph. Thus the tree-width of a tree is one.

In a tree-decomposition we can easily identify separators as the following lemma states.

**Lemma 2.17** For a graph $G$ with tree-decomposition $(T, (N_t)_{t \in T})$ let $t_1t_2$ be any edge of $T$. Then $N_{t_1} \cap N_{t_2}$ is a separator in $G$.

**Proof.** See, e. g., [20], Lemma 12.3.1.

We obtain a graph $G/\{ij\} = (N', E')$ from $G = (N, E)$ by contracting an edge $ij \in E$ as follows: we identify the two nodes $i$ and $j$ and replace them by a new node $i'$. Hence $N' := (N \setminus \{i, j\}) \cup \{i'\}$. The new node $i'$ is adjacent to all neighbors of $i$ and $j$ (if they have a common neighbor there is only one edge), for that reason $E' := \{xy \in E : \{x, y\} \cap \{i, j\} = \emptyset\} \cup \{i'x : ix \in E \setminus \{ij\}\}$.

We call a graph $G_M$ a minor of $G$ if we obtain $G_M$ from $G$ by a sequence of edge contractions, edge deletions, and deletions of isolated nodes.

A graph invariant $\sigma(G)$ is called minor monotone, if $\sigma(G_M) \leq \sigma(G)$ for any minor $G_M$ of $G$.

Finally we summarize and generalize some notions concerning the symmetry of a graph in the same way we have already done in [37].

An automorphism $\varphi$ of a graph $G = (N, E)$ is a permutation of the vertices $N$ that leaves the edge set $E$ invariant, i. e., $\varphi : N \to N$ bijectively and $ij \in E$ if and only if $\varphi(i)\varphi(j) \in E$. For simplicity, for the image of an edge $ij \in E$ we write $\varphi(ij)$ instead of $\varphi(i)\varphi(j)$.

If there are given node weights $s_i$ ($i \in N$) and edge weights $l_{ij}$ ($ij \in E$) then we extend the definition by requiring that a bijective $\varphi : N \to N$ is an automorphism of $G$ with weights $s$ and $l$ if $ij \in E$ if and only if $\varphi(ij) \in E$, $s_k = s_{\varphi(k)}$ ($k \in \{i, j\}$), and $l_{ij} = l_{\varphi(ij)}$ (see also [10]).

It is well known that the set of all automorphisms of $G$ forms the automorphism group $\text{Aut}(G)$. The same holds for the automorphisms of $G$ with weights $s$ and $l$. We denote this group by $\text{Aut}(G, s, l)$.

Note that $\text{Aut}(G, s, l) \subseteq \text{Aut}(G)$ and $\text{Aut}(G, c_s1, c_l1) = \text{Aut}(G)$ for $c_s, c_l \in \mathbb{R}$.

The orbits $E_1, \ldots, E_k$ of the edge set $E$ under the action of $\text{Aut}(G, s, l)$ give rise to a partition of $E$. Furthermore if the edges $e_1, e_2, e_3, e_4$ (not necessarily different) lie in the same orbit, then

$$|\{\varphi \in \text{Aut}(G, s, l) : \varphi(e_1) = e_2\}| = |\{\varphi \in \text{Aut}(G, s, l) : \varphi(e_3) = e_4\}| \neq 0,$$
i. e., the number of automorphisms that maps an edge onto another edge of the same orbit is the same for all pairs of edges of this orbit. We assign to each orbit $E_r$ ($r = 1, \ldots, k$) this number of automorphisms $a_r$, i. e., $a_r = |\{ \varphi \in \text{Aut}(G, s, l) : \varphi(e) = e' \}|$ with $e, e' \in E_r$. This leads to the following lemma (which may also be seen as a direct consequence of Lagrange’s theorem in group theory).

**Lemma 2.18** Let $G$ be a graph with weights $s$ and $l$, $\text{Aut}(G, s, l)$ its automorphism group and $E_1, \ldots, E_k$ the orbits of the edge set $E$. Then $|\text{Aut}(G, s, l)| = a_r \cdot |E_r|$ for $r = 1, \ldots, k$.

**Proof.** Enumerate the edges, $E = \{e_1, \ldots, e_m\}$, and let $e_1 \in E_r$ for some $r \in \{1, \ldots, k\}$.

\[
|\text{Aut}(G, s, l)| = \sum_{\varphi \in \text{Aut}(G, s, l)} 1 = \sum_{e_i \in E} \sum_{\varphi \in \text{Aut}(G, s, l)} 1 = \sum_{e_i \in E_r} \sum_{\varphi \in \text{Aut}(G, s, l)} 1 = \sum_{e_i \in E_r} a_r = a_r \cdot |E_r|. \]

A graph $G = (N, E)$ whose automorphism group consists of only one orbit is called *edge transitive*, i. e., for $e_1, e_2 \in E$ there is an automorphism $\varphi \in \text{Aut}(G)$ such that $\varphi(e_1) = e_2$. 
Chapter 3

The Second Smallest Eigenvalue of the Laplacian

The Laplacian of a graph provides various information about the graph and its structure. In this context the Laplacian spectrum, in particular the extremal eigenvalues, are of great interest. As the smallest eigenvalue equals zero, the second smallest eigenvalue is of more significance. In this chapter our main concern is to examine properties of the graph given by the second smallest eigenvalue and the corresponding eigenspace.

The considerations are based on an approach of Fiedler who weighted the edges of a graph $G = (N, E \neq \emptyset)$ such that the total edge weight equals the number of edges. He introduced the absolute algebraic connectivity in \[\hat{\alpha}(G) := \max \left\{ \lambda_2(L_w) : \sum_{ij \in E} w_{ij} = |E|, \ w_{ij} \geq 0 \ (ij \in E) \right\}, \quad (3.1)\]

which is the maximal second smallest eigenvalue of these weighted Laplacians.

Göring et al. formulated this problem as a pair of primal-dual semidefinite programs and proved relations of optimal solutions to structural graph properties. In this chapter we give a summary of these results following and adapting [39, 40].

In the first section a generalization of (3.1) is formulated by a semidefinite pair of primal-dual programs ((P$_{\lambda_2}$) and (D$_{\lambda_2}$)) for which strong duality is analyzed. It turns out that the dual is equivalent to a graph realization problem which assigns each node a vector in $\mathbb{R}^n$ under some constraints. An interpretation of optimal realizations as maps of eigenvectors to the maximal second smallest eigenvalue of the (optimal) weighted Laplacian and optimal realizations of nonconnected graphs concludes this section. Even though Göring et al. did not deal with (P$_{\lambda_2}$) and (D$_{\lambda_2}$) most results of this section are based on approaches of their work [39, 40].
The programs of [40] which are scaled versions of $(P_{\lambda_2})$ and $(D_{\lambda_2})$ and relations to them are given in the next section.

In Section 3.3 properties of optimal realizations are discussed. Separators play an important role as there is a result that implies an unfolding property of optimal realizations (Separator-Shadow Theorem, Theorem 3.10). As the existence of low dimensional realizations is of great interest the rotational dimension of a graph is introduced and proven to be a minor monotone graph parameter. Separators are closely linked to the graph’s tree-width which establishes an upper bound for the dimension of an optimal realization and for the rotational dimension (Theorem 3.14). Finally we identify a special optimal primal edge weighting for graphs exhibiting special symmetry properties and apply it to edge transitive graphs.

While most results of these sections are based on [39, 40] we want to mention that we analyze strong duality and attainment of optimal solutions of $(P_{\lambda_2})$ and $(D_{\lambda_2})$ in more generality and more detail. Our characterization of optimal solutions of nonconnected graphs, Proposition 3.8, is a new result. Also the considerations on the graph’s symmetry, Section 3.3, were of no interest for Göring et al.. However, note that Fiedler already proved a special case of Proposition 3.17 that we cite in Proposition 3.16.

The final section of this chapter is based on joint work with Christoph Helmberg. Results are mainly taken from [50] and presented in this thesis in more detail. We consider another new primal-dual pair of semidefinite programs together with a formulation via graph realizations. On the one hand optimal realizations are proven to be maps of eigenvectors to the second smallest eigenvalue of the unweighted Laplacian, Theorem 3.22. On the other hand each eigenvector gives rise to an optimal realization, Theorem 3.23.

Let us observe that minimizing the second smallest eigenvalue of the weighted Laplacian of a graph with nonempty edge set is of little interest. As the weighted Laplacian is positive semidefinite the minimum of the second smallest eigenvalue is zero. For a graph with at least three nodes it is attained if the graph is not connected, e. g., we put all weight onto one edge. The second smallest eigenvalue of the complete graph on two nodes is fixed by the single constraint.

3.1 Primal-Dual Formulation and Basic Properties

Let $G = (N, E)$ be a graph with at least one edge. Our starting point is the absolute algebraic connectivity $\hat{a}(G)$ which was introduced by Fiedler. While he proved close connections between $\hat{a}(G)$ and the node and edge connectivity of the graph we recall a less powerful but basic result. An edge weighted graph is connected if and only if the smallest eigenvalue of the weighted Laplacian is simple.
Theorem 3.1 ([25], Theorem 6.1) Let $G = (N, E)$ be a graph and $w_{ij} \geq 0$ $(ij \in E)$ a nonnegative edge weighting. Then $\lambda_2(L_w) \geq 0$, and $\lambda_2(L_w) > 0$ if and only if $G_w = (N, \{ij \in E : w_{ij} > 0\})$ is connected.

Note that in the following we will call $G_w$ the strictly active subgraph (with respect to $w$).

Inspired by Fiedler’s work, Göring et al. considered a generalization of (3.1) by introducing node weights $s \in \mathbb{R}^{|N|}$, $s > 0$ and edge length parameters $l \in \mathbb{R}^{|E|}$, $0 \neq l \geq 0$ (see [40]). With $D := \text{diag}(s_1^{-1/2}, \ldots, s_n^{-1/2})$ the problem reads

$$\max \left\{ \lambda_2(DL_w D) : \sum_{ij \in E} l_{ij}^2 w_{ij} = |E|, \ w_{ij} \geq 0 \ (ij \in E) \right\}.$$  

(3.2)

Using a semidefinite approach, they reformulated (3.2) and got the semidefinite primal program $(P_{\lambda_2})$ listed in Table 3.1.

Thereby the semidefinite constraint

$$DL_w D + \mu D^{-1}1 1^\top D^{-1} \succeq \lambda_2 I,$$

(3.3)

is equivalent to the property that all eigenvalues of $DL_w D + \mu D^{-1}1 1^\top D^{-1}$ are greater or equal to the variable $\lambda_2$. The free variable $\mu$ serves to shift the zero eigenvalue with corresponding eigenvector $D^{-1}1$ of $DL_w D$. As $\lambda_2$ is maximized, optimal $\lambda_2^*$ will be the smallest eigenvalue of $DL_{w^*} D + \mu^* D^{-1}1 1^\top D^{-1}$ or the second smallest of $DL_{w^*} D$, respectively, if an optimal solution $(\lambda_2^*, \mu^*, w^*)$ exists.

| Graph $G = (N, E \neq \emptyset)$, data $s \in \mathbb{R}^{|N|}$, $s > 0$ and proper $l \in \mathbb{R}^{|E|}$. | primal | dual |
|-------------------------------------------------|-------|------|
| $\min \ -\lambda_2$ | $\max \ \xi$ | $\max \ \xi$ |
| s.t. $DL_w D + \mu D^{-1}1 1^\top D^{-1} \succeq \lambda_2 I$, | s.t. $\langle I, X \rangle = 1$, $\langle D^{-1}1 1^\top D^{-1}, X \rangle = 0$, $\langle DE_{ij} D, X \rangle \leq -l_{ij}^2 \xi \ (ij \in E)$, | $\langle I, X \rangle = 1$, $\langle D^{-1}1 1^\top D^{-1}, X \rangle = 0$, $\langle DE_{ij} D, X \rangle \leq -l_{ij}^2 \xi \ (ij \in E)$, |
| $\sum_{ij \in E} l_{ij}^2 w_{ij} = 1$, | $\xi \in \mathbb{R}, X \succeq 0$. | $\xi \in \mathbb{R}, X \succeq 0$. |
| $\lambda_2, \mu \in \mathbb{R}, w \geq 0$. | | $(D_{\lambda_2})$ |

(P$_{\lambda_2}$) 

Table 3.1: A reformulation of (3.2) and the corresponding dual program (cf. [39, 40]).

By the usual Lagrangian approach, the dual program $(D_{\lambda_2})$ of $(P_{\lambda_2})$ is formulated and listed on the right hand side of Table 3.1.

Note that for $l = 0$ the primal feasible set is empty because the equality constraint does not hold. On the other hand we may choose $l$ in such a way that the dual feasible set is
empty. This is the case if the edge length parameters are zero on the edges of a spanning tree of the graph. Then the second equality constraint and the inequality constraints fix a feasible matrix to zero which contradicts the first constraint. In this chapter we want to avoid both cases and choose a proper edge length parameter \( l \), defined via the properties that each spanning tree of the graph has an edge with positive parameter and \( l \neq 0 \). Note that the latter property is important in the case of nonconnected graphs, because then the set of spanning trees is empty.

For properly chosen edge length parameters we are able to partition the graph’s node set in the following way.

**Lemma 3.2** Let \( G = (N, E \neq \emptyset) \) be a graph with given data \( s > 0 \) and proper \( l \). There exists a partition of the node set \( N \) into two nonempty disjoint subsets \( A \) and \( B = N \setminus A \), such that there is no edge \( ij \in E \) with \( i \in A, j \in B \) and \( l_{ij} = 0 \).

**Proof.** If the graph is not connected let \( A \) be a connected component and \( B \) be the remaining nodes. As there is no edge connecting the node sets \( A \) and \( B \) this is a required partition.

If the graph is connected assume for contradiction, that it is not possible to find such a partition. That means that for all partitions \( A, B = N \setminus A \) there is an edge \( ij \in E \) with \( i \in A, j \in B \) and \( l_{ij} = 0 \). Then we find a spanning tree with zero edge length parameters, e.g., by the well known minimum spanning tree algorithm of Prim (cf. [83]). This contradicts the proper choice of \( l \).

For the sake of completeness let us recall and apply the algorithm, which constructs a sequence of trees \( T_k = (N_k, E_k) \) \((k = 1, \ldots, n)\). Then \( T_n \) will be a minimum spanning tree of \( G \), in our case a spanning tree of \( G \) having zero edge length parameters.

Choose \( v_0 \in N \) and set \( T_1 = (N_1, E_1) \) with \( N_1 = \{v_0\} \) and \( E_1 = \emptyset \).

For \( k = 1, \ldots, n-1 \) let \( v_i v_j \in E \) with \( v_i \in N_k, v_j \in N \setminus N_k \) and \( l_{v_i v_j} = 0 \) (this is possible because of the assumption). Set \( T_{k+1} = (N_{k+1}, E_{k+1}) \) with \( N_{k+1} = N_k \cup \{v_j\} \) and \( E_{k+1} = E_k \cup \{v_i v_j\} \).

We prove next that the dual feasible set is not empty in the case of proper edge length parameters.

**Lemma 3.3 (Feasible Dual Solution)** Let \( G = (N, E \neq \emptyset) \) be a graph with given data \( s > 0 \) and proper \( l \). Then the feasible set of \((D_{\lambda_2})\) is not empty.

**Proof.** By Lemma 3.2 we partition the node set \( N \) in two nonempty disjoint subsets \( N_1 \) and \( N_2 = N \setminus N_1 \), such that there is no edge \( ij \) with \( i \in N_1, j \in N_2 \) and \( l_{ij} = 0 \).
3.1. PRIMAL-DUAL FORMULATION AND BASIC PROPERTIES

W.l.o.g. let $N_1 = \{1, \ldots, |N_1|\}$. Let $h \in \mathbb{R}^n$ with $\|h\| = 1$ and put, for parameters $\alpha, \beta \in \mathbb{R}$ to be determined below,

$$u_i = \begin{cases} \sqrt{s_i} \alpha h & \text{if } i \in N_1 \\ \sqrt{s_i} \beta h & \text{if } i \in N_2 \end{cases}, \quad X := [u_1, \ldots, u_n]^\top [u_1, \ldots, u_n] \quad (\alpha, \beta \in \mathbb{R}). \quad (3.4)$$

$X$ is positive semidefinite as it is a Gram matrix. Recall the notation $\bar{s}(N_i)$ on page 24. If $\alpha$ and $\beta$ exist with

$$\langle I, X \rangle = \bar{s}(N_1)\alpha^2 + \bar{s}(N_2)\beta^2 = 1,$$
$$\langle D^{-1}\mathbf{1}\mathbf{1}^\top D^{-1}, X \rangle = (\bar{s}(N_1)\alpha + \bar{s}(N_2)\beta)^2 = 0 \quad (3.5)$$

then we may choose $\xi \leq \min\{-(\alpha - \beta)^2 l_{ij}^2 : ij \in E, i \in N_1, j \in N_2\}$ and $X$ is feasible for $(D_{\lambda_2})$.

The system of equations (3.5) is solvable, because $\bar{s}(N_1), \bar{s}(N_2) > 0$, the first equation describes an ellipse whose center is the origin and the second equation describes just a straight line through the origin.

In order to prove strong duality for $(P_{\lambda_2})$ and $(D_{\lambda_2})$ we observe that for $G = (N, E \neq \emptyset)$ with given data $s > 0$ and proper $l$, $(\hat{\lambda}_2 < 0, \hat{\mu} \geq 0, \hat{w} \geq 0)$ is a strictly feasible primal solution with respect to the semidefinite constraint, whenever $\sum_{ij \in E} l_{ij}^2 \hat{w}_{ij} = 1$.

We are now able to establish strong duality for $(P_{\lambda_2})$ and $(D_{\lambda_2})$. Note that in comparison to [39, 40] we allow some edge length parameters to be zero.

**Proposition 3.4 (Strong Duality, cf. [39, 40])** Let $G = (N, E \neq \emptyset)$ be a graph with given data $s > 0$ and proper $l$. Strong duality holds for $(P_{\lambda_2})$ and $(D_{\lambda_2})$ and the dual program attains its optimal solution. Primal attainment holds if $l > 0$.

**Proof.** Strong duality follows from Corollary 2.15 and the mentioned strictly feasible solutions $(\hat{\lambda}_2, \hat{\mu}, \hat{w})$ of $(P_{\lambda_2})$ with respect to the semidefinite constraint. As both feasible sets are not empty (because of $(\hat{\lambda}_2, \hat{\mu}, \hat{w})$ and Lemma 3.3) the optimal value is finite, thus the dual attains its optimal solution. In the case of $l > 0$ the primal constraint $\sum_{ij \in E} l_{ij}^2 \hat{w}_{ij} = 1$ yields $w_{ij} \leq l_{ij}^{-2} (ij \in E)$. Thus the weights remain in a compact subset which completes the proof.

If an edge parameter equals zero, primal attainment is not guaranteed.

**Example 3.5 (No Primal Attainment, [30])** Let $G = (\{1, 2, 3\}, \{12, 23\})$ be a path with data $s = 1$ and $l_{12} = 0$, $l_{23} = 1$. 
Let \( h \in \mathbb{R}^n \), \( \|h\|^2 = 1 \), \( u_1 = u_2 = h/\sqrt{6} \), \( u_3 = -2h/\sqrt{6} \). Then \( X = [u_1, u_2, u_3]^\top [u_1, u_2, u_3] \), \( \xi = -3/2 \) is an optimal dual solution:

\[
\langle E_{12}, X \rangle = \|u_1 - u_2\|^2 \leq 0 \text{ requires } u_1 = u_2. \text{ The precise values follow from }
\langle I, X \rangle = \|u_1\|^2 + \|u_2\|^2 + \|u_3\|^2 = 1 \text{ and } \langle 11^\top, X \rangle = \|u_1 + u_2 + u_3\|^2 = 0.
\]

Finally \( \xi \) follows from \( \langle E_{23}, X \rangle = \|u_2 - u_3\|^2 = 3/2 \leq -\xi \). \( X \) is positive semidefinite as it is the Gram matrix of \( u_i \) \((i = 1, 2, 3)\).

Assume, for contradiction, that there exists an optimal primal solution \((\lambda^*_2, \mu^*, w^*)\). As strong duality holds, \( \lambda^*_2 = 3/2 \). Furthermore \( w^*_{23} = 1 \). Then the semidefinite constraint reads

\[
\begin{pmatrix}
  w^*_{12} + \mu^* - \frac{3}{2} & \mu^* - w^*_{12} & \mu^* \\
  \mu^* - w^*_{12} & w^*_{12} + \mu^* - \frac{3}{2} & \mu^* \\
  \mu^* & \mu^* & \mu^* - \frac{3}{2}
\end{pmatrix} \succeq 0.
\]

The determinant equals \(-\frac{9}{2} \mu^* + \frac{9}{2} \) \((w^*_{12} \text{ cancels out})\) and has to be greater or equal to zero, thus \( \mu^* \leq \frac{1}{2} \). Also the main diagonal has to be greater or equal to zero, thus \( \mu^* \geq \frac{1}{2} \) and \( \mu^* = \frac{1}{2} \) follows. Hence the semidefinite constraint does not hold as the third main diagonal element equals zero but the corresponding column and row are not equal to zero. (Alternatively, evaluating the eigenvalues in dependence of \( w^*_{12} \), one eigenvalue proves to be negative.) This contradicts the existence of an optimal primal solution.

In the previous lemma and example we already used a Gram representation of the dual matrix to get a more illustrative representation of the dual program as a graph realization problem. Let us deduce this interpretation in general from the dual program.

As \( DXD \) is symmetric, there exists a Gram representation \( DXD = U^\top U \) in which we denote the \( i \)-th column of \( U \) by \( u_i \in \mathbb{R}^n \) \((i \in N)\). Using \([DXD]_{ij} = u_i^\top u_j\) we obtain with

\[
\langle I, X \rangle = \sum_{i \in N} s_i \|u_i\|^2,
\]

\[
\langle D^{-1}11^\top D^{-1}, X \rangle = \left\| \sum_{i \in N} s_i u_i \right\|^2
\]

and

\[
\langle DE_{ij}D, X \rangle = \|u_i - u_j\|^2
\]
a graph realization (embedding) formulation of \((D_{\lambda_2})\)

\[
\begin{align*}
\text{maximize} & \quad \xi \\
\text{subject to} & \quad \sum_{i \in N} s_i \|u_i\|^2 = 1, \\
& \quad \sum_{i \in N} s_i u_i = 0, \\
& \quad \|u_i - u_j\|^2 \leq -l^2_{ij} \xi \quad (ij \in E), \\
& \quad \xi \in \mathbb{R}, \quad u_i \in \mathbb{R}^n \quad (i \in N).
\end{align*}
\]
So we search for a realization of the graph in $\mathbb{R}^n$ such that the weighted barycenter is in the origin, the largest scaled edge is as short as possible (we call this the *distance constraints*) but the sum of the weighted squared norms equals one (the *normalization constraint*), i.e., not all nodes can be embedded in the origin.

Note, that a zero edge length parameter forces the corresponding adjacent nodes to lie on the same point, i.e., the edge has zero length.

For an illustration of the primal and the graph realization problem we consider the following example.

**Example 3.6** Let $G$ be the graph of Figure 3.1, having all node and edge parameters equal to one. It was generated by randomly choosing thirty nodes in $[0,1]^2$ and by adding an edge if the Euclidean distance of two nodes is at most 0.3.

![Figure 3.1](image)

*Figure 3.1:* The graph corresponding to Example 3.6 with parameters $s = 1$ and $l = 1$: 30 randomly chosen nodes in $[0,1]^2$, two nodes are adjacent if the Euclidean distance is at most 0.3.

The optimal weighted graph is illustrated on the left hand side of Figure 3.2. Thereby the weights are given by gray shades, i.e., white corresponds to weight 0 and black to the maximum weight. The right hand side of Figure 3.2 presents an optimal two-dimensional realization, which is computed using SeDuMi [88]. The red circle displays the origin. For a better understanding of the relation of the primal solution to the graph realization the edges are again weighted. So effectively we see an optimal graph realization of the strictly active subgraph (cf. page 37) because zero weighted edges are colored white, thus they are not visible (e.g. edge $\{8,11\}$).
Figure 3.2: Optimal edge weighted graph of the graph of Figure 3.1 and a corresponding optimal 2-dimensional realization for \((P_{\lambda_2})\) and \((E_{\lambda_2})\), respectively (cf. Example 3.6).

Göring et al. observed a relation between optimal realizations and the eigenspace of the maximum second smallest eigenvalue.

**Proposition 3.7 (cf. [39, 40])** Given a graph \(G = (N,E \neq \emptyset)\) with data \(s > 0\) and proper \(l\). Let \(U\) be an optimal realization of \((E_{\lambda_2})\) and suppose there is an optimal solution \((\lambda_2,w)\) for \((P_{\lambda_2})\). For any \(h \in \mathbb{R}^n\) the scaled projection \(D^{-1}U^\top h\) onto the one-dimensional subspace spanned by \(h\) yields an eigenvector to \(\lambda_2(DL_wD)\), unless it is the zero vector.

Proposition 3.7 is illustrated in Figure 3.3. The optimal realization of Figure 3.2 is mapped onto a one-dimensional subspace (the blue line). The distances of the mapped nodes (the green dots on the line) to the origin are the absolute values of the corresponding eigenvector’s components.

In the following we want to investigate graphs with optimal value zero. Note that, as \(D\) is nonsingular, \(\lambda_2(DL_wD) \geq 0\) for all feasible edge weights \(w\). Furthermore \(\lambda_2(DL_wD) > 0\) if and only if \(\lambda_2(L_w) > 0\) which is equivalent to the strictly active subgraph \(G_w\) being connected.

So let \(G\) be a connected graph with given proper edge length parameter \(l\). The feasible edge weights \(w = (\sum_{ij \in E} l_{ij}^2)^{-1}1\) keep the weighted graph connected, thus \(\lambda_2(L_w) > 0\). Because \((P_{\lambda_2})\) maximizes the second smallest eigenvalue the optimal value is strictly positive.

In the case of a nonconnected graph the optimal value is zero, optimal realizations have special structure and there exists a one-dimensional optimal realization:
Proposition 3.8 Let \( G = (N, E \neq \emptyset) \) be a nonconnected graph with given data \( s > 0 \) and proper \( l \). Each edge \( ij \in E \) has zero length in an optimal realization \( U = [u_1, \ldots, u_n] \) of \( (E_{\lambda_2}) \), i.e., \( u_i = u_j \) for \( ij \in E \). In addition there exists an optimal one-dimensional realization.

Proof. The dual optimal value \( \xi = 0 \) follows from optimal \( \lambda_2 = 0 \) because the graph is not connected and strong duality holds. Thus, the distance constraints require \( u_i = u_j \) \((ij \in E)\) for all optimal realizations.

An optimal one-dimensional realization may be constructed as follows. Let \( N_1 \subset N \) be the node set of a connected component of the graph, \( N_2 = N \setminus N_1 \) and \( h \in \mathbb{R}^n \) with \( \|h\| = 1 \). In order to satisfy \( u_i = u_j \) \((ij \in E)\) we choose \( \alpha, \beta \in \mathbb{R} \) and put \( u_i = \alpha h \) for \( i \in N_1 \), \( u_i = \beta h \) otherwise. The two remaining constraints of \( (E_{\lambda_2}) \) lead to the system of equations

\[
\bar{s}(N_1)\alpha^2 + \bar{s}(N_2)\beta^2 = 1,
\]

\[
(\bar{s}(N_1)\alpha + \bar{s}(N_2)\beta)^2 = 0
\]

which is solvable giving \( \alpha \) and \( \beta \) (cf. the proof of Lemma 3.3).

3.2 A Scaled Primal-Dual Pair

In fact, in [39, 40] Göring et al. considered slightly different problems than \( (P_{\lambda_2}), (D_{\lambda_2}) \) and \( (E_{\lambda_2}) \). If we disregard nonconnected graphs, the optimal value of \( (P_{\lambda_2}) \) is greater than
zero. So by dividing all constraints by the optimal value of \((P_{\lambda_2})\) and by replacing the objective function by the scaled equality constraint we get a scaled primal program having fewer variables. By the same procedure or alternatively by duality theory we get a dual program and an embedding formulation. The programs are listed in Table 3.2.

<table>
<thead>
<tr>
<th>primal</th>
<th>dual</th>
</tr>
</thead>
<tbody>
<tr>
<td>min ( \sum_{ij \in E} l_{ij}^2 \hat{w}_{ij} )</td>
<td>max ( \langle I, \hat{X} \rangle )</td>
</tr>
<tr>
<td>s.t. ( DL_{\hat{w}} D + \hat{\mu} D^{-1} 11^\top D^{-1} \geq I, ) ( \hat{\mu} \in \mathbb{R}, \hat{w} \geq 0. )</td>
<td>s.t. ( \langle D^{-1} 11^\top D^{-1}, \hat{X} \rangle = 0, ) ( \langle DE_{ij} D, \hat{X} \rangle \leq l_{ij}^2 ) ( (ij \in E), ) ( \hat{X} \succeq 0 )</td>
</tr>
</tbody>
</table>

Table 3.2: Scaled versions of \((P_{\lambda_2}), (D_{\lambda_2})\) and \((E_{\lambda_2})\) for a connected graph \(G\) (see [39, 40]).

Note that now the optimal values coincide independently of whether \(l\) is proper or not. If there is a spanning tree, having all edge length parameters equal to zero, the optimal value equals zero.

As \((P_{\lambda_2}-s)\) has strictly feasible solutions (use sufficiently large \(\hat{w}\) and \(\hat{\mu}\)) strong duality also hold for \((P_{\lambda_2}-s)\) and \((D_{\lambda_2}-s)\) (cf. [40], Observation 3.2). The primal solution, however, need not to be attained if there is an edge length parameter equal to zero.

The next proposition states the connection of the scaled programs to the corresponding unscaled ones.

**Proposition 3.9 (cf. [39, 40])** Let \(G = (N, E \neq \emptyset)\) be a connected graph with given data \(s > 0\) and proper \(l\). There exist transformations, that map optimal solutions of \((D_{\lambda_2})\) and \((E_{\lambda_2})\) to optimal solutions of \((D_{\lambda_2}-s)\) and \((E_{\lambda_2}-s)\) for the same data \(s\) and \(l\), and vice versa. In the case of primal attainment the same holds for \((P_{\lambda_2})\) and \((P_{\lambda_2}-s)\). In addition the strictly active subgraphs are the same.
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Proof. As the graph is connected and the edge weight parameters are proper, the optimal values of the programs are not equal to zero. The transformations are listed in Table 3.3. Feasibility follows by direct calculation and optimality by strong duality.

<table>
<thead>
<tr>
<th>Optimal solutions</th>
<th>⇒</th>
<th>⇐</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda_2^<em>, \mu^</em>, w^* ) of ( (P_{\lambda_2}) ), ( \xi^<em>, X^</em> ) of ( (D_{\lambda_2}) ) and ( \xi^<em>, [u_1^</em>, \ldots, u_n^<em>] ) of ( (E_{\lambda_2}) ), ( \hat{\mu}^</em>, \hat{w}^* ) of ( (P_{\lambda_2-s}) ), ( \hat{X}^* ) of ( (D_{\lambda_2-s}) ) and ( [\hat{u}<em>1^<em>, \ldots, \hat{u}_n^</em>] ) of ( (E</em>{\lambda_2-s}) ).</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \lambda_2 = \frac{1}{\sum_{ij \in E} \hat{w}<em>{ij}^<em>}, \mu = \frac{\hat{\mu}^</em>}{\sum</em>{ij \in E} \hat{w}_{ij}^*} )</td>
<td></td>
<td>( \hat{\mu}^* = \mu^<em>, \lambda_2^</em> = \frac{1}{\sum_{ij \in E} w_{ij}^*} )</td>
</tr>
<tr>
<td>( \hat{w}<em>{ij} = \frac{w</em>{ij}^<em>}{\lambda_2^</em>} ) ((ij \in E))</td>
<td>( w_{ij} = \frac{\hat{w}<em>{ij}^*}{\sum</em>{ij \in E} \hat{w}_{ij}^*} ) ((ij \in E))</td>
<td></td>
</tr>
<tr>
<td>( \hat{X} = \frac{1}{\xi^<em>} X^</em> )</td>
<td></td>
<td>( \xi = \frac{1}{\langle I, X^* \rangle}, X = \frac{1}{\langle I, X^* \rangle} \hat{X}^* )</td>
</tr>
<tr>
<td>( \hat{u}_i = \frac{1}{\sqrt{\xi^<em>}} u_i^</em> ) ((i \in N))</td>
<td></td>
<td>( \xi = \frac{1}{\sum_{i \in N} s_i |u_i^<em>|^2}, u_i = \frac{1}{\sum_{i \in N} s_i |u_i^</em>|^2} \hat{u}_i^* ) ((ij \in E))</td>
</tr>
</tbody>
</table>

Table 3.3: Transformations for optimal solutions of \( (P_{\lambda_2}) \), \( (D_{\lambda_2}) \) and \( (E_{\lambda_2}) \) on \( (P_{\lambda_2-s}) \), \( (D_{\lambda_2-s}) \) and \( (E_{\lambda_2-s}) \) and vice versa (cf. the steps of transformations in [39, 40]).

We observe, that by the transformations of Proposition 3.9 a primal optimal solution of \( (P_{\lambda_2}) \) is attained if and only if a primal optimal solution of \( (P_{\lambda_2-s}) \) is attained.

At the end of this section we want to refer to [89]. Sun et al. considered a similar problem to \( (P_{\lambda_2-s}) \) in the context of Markov processes and interpreted optimal edge weights as optimal transition rates that maximize the mixing process. In addition they get similar dual graph realization programs to \( (D_{\lambda_2-s}) \) and \( (E_{\lambda_2-s}) \) and related the latter one to a maximum variance unfolding problem.

3.3 Structural Properties

As mentioned, considerations were made about the spectrum of the Laplacian, e. g., to get a better insight into connections to graph properties, concerning the connectivity of the graph. In particular, Göring et al. proved the following important result about optimal realizations and the separator structure of the graph. While the Separator-Shadow Theorem in [40] was formulated for data \( l > 0 \) their proof also works for the following theorem.
Theorem 3.10 (Separator-Shadow) Given optimal $u_i \in \mathbb{R}^n$ ($i \in N$) of $(E_{\lambda_2^{-}}s)$ for a connected graph $G = (N, E \neq \emptyset)$ with node weights $s > 0$ and edge length parameter $0 \neq l \geq 0$, let $S$ be a separator in $G$ giving rise to a partition $N = S \cup C_1 \cup C_2$ where there is no edge in $E$ between $C_1$ and $C_2$. For at least one $C_j$ with $j \in \{1, 2\}$

$$\text{conv}\{0, u_i\} \cap \text{conv}\{u_s : s \in S\} \neq \emptyset \quad \forall i \in C_j.$$ 

In words, the straight line segments $\text{conv}\{0, u_i\}$ of all nodes $i \in C_j$ intersect the convex hull of the points in $S$.

If there are optimal $w_{ij}$ ($ij \in E$) of $(P_{\lambda_2^{-}}s)$ the same holds for separators $S$ in the strictly active subgraph $G_w = (N, E_w)$.

Proposition 3.9 ensures the following similar result for the unscaled programs.

Corollary 3.11 Let $G = (N, E \neq \emptyset)$ be a connected graph with given data $s > 0$ and proper $l$. The Separator-Shadow Theorem also holds for optimal solutions of $(E_{\lambda_2})$ and if a primal optimal solution $w$ exists then also for $G_w$.

Theorem 3.10 and the previous corollary say, that considering the origin as a light source, like the sun, and the convex hull of the separator as a solid object, like a wall, then in an optimal realization all but one of the components must be embedded in the shadow of the separator. Thus Theorem 3.10 and Corollary 3.11 characterize an unfolding property of optimal realizations of $(E_{\lambda_2^{-}}s)$ and $(E_{\lambda_2})$, respectively.

One may check the separator property on the optimal realization, given in Figure 3.2, of the graph of Figure 3.1. For example, node 11 separates the graph into two components and the node set $\{8, 23, 27, 29\}$ leads to three components, respectively. Figure 3.4 illustrates both situations. The dotted lines are the bounds of the shadow. In both cases only the orange marked component lies not in the shadow of the separator.

A second important aspect is the existence of low dimensional optimal realizations, thus optimal matrices of $(D_{\lambda_2})$ having low rank. It is related to the matrix rank minimization problem, i.e., finding a matrix of minimal rank within a convex set of matrices. Various of its applications and corresponding references can be found in [21, 79].

Göring et al. introduced the rotational dimension of a graph $G$ which is the maximal minimum dimension of an optimal graph realization under all possible node and edge parameters.

Definition 3.12 For a connected graph $G = (N, E \neq \emptyset)$, the rotational dimension of $G$ with respect to node weights $s \in \mathbb{R}^{|N|}$ and edge length parameters $l \in \mathbb{R}^{|E|}$ is

$$\text{rotdim}_G(s, l) := \min\{\dim \text{span}\{v_i, i \in N\} : v_i, i \in N, \text{ is an optimal solution of } (E_{\lambda_2^{-}}s)\}$$
3.3. STRUCTURAL PROPERTIES

\[ \begin{align*}
\text{rotdim}(G) &:= \max\{ \text{rotdim}_G(s, l) : s \in \mathbb{N}_0, l \in \mathbb{N}_0 \}.
\end{align*} \]

For a graph \( G \) consisting of several connected components the rotational dimension of \( G \) is
\[ \text{rotdim}(G) := \max\{ \text{rotdim}(C) : C \text{ is a connected component of } G \} \]

A graph \( G \) is called \( d \)-embeddable if \( \text{rotdim}(G) \leq d \).

There are some similarities of the rotational dimension of a graph to the Colin de Verdière number (see [91]). So, e.g., both can be shown to be minor monotone.

**Theorem 3.13** ([40], Theorem 1.2) \textit{The rotational dimension is a minor monotone graph parameter and \( d \)-embeddability is a minor monotone graph property.}

The tree-width of a graph gives rise to a bound on the minimal dimension of optimal realizations of \((E_{\lambda_2} \cdot s)\), thus on the rotational dimension of the graph.

**Theorem 3.14** (Tree-Width Bound, [40], Theorem 1.5) \textit{Let } \( G = (N, E \neq \emptyset) \text{ be a connected graph and } s > 0 \text{ and } 0 \neq l \geq 0 \text{ be given data. There exists an optimal realization of } (E_{\lambda_2} \cdot s) \text{ of dimension at most the tree-width of } G \text{ plus one.}
Corollary 3.15 Let $G = (N, E \neq \emptyset)$ be a connected graph with given data $s > 0$ and proper $l$. The tree-width bound, Theorem 3.14 also holds for $(E_{\lambda_2})$.

Considering the graph of Figure 3.1 we notice that its tree-width is at least 5, because the induced subgraph of the nodes $\{1, 7, 9, 13, 14, 30\}$ is complete. By the two-dimensional optimal realization of Figure 3.2 we observe, that in this case the tree-width bound is not tight. However, Göring et al. specify a class of graphs with tight dimension bound, see therefore Example 8 in [39].

The symmetry of the input data in SDP and resulting special solutions are of great interest as, e. g., the problem size may be reduced [2, 19]. Therefore we consider graphs and graph automorphisms in conjunction with special optimal solutions for $(P_{\lambda_2})$.

Fiedler already showed that there exists an optimal solution of (3.1) which is invariant under the group action.

Proposition 3.16 ([25], Lemma 6.7) Let $G$ be a graph. There exists an optimal edge weighting of (3.1) for which edges of the same orbit under the action of the automorphism group $\text{Aut}(G)$ have the same value.

We may extend the previous proposition to the parametrized primal problem $(P_{\lambda_2})$ by using the generalized automorphism group $\text{Aut}(G, s, l)$. For the sake of completeness we add a proof which follows that of Fiedler’s result.

Proposition 3.17 Let $G$ be a graph with given data $s > 0$ and proper $l$. If primal attainment holds, there exists an optimal edge weighting of $(P_{\lambda_2})$ for which edges of the same orbit under the action of the automorphism group $\text{Aut}(G, s, l)$ have the same value.

Proof. Let $\lambda_2$, $w_{ij}$ ($ij \in E$) be optimal for $(P_{\lambda_2})$ and let $E_1, \ldots, E_k$ be the orbits of the edge set $E$ under the action of the automorphism group $\text{Aut}(G, s, l)$. Because an automorphism $\varphi \in \text{Aut}(G, s, l)$ does not change the graph’s structure, $\lambda_2$ and $w_{\varphi(ij)}$ ($ij \in E$) is also optimal for $(P_{\lambda_2})$.

Using Lemma 2.18 define new weights $\hat{w}_{ij}$ for $ij \in E_r$ ($r \in \{1, \ldots, k\}$) via

$$|\text{Aut}(G, s, l)|\hat{w}_{ij} = \sum_\varphi w_{\varphi(ij)} = \sum_{xy \in E} \sum_{\varphi(ij) = xy} w_{\varphi(ij)} = \sum_{xy \in E_r} \sum_{\varphi(ij) = xy} w_{xy} = a_r \cdot \sum_{xy \in E_r} w_{xy}. \quad (3.6)$$

Because this is a convex combination of optimal solutions, it is optimal, too.

For edge transitive graphs and a special choice of data, like the cube graph of Figure 3.5 with $s = 1$ and $l = 1$, we get the following corollaries. The first one says, that there is an optimal primal solution with the same weight on each edge. The second interprets each optimal realization as a map of eigenvectors of the second smallest eigenvalue of the Laplacian of the graph.
Corollary 3.18 (Edge Transitive Graphs) Let $G = (N, E \neq \emptyset)$ be an edge transitive graph and $s = c_s \mathbf{1}$, $l = c_l \mathbf{1}$ with real $c_s, c_l > 0$ be given data. There is an optimal solution of $(P_{\lambda_2})$ with edge weights $w_{ij} = (|E| c_t^2)^{-1}$ ($ij \in E$).

Figure 3.5: A cube graph with data $s = 1$ and $l = 1$ and an optimal 3-dimensional realization for $(E_{\lambda_2})$. As the graph is edge transitive there is an optimal primal solution with equal weight for all edges (cf. Corollary 3.18).

Corollary 3.19 Let $G = (N, E \neq \emptyset)$ be an edge transitive graph, $s = c_s \mathbf{1}$, $l = c_l \mathbf{1}$ with real $c_s, c_l > 0$ be given data and $U$ an optimal realization of $(E_{\lambda_2})$. For $h \in \mathbb{R}^n$ the vector $U^\top h$ is an eigenvector of $\lambda_2(L(G))$, unless it is the zero vector.

Proof. We use the special primal solution of the previous corollary, i.e., $\lambda_2$ and $w_{ij} = (|E| c_t^2)^{-1}$ ($ij \in E$). Because of Proposition 3.7 and $D = c_s^{-1/2} I$ we get

$$0 = (\lambda_2 I - DLwD) D^{-1} U^\top h = \sqrt{c_s} \left( \lambda_2 I - \frac{1}{c_s} \cdot \frac{1}{|E| c_t^2} L \right) U^\top h$$

$$= \frac{1}{|E| c_t^2 \sqrt{c_s}} (|E| c_t^2 c_s \lambda_2 I - L) U^\top h.$$

Thus $\lambda_2(L(G)) = c_s c_t^2 |E| \lambda_2$ with eigenvector $U^\top h$. □

Complete graphs have in some sense a high measure of symmetry. They are edge as well as node transitive graphs. An optimal realization of $(E_{\lambda_2})$ of a complete graph with data $s = 1$ and $l = 1$ is characterized in [39]. To complete and close this section we finally want to extend the result for arbitrary data $s$ and $l = c_l \mathbf{1}$ with real $c_l > 0$. 
Example 3.20 (Complete Graph) An optimal realization of \((E_{\lambda_2}-s)\) of the complete graph \(K_n\) with data \(s > 0\) and \(l = c_1\), for real \(c_1 > 0\), is a regular \((n-1)\)-dimensional simplex: the barycenter of an optimal realization must be in the origin, thus \(\bar{u}(N) = 0\). Employing Lemma 2.10 we rewrite the sum of the weighted squared norms and bound it via the edge length constraints,

\[
\sum_{i \in N} s_i \|u_i\|^2 = \frac{1}{2s(N)} \sum_{i,j \in N} s_i s_j \|u_i - u_j\|^2 \leq \frac{c_i^2}{2s(N)} \sum_{i,j \in N} s_i s_j = \frac{c_i^2}{2s(N)} (s(N)^2 - \|s\|^2).
\]

Equality holds if and only if \(\|u_i - u_j\|^2 = c_i^2\) for all \(ij \in E\).

Because of Proposition 3.9 an optimal realization of \((E_{\lambda_2})\) has the same structure.

3.4 Variable Edge Length Parameters

In this section we want to investigate the eigenspace of the second smallest eigenvalue of a connected graph in more detail. Proposition 3.7 states that optimal realizations of \((E_{\lambda_2})\) may be seen as maps of eigenvectors to the second smallest eigenvalue of the optimal weighted Laplacian. For edge transitive graphs with special parameters it turned out in Corollary 3.19 that they are even maps of eigenvectors of the (unweighted) Laplacian itself. That is, optimal realizations are maps of Fiedler vectors.

So we may ask whether there is a formulation of a graph realization problem such that optimal realizations may be seen as maps of eigenvectors to the second smallest eigenvalue of the Laplacian itself for arbitrary graphs. On the other hand we may ask for optimal edge parameters that maximize the spread of a graph realization.

The answer to both questions proves to be the following. Let \(G = (N, E \neq \emptyset)\) be a connected graph. We consider the scaled program \((E_{\lambda_2}-s)\) with \(s = 1\) and interchange the squared edge length parameters \(l_{ij}^2\) for distance variables \(d_{ij} \in \mathbb{R} (ij \in E)\). As otherwise the optimal value is unbounded we need an additional normalization constraint, say \(\sum_{ij \in E} d_{ij} \leq 1\). This results in the following graph realization formulation

\[
\begin{align*}
\text{maximize} & \quad \sum_{i \in N} \|u_i\|^2 \\
\text{subject to} & \quad \sum_{i \in N} u_i = 0, \\
& \quad \sum_{ij \in E} d_{ij} \leq 1, \\
& \quad \|u_i - u_j\|^2 \leq d_{ij} (ij \in E), \\
& \quad d_{ij} \in \mathbb{R} (ij \in E), \\
& \quad u_i \in \mathbb{R}^n (i \in N).
\end{align*}
\]
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Figure 3.6: A one-dimensional optimal realization of the graph of Figure 3.1 for \((E_{\lambda_2,l})\).

Considering the graph of Figure 3.1, an optimal one-dimensional realization for \((E_{\lambda_2,l})\) is illustrated in Figure 3.6. The order of the nodes is given below the realization of the graph.

Setting \(X = U^\top U\) in \((E_{\lambda_2})\) as before, the corresponding semidefinite problem reads

\[
\begin{align*}
\text{maximize} & \quad \langle I, X \rangle \\
\text{subject to} & \quad \langle 11^\top, X \rangle = 0, \\
& \quad \sum_{i,j \in E} d_{ij} \leq 1, \\
& \quad \langle E_{ij}, X \rangle \leq d_{ij} \quad (ij \in E), \\
& \quad d_{ij} \in \mathbb{R} \quad (ij \in E), \\
& \quad X \succeq 0.
\end{align*}
\]

\((D_{\lambda_2,l})\)

As \(X = 0\) and \(d = 0\) is feasible for \((D_{\lambda_2,l})\) the feasible set is not empty.

The semidefinite dual of \((D_{\lambda_2})\) reads

\[
\begin{align*}
\text{minimize} & \quad \rho \\
\text{subject to} & \quad \sum_{i,j \in E} w_{ij} E_{ij} + \mu 11^\top \succeq I, \\
& \quad \rho - w_{ij} = 0 \quad (ij \in E), \\
& \quad w \geq 0, \rho \geq 0, \mu \in \mathbb{R}.
\end{align*}
\]

\((P_{\lambda_2,l})\)

Note that the feasible set of \((P_{\lambda_2,l})\) is equivalent to

\[\{(w = \rho 1, \rho, \mu) : \rho L + \mu 11^\top \succeq I, \rho \geq 0, \mu \in \mathbb{R}\}.
\]
Thus all edges have the same weight which is equal to the objective value.

Furthermore \( \tilde{w} = \tilde{\rho} \mathbf{1}, \tilde{\rho} > \lambda_2(L(G))^{-1} \) and \( \tilde{\mu} = 1 \) are strictly feasible solutions of \((P_{\lambda_2})\) with respect to the semidefinite constraint: eigenvectors of \( L(G) \) are also eigenvectors of \( \tilde{\rho} L + \mathbf{1}\mathbf{1}^\top - I \). Calculating the corresponding eigenvalues yields the claim.

Now we are able to establish strong duality.

**Proposition 3.21 (Strong Duality)** Let \( G = (N, E \neq \emptyset) \) be a connected graph. Strong duality holds for \((P_{\lambda_2})\) and \((D_{\lambda_2})\) and both programs attain their optimal solution.

**Proof.** Strong duality follows from Corollary 2.15 and the mentioned strictly feasible solutions \((\tilde{w}, \tilde{\rho}, \tilde{\mu})\) of \((P_{\lambda_2})\) with respect to the semidefinite constraint. As both feasible sets are not empty the optimal value is finite, thus the dual attains its optimal solution. Because \( w_{ij} = \rho \) for \( ij \in E \), optimal edge weights remain in a compact set, thus the primal solution is attained, as well.

Observe that the optimal value of \((P_{\lambda_2})\) is strictly greater than zero because otherwise \( w = 0 \) and \( \mu \mathbf{1}\mathbf{1}^\top \not\preceq I \) for all \( \mu \in \mathbb{R} \). Due to \( w = \rho \mathbf{1} \) in an optimal solution all edge weights are strictly positive. Thus complementarity requires \( \|u_i - u_j\|^2 = d_{ij} \) for \( ij \in E \) for optimal graph realizations and corresponding distance variables.

Our next result gives the answer to the above question. Indeed, the optimal value of \((E_{\lambda_2})\) is the reciprocal of \( \lambda_2(L(G)) \) and optimal realizations may be interpreted as maps of eigenvectors to \( \lambda_2(L(G)) \).

**Theorem 3.22** Given a connected graph \( G = (N, E \neq \emptyset) \), let \( U = [u_1, \ldots, u_n] \) be an optimal solution of \((E_{\lambda_2})\). Then

\[
\sum_{i \in N} \|u_i\|^2 = \frac{1}{\lambda_2(L(G))}
\]

and for \( h \in \mathbb{R}^n \) the vector \( U^\top h \) is an eigenvector of \( \lambda_2(L(G)) \), unless it is the zero vector.

The proof follows that of Proposition 3.7.

**Proof.** Because of strong duality \( \sum_{i \in N} \|u_i\|^2 = \rho \) for optimal primal and dual solutions. The semidefinite constraint of \((P_{\lambda_2})\) then equals \( L - \frac{\rho}{\tilde{\rho}} \mathbf{1}\mathbf{1}^\top - \frac{1}{\tilde{\rho}} I \succeq 0 \), thus \( \rho = \sum_{i \in N} \|u_i\|^2 = \frac{1}{\lambda_2(L)} \) (see the comments about the semidefinite constraint (3.3) on page 37).
3.4. VARIABLE EDGE LENGTH PARAMETERS

By semidefinite complementarity and an eigenvalue decomposition \( P\Omega P^\top \) of \( L - \frac{\mu}{\rho} 11^\top - \frac{1}{\rho} I \) with eigenvalues \( \omega_i \geq 0 \) \((i = 1, \ldots, n)\) we obtain

\[
0 = \left\langle U^\top U, L - \frac{\mu}{\rho} 11^\top - \frac{1}{\rho} I \right\rangle = \left\langle U^\top U, P\Omega P^\top \right\rangle = \left\langle I, UP\Omega P^\top U^\top \right\rangle = \sum_{i=1}^{n} \omega_i (Up_i)^\top Up_i,
\]

thus either \( \omega_i = 0 \) or \( Up_i = 0 \) for \( i \in N \). Because of \( \langle 11^\top, U^\top U \rangle = 0 \) it follows that

\[
\left( L - \frac{1}{\rho} I \right) U^\top = P\Omega(UP)^\top = P[\omega_1 Up_1, \ldots, \omega_n Up_n] = 0
\]

which proves, that the columns of \( U^\top \) are contained in the eigenspace of \( \lambda_2(L) = \frac{1}{\rho} \).

Theorem 3.22 states, that a projection onto a one-dimensional subspace yields eigenvectors to \( \lambda_2(L(G)) \). For the graph of Example 3.6 it is illustrated in Figure 3.7. The green dots are the maps of the graph’s nodes onto the blue marked subspace. The distances of the mapped nodes to the origin are the absolute values of the corresponding eigenvector’s components.

![Figure 3.7: Projection of an optimal realization of the graph of Example 3.6 for \((E_{\lambda_2} - l)\) onto a one-dimensional subspace.](image)

Conversely, each eigenvector to \( \lambda_2(L(G)) \) gives rise to an optimal solution of \( (E_{\lambda_2} - l) \), as we show next.

**Theorem 3.23** Given a connected graph \( G = (N, E \neq \emptyset) \), let \( u \in \mathbb{R}^n, \|u\| = 1 \), be an eigenvector to \( \lambda_2(L(G)) \). An optimal solution of \( (D_{\lambda_2} - l) \) is

\[
X = \frac{1}{\lambda_2(L(G))} uu^\top \text{ and } d_{ij} = \frac{1}{\lambda_2(L(G))} ([u]_i - [u]_j)^2 \text{ for } ij \in E.
\]
Proof. To check feasibility, observe that \( u \) is orthogonal to the eigenvector \( \mathbf{1} \) of \( \lambda_1(L) = 0 \), so \( \langle \mathbf{1}^\top, X \rangle = 0 \).

For \( ij \in E \),
\[
\langle E_{ij}, X \rangle = \frac{1}{\lambda_2(L)} u^\top E_{ij} u = \frac{1}{\lambda_2(L)} ([u]_i - [u]_j)^2 = d_{ij},
\]
thus \( \sum_{ij \in E} d_{ij} = \frac{1}{\lambda_2(L)} u^\top Lu = 1 \). As \( \langle I, X \rangle = \frac{1}{\lambda_2(L)} \), optimality follows from Theorem 3.22.

The two theorems together assert that an optimal solution of maximum rank to \((D_{\lambda_2^{-1}})\) (as delivered, e.g., by interior point methods) gives a geometric view of the entire eigenspace of \( \lambda_2(L(G)) \). Indeed, suppose the columns of \( \hat{U} \in \mathbb{R}^{n \times k} \) with \( \hat{U}^\top \hat{U} = I \in \mathbb{R}^{k \times k} \) span the eigenspace to \( \lambda_2(L(G)) \), then the convex combination
\[
X = \frac{1}{k\lambda_2(L(G))} \hat{U} \hat{U}^\top \text{ with } d_{ij} = \langle E_{ij}, X \rangle \text{ for } ij \in E
\]
is a corresponding maximum rank solution of \((D_{\lambda_2^{-1}})\) and its \( k \)-dimensional realization \((E_{\lambda_2^{-1}})\) is given by the columns of
\[
U = \frac{1}{\sqrt{k\lambda_2(L(G))}} \hat{U}^\top.
\]

Theorems 3.22 and 3.23 and the previous considerations prove the following corollary.

**Corollary 3.24** Let \( G = (N, E \neq \emptyset) \) be a connected graph, with \( \lambda_2(L(G)) \) having multiplicity one. Then all optimal solutions of \((E_{\lambda_2^{-1}})\) are rank one (i.e., an optimal graph realization is one-dimensional).

Observe, that the example graph of Figure 3.1 has a simple second smallest Laplacian eigenvalue, thus an optimal realization of \((E_{\lambda_2^{-1}})\) has to be one-dimensional, cf. Figure 3.6.

The second smallest eigenvalue of the cube graph of Figure 3.5 has multiplicity three. Figure 3.8 illustrates a one-, a two- and a three dimensional optimal realization for \((E_{\lambda_2^{-1}})\).
3.4. VARIABLE EDGE LENGTH PARAMETERS

Figure 3.8: A one-, a two- and a three-dimensional optimal realization of the cube graph for \((E_{\lambda^2-1})\).
Chapter 4

Minimizing the Maximum Eigenvalue

So far we have elaborated relations between structural graph properties and eigenvectors to the maximal second smallest eigenvalue of the weighted Laplacian using a semidefinite approach. We may proceed in an analogous manner with the maximum eigenvalue and consider the problem

$$\min \left\{ \lambda_{\text{max}}(D L_w D) : \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \ w_{ij} \geq 0 \ (ij \in E) \right\}$$

(4.1)

for a graph \( G = (N, E \neq \emptyset) \) with node weights \( s \in \mathbb{R}^{|N|}, s > 0 \) and edge length parameters \( l \in \mathbb{R}^{|E|}, 0 \neq l \geq 0 \). We put again \( D := \text{diag}(s_1^{-1/2}, \ldots, s_n^{-1/2}) \).

Note that already Fiedler considered a slightly different version of (4.1) for \( s = 1 \) and \( l = 1 \) in [27]. The difference to (4.1) is that the edge weights have to sum up to the number of edges in the graph. So, if the edge set of the graph is not empty, it is just a scaled version of (4.1). Fiedler analyzed optimal edge weights and the corresponding minimal maximum eigenvalue of the so weighted Laplacian. He established some bounds on the optimal value and considered the symmetry of the graph. So he proved that there is an optimal edge weighting such that edges of the same orbit have the same weight. For bipartite graphs and especially for trees he related optimal edge weightings to generalized doubly stochastic matrices, i.e., nonnegative matrices having all row sums equal and all column sums equal. In that cases where our considerations will touch these of Fiedler we will mention it in the text.

In this chapter we formulate the primal, dual as well as the graph realization problem of (4.1) and discuss strong duality and different interpretations of optimal solutions.

We continue in Section 4.2 with basic properties of optimal solutions, e.g., the identification of the origin as the realization’s barycenter (Proposition 4.4), upper bounds on the realization’s vector length (Proposition 4.5) and the characterization of optimal realizations.
of isolated nodes (Theorem 4.7). Note that Theorem 4.7 holds for arbitrary graphs with
nonempty edge set and in particular generalizes a result of Fiedler that was proven only
for a special family of graphs. Results about special graph classes, like bipartite graphs
and graphs with some symmetry follow. We want to point out Theorem 4.8 which proves
the existence of a one-dimensional optimal realization for bipartite graphs.

In sections 4.3 and 4.4 we establish relations of the graph’s separator structure and optimal
realizations. The Sunny-Side Theorem, Theorem 4.13, states a folding property of optimal
realizations which is in some sense dual to the unfolding property specified by the Separator-
Shadow Theorem, Theorem 3.10, for \((E_{\lambda})\). We may also ensure the existence of a low
dimensional realization, depending on the graph’s tree-width, see Theorem 4.15. That the
bound may not be improved in general follows by a family of graphs with tight dimension
bound. At the end we discuss a graph parameter according to the rotational dimension.

In order to get rid of one variable of the primary programs of the first section we present
scaled versions of them in the following section. Some readers may be more familiar with
the underlying interpretation and get a better understanding of the explanations of the
previous sections.

In the last section we adapt the scaled graph realization problem so, that optimal realiza-
tions are maps of eigenvectors to the maximum eigenvalue of the unweighted Laplacian.
Also, each eigenvector gives rise to an optimal realization.

The theory presented in sections 4.1 to 4.5 is joint work with Frank Göring and Christoph
Helmberg and is based on [38] (sometimes taken verbatim). We want to point out that
[38] starts with the scaled programs of Section 4.5 and the results are formulated for
these programs. For a better comparison of the optimization problems considered in this
thesis, we start with slightly other programs and adapt all results and proofs of [38]. The
presentation here is often in more detail and often illustrated by examples. We want to
spotlight the different proof of the Sunny-Side Theorem, Theorem 4.13. Furthermore the
results concerning optimal solutions depending on the symmetry of the graph and the
interpretation of optimal realizations as maps of eigenvectors are new.

The last section of this chapter is joint work with Christoph Helmberg. The results are
mostly taken from [50] but are presented in more detail.

### 4.1 Primal-Dual Formulation

In this chapter we consider a graph \( G = (N, E \neq \emptyset) \), not necessarily connected, with node
weights \( s \in \mathbb{R}^{|N|}, s > 0 \) and edge length parameters \( l \in \mathbb{R}^{|E|}, 0 \neq l \geq 0 \).

We follow the usual approach which we have presented in Chapter 3 for the case of the
second smallest eigenvalue to find a pair of semidefinite primal and dual programs followed
by a graph realization formulation of (4.1). If the semidefinite inequality
\[ \lambda_n I \succeq \sum_{ij \in E} w_{ij} DE_{ij} D \]
holds, it bounds the maximum eigenvalue of \( DL_w D = \sum_{ij \in E} w_{ij} DE_{ij} D \) by \( \lambda_n \) (cf. inequality (3.3) on page 37). Minimizing this bound the semidefinite formulation of (4.1) reads
\[
\begin{align*}
\text{minimize} & \quad \lambda_n \\
\text{subject to} & \quad \lambda_n I - \sum_{ij \in E} w_{ij} DE_{ij} D \succeq 0, \\
& \quad \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \\
& \quad \lambda_n \in \mathbb{R}, \quad w \geq 0.
\end{align*}
\]
(P\(_{\lambda_n}\))

The feasible set of (P\(_{\lambda_n}\)) is not empty as the graph’s edge set is not empty and \( l \neq 0 \): choosing nonnegative feasible edge weights \( \tilde{w} \) and
\[ \tilde{\lambda}_n > \sum_{ij \in E} \tilde{w}_{ij} (s_i^{-1} + s_j^{-1}) \]
yields strictly feasible solutions with respect to the semidefinite constraint because of Weyl’s Theorem, Theorem 2.3.

Furthermore the objective value is greater than zero because at least one edge weight is greater than zero due to the equality constraint. Thus the weighted Laplacian is not the zero matrix which causes a positive maximum eigenvalue.

The Lagrangian dual of (P\(_{\lambda_n}\)) reads
\[
\begin{align*}
\text{maximize} & \quad \xi \\
\text{subject to} & \quad \langle I, Y \rangle = 1, \\
& \quad \langle DE_{ij} D, Y \rangle - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \quad \xi \in \mathbb{R}, \quad Y \succeq 0.
\end{align*}
\]
(D\(_{\lambda_n}\))

Also the feasible set of (D\(_{\lambda_n}\)) is not empty as, e. g., \( \xi = 0 \) and \( Y = \frac{1}{n} I \) is feasible.

Because of the positive semidefiniteness of \( Y \), the matrix \( DYD \) admits a Gram representation \( DYD = V^TV \) with \( V \in \mathbb{R}^{n \times n} \). We denote the \( i \)-th column of \( V \) by \( v_i \), i. e., \( V = [v_1, \ldots, v_n] \).

With \( (DYD)_{ij} = v_i^T v_j \) and
\[ \langle DE_{ij} D, Y \rangle = \langle E_{ij}, DYD \rangle = \|v_i\|^2 - 2v_i^T v_j + \|v_j\|^2 = \|v_i - v_j\|^2 \]
we arrive at the corresponding graph realization problem of (D\(_{\lambda_n}\))
\[
\begin{align*}
\text{maximize} & \quad \xi \\
\text{subject to} & \quad \sum_{i \in N} s_i \|v_i\|^2 = 1, \\
& \quad \|v_i - v_j\|^2 - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \quad \xi \in \mathbb{R}, \quad v_i \in \mathbb{R}^n \quad (i \in N).
\end{align*}
\]
(E\(_{\lambda_n}\))
CHAPTER 4. MINIMIZING $\lambda_{\text{MAX}}$

So the dual problem of (4.1) or rather $(P_{\lambda_n})$ is equivalent to finding a realization of the graph’s nodes in $n$-space such that the sum of the node weighted squared norms is one (we call this the *normalization constraint*) and the distances of adjacent nodes are lower bounded by the weighted variable $\xi$ (the *distance constraints*). In optimal solutions the minimal ratio of distance to $l_{ij}$ of adjacent nodes $i$ and $j$ with $l_{ij} > 0$ is as large as possible.

What effect have edge parameters that are equal to zero in the primal and dual (graph realization) program? Well, such a parameter causes a trivial constraint in $(D_{\lambda_n})$ and $(E_{\lambda_n})$ as edge lengths are always nonnegative. On the primal side we may fix the corresponding edge weight to zero without endangering feasibility or optimality. So we may interpret zero edge length parameters as deleting the edge $ij$ from the graph. In consequence requiring $l > 0$ would be no momentous restriction.

Next we analyze Lagrangian duality of the primal and the dual program. By the Lagrangian approach weak duality holds for $(P_{\lambda_n})$ and $(D_{\lambda_n})$ or $(E_{\lambda_n})$ respectively. That is $\lambda_n \geq \xi$ for feasible $\lambda_n$ of $(P_{\lambda_n})$ and feasible $\xi$ of $(D_{\lambda_n})$ or $(E_{\lambda_n})$ respectively. In fact, equality holds for optimal solutions.

**Proposition 4.1 (Strong Duality)** Let $G = (N, E \neq \emptyset)$ be a graph with given data $s > 0$ and $0 \neq l \geq 0$. Strong duality holds for $(P_{\lambda_n})$ and $(D_{\lambda_n})$ and both programs attain their optimal value (i.e., optimal solutions exist).

**Proof.** Strong duality follows from Corollary 2.15 and the strictly feasible solution $(\tilde{\lambda}_n, \tilde{w})$ of $(P_{\lambda_n})$ with respect to the semidefinite constraint. As both feasible sets are not empty the optimal value is finite, thus the dual attains its optimal value. The primal attains its optimal value because, by Weyl’s Theorem (Theorem 2.3) and the semidefinite inequality constraint for finite $\lambda_n$,

$$\lambda_n \geq \lambda_{\text{max}} \left( \sum_{ij \in E} w_{ij}DE_{ij}D \right) \geq w_{kl}\lambda_{\text{max}}(DE_{kl}D) + \lambda_1 \left( \sum_{ij \in E \setminus \{kl\}} w_{ij}DE_{ij}D \right) = \left( \frac{1}{s_k} + \frac{1}{s_l} \right) w_{kl}$$

follows for $kl \in E$. Hence the feasible weights lie in a closed and bounded, thus compact subset of $\mathbb{R}^{|E|}$.

To give an example of optimal primal and dual solutions, thus optimal realizations, let us recall the graph of Example 3.6 on page 41 and let the node and edge parameters all be equal to one. An optimal edge weighting for $(P_{\lambda_n})$ is illustrated at the left hand side of Figure 4.1. Like in Section 3.1 the weights are given by gray shades. An optimal (probably
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Figure 4.1: Optimal edge weighting of the graph of Example 3.6 by gray shades and a corresponding optimal realization for \((P_{\lambda_n})\) and \((E_{\lambda_n})\), respectively.

15-dimensional) realization for \((E_{\lambda_n})\) is presented at the right hand side of Figure 4.1. The solution is computed by SeDuMi [88]. Remember, the red circle displays the origin.

Comparing the optimal solutions of the graph of \((P_{\lambda_2})\) and \((E_{\lambda_2})\) illustrated in Figure 3.2 with the optimal solutions from above, Figure 4.1, we observe some in a certain sense dual aspects. Edges which are important for one problem, i.e., which have large weight in comparison to the other edge weights in a solution, seem to be not so important for the other problem, i.e., they have small weight. For example the edges \(\{3, 28\}\) and \(\{24, 25\}\) are important for \((P_{\lambda_n})\) but not so for \((P_{\lambda_2})\). Otherwise, the edges \(\{11, 19\}\) and \(\{11, 29\}\) are important for \((P_{\lambda_2})\) but not so for \((P_{\lambda_n})\). Indeed, the edge \(\{11, 29\}\) has zero weight in \((P_{\lambda_n})\).

Furthermore we observe that important edges for \((P_{\lambda_2})\) are in some sense central edges, whereas the important edges for \((P_{\lambda_n})\) are often such ones connecting only one node to the graph.

Differences of the presented optimal realizations are obvious. First we have an optimal two- versus an optimal high-dimensional solution. And second, the realization of \((E_{\lambda_2})\) is in some sense unfolded whereas the realization of \((E_{\lambda_n})\) seems to be folded.

Whether we may observe the above aspects for arbitrary graphs or whether they only hold for some graphs we want to analyze in the remainder of this chapter and hopefully want to find reasons for these observations.

Firstly, considering the Karush-Kuhn-Tucker conditions of \((P_{\lambda_n})\) and \((E_{\lambda_n})\) leads to a
physical view of the primal-dual pair of programs. Without feasibility, they read

$$\lambda_n s_i v_i = \sum_{ij \in E} w_{ij} (v_i - v_j) \quad (i \in N),$$  \hspace{1cm} (4.2)

$$w_{ij} (\|v_i - v_j\|^2 - l_{ij}^2 \xi) = 0 \quad (ij \in E).$$  \hspace{1cm} (4.3)

Because of equation (4.2) we may see problem \((E_{\lambda_n})\) from the perspective of forces. Consider each edge \(ij\) as being a spring between adjacent nodes at positions \(v_i\) and \(v_j\). Then \(l_{ij} \sqrt{\xi}\) is a lower bound for the spring’s length. The node weights \(s_i\) may reflect the importance of the nodes in the sense that there are additional \(s_i\) springs between node \(i\) at position \(v_i\) and the origin. Now optimal solutions of \((E_{\lambda_n})\) and \((P_{\lambda_n})\) correspond to an equilibrium configuration. The edge weight \(w_{ij}\) may be interpreted as the spring constant of spring \(ij\) and optimal \(\lambda_n\) is the spring constant of all springs between a node and the origin (cf. rigidity theory [84]). In particular, the forces are in equilibrium in each node, by equation (4.2).

Note that there is also a physical interpretation of optimal solutions of \((P_{\lambda_2-s})\) and \((E_{\lambda_2-s})\) in [39]. Also Sun et al. [89] linked \((P_{\lambda_2-s})\) and \((E_{\lambda_2-s})\) with different contexts. In a mechanics interpretation they called the force between the nodes and the origin centripetal.

The Karush-Kuhn-Tucker conditions provide a connection of optimal realizations and the eigenspace of an optimal maximum eigenvalue. One may view optimal realizations as a map of eigenvectors to this eigenvalue (cf. Proposition 3.7 and Figure 3.3).

**Proposition 4.2** Let \(G = (N, E \neq \emptyset)\) be a graph with given data \(s > 0\) and \(0 \neq l \geq 0\). Let \(V = [v_1, \ldots, v_n]\) be an optimal realization for \((E_{\lambda_n})\) and let \((\lambda_n, w)\) be optimal for \((P_{\lambda_n})\). For any \(h \in \mathbb{R}^n\) the scaled projection \(D^{-1}V^\top h\) onto the one-dimensional subspace spanned by \(h\) yields an eigenvector to \(\lambda_{\max}(DL_wD)\), unless it is the zero vector.

**Proof.**

\[
(\lambda_n I - DL_wD)D^{-1}V^\top h = \lambda_n D^{-1}V^\top h - \sum_{ij \in E} w_{ij} DE_{ij} V^\top h \\
= D \left( \lambda_n D^{-2} V^\top - \sum_{ij \in E} w_{ij} E_{ij} V^\top \right) h = 0
\]

The last equation follows from (4.2) as the \(i\)-th row of \(\lambda_n D^{-2} V^\top - \sum_{ij \in E} w_{ij} E_{ij} V^\top\) equals the (transposed) KKT condition of node \(i\).

Before we go into more detail concerning the properties of optimal solutions of \((P_{\lambda_n})\), \((D_{\lambda_n})\) and \((E_{\lambda_n})\) let us shortly think about maximizing the maximum eigenvalue, i. e.,

\[
\max \left\{ \lambda_{\max}(DL_wD) : \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \ w_{ij} \geq 0 \ (ij \in E) \right\}.
\]
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We have to consider the two cases that there exists an edge $\hat{e} \in E$ with $l_{\hat{e}} = 0$ on the one hand and $l > 0$ on the other hand. In both cases we may state an optimal solution, because Weyl's Theorem, Theorem 2.3, yields for $kl \in E$

$$w_{kl}\lambda_{\text{max}}(DE_{kl}D) \leq \lambda_{\text{max}}(DL_wD) \leq \sum_{ij \in E} w_{ij}(s_i^{-1} + s_j^{-1}).$$

As there is no upper bound on $w_{\hat{e}}$ in the first case, it may increase to infinity, thus the maximum eigenvalue of the weighted Laplacian increases to infinity, too.

In the case of $l > 0$ the edge weights are bounded by $w_{ij} \leq l_{ij}^{-2}$. We give an upper bound on the maximum eigenvalue which is independent of the edge weights and which can be reached. The bound reads

$$\sum_{ij \in E} l_{ij}^2 w_{ij}l_{ij}^{-2}(s_i^{-1} + s_j^{-1}) \leq \max\{l_{ij}^2(s_i^{-1} + s_j^{-1}) : ij \in E\} = l_{kl}^2(s_k^{-1} + s_l^{-1})$$

for appropriate $k$ and $l$ realizing the maximum. Indeed $w_{kl} = l_{kl}^{-2}$ and $w_{ij} = 0$ otherwise is such a maximizing edge weighting.

4.2 Basic Properties

We start this section by the definition of subgraphs which depend on optimal solutions. This is motivated by the fact that edges whose distance constraints are inactive or whose weights are zero in optimal solutions, are mostly of no importance in the considerations to follow and may be dropped.

**Definition 4.3** For $G = (N, E \neq \emptyset)$ with given data $s > 0$ and $0 \neq l \geq 0$ let $\xi, V = [v_1, \ldots, v_n]$ be an optimal solution of $(E_{\lambda_n})$ and $w_{ij}$ $(ij \in E)$ be a corresponding optimal solution of $(P_{\lambda_n})$.

The edge set $E_{V,\xi,l} := \{ij \in E : \|v_i - v_j\|^2 = l_{ij}^2 \xi\}$ gives rise to the active subgraph $G_{V,\xi,l} = (N, E_{V,\xi,l})$ of $G$ with respect to $V$ and $\xi$.

The strictly active subgraph $G_w = (N, E_w)$ of $G$ with respect to $w$ has edge set $E_w := \{ij \in E : w_{ij} > 0\}$.

By the definitions of $E_{V,\xi,l}$ and $E_w$ both sets are subsets of the graph's edge set. Furthermore $E_w \subseteq E_{V,\xi,l}$ holds because of the complementarity conditions (4.3), thus $E_w \subseteq E_{V,\xi,l} \subseteq E$ for optimal $w$, and optimal $V, \xi$.

Recall that a component of a graph is a maximal connected subgraph, and so a component of $G$ may split into several components in $G_{V,\xi,l}$ which may again split into several components in $G_w$. 
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Let us now specify basic properties of optimal realizations. While, in contrast to $(E_{\lambda_2})$, there is no constraint concerning the realization’s barycenter in $(E_{\lambda_n})$ it is in the origin for optimal solutions, too. Moreover each component is centered at the origin.

Proposition 4.4 Given optimal solutions to $(E_{\lambda_n})$ and $(P_{\lambda_n})$, the barycenter of each component of the strictly active subgraph as well as of the active subgraph as well as of the graph itself is in the origin. Hence, any optimal realization is at most $(n - 1)$-dimensional.

Proof. Let $C \subseteq N$ be a component of the strictly active subgraph or a component of the active subgraph or the graph itself. Taking the sum of the KKT conditions (4.2) over the component’s nodes, we get

$$\sum_{i \in C} \lambda_n s_i v_i = \sum_{i \in C} \sum_{ij \in E} w_{ij} (v_i - v_j) = 0$$

because each edge $ij \in E$ with $i, j \in C$ occurs twice, the corresponding summands have opposite sign and $ij \in E$ with $i \in C$, $j \notin C$ has zero weight, thus all $w_{ij}$ cancel out.

The next result states that any optimal realization of $(E_{\lambda_n})$ is contained within a ball.

Proposition 4.5 Let $G = (N,E \neq \emptyset)$ be a graph with given data $s > 0$ and $0 \neq l \geq 0$. Define $\hat{s} := \min\{s_k : k \in N\}$ and $\hat{l} := \max\{l_{ij} : ij \in E\}$. All optimal solutions $\xi, [v_1, \ldots, v_n]$ of $(E_{\lambda_n})$ satisfy $\|v_i\| < \min\{\hat{s}^{-1/2}, \hat{l} \sqrt{\xi}\}$ for $i \in N$.

Proof. The inequality $\hat{s}\|v_i\|^2 \leq s_i\|v_i\|^2 \leq 1$ follows from the normalization constraint. Assume, for contradiction, that $\hat{s}\|v_k\|^2 = 1$ for some $k \in N$. Then $v_i = 0$ for $i \in N \setminus \{k\}$ follows from $s > 0$ and the normalization constraint. As this is a contradiction to Proposition 4.4, the first part $\|v_i\| < \hat{s}^{-1/2}$ is true.

Given an optimal solution $\xi, [v_1, \ldots, v_n]$, assume, for contradiction, there exists a vector $v_k$ for some $k \in N$ with $\|v_k\| = \hat{l} \sqrt{\xi} + \epsilon \geq \hat{l} \sqrt{\xi}$. By Proposition 4.4 we may choose a vector $h \in \mathbb{R}^n$, $\|h\| = 1$, with $h$ perpendicular to all $v_i$ ($i \in N$). Because of the normalization constraint $s_k\|v_k\|^2 = s_k(\hat{l} \sqrt{\xi} + \epsilon)^2 \leq 1$, thus $0 \leq s_k(2\hat{l} \sqrt{\xi} \epsilon + \epsilon^2) < 1$. Define a new realization $[v'_1, \ldots, v'_n]$ which satisfies the normalization constraint via

$$v'_i := \frac{1}{\sqrt{1 - s_k(2\hat{l} \sqrt{\xi} \epsilon + \epsilon^2)}} \begin{cases} v_i, & i \in N \setminus \{k\} \\ \hat{l} \sqrt{\xi} h, & i = k. \end{cases}$$

Because the scaling factor is greater than or equal to one, edges $ij \in E$, $i,j \neq k$ do not become shorter. Edges which are incident with node $k$ also do not become shorter, as
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\[ \|v'_i - v'_k\|^2 \geq \|\hat{l}\sqrt{\xi}h\|^2 = \hat{l}^2\xi. \]
So the new realization is feasible with the same \(\xi\), thus it is optimal, too. The barycenter of the new realization, however, is not in the origin. Indeed,

\[ h^T\bar{v}'(N) = \frac{s_k\hat{l}\sqrt{\xi}}{\bar{s}(N)\sqrt{1 - s_k(2\hat{l}\sqrt{\xi}\epsilon + \epsilon^2)}} \neq 0, \]
so by Proposition 4.4 the new realization is not optimal. This contradicts optimality of the original one.

In the following we will sometimes use the argument of the preceding proof to show optimality of a realization of \((E_{\lambda_n})\). It is a transformation which expands the graph. To memorize it we outline it once more.

**Remark 4.6** Let \( G = (N, E \neq \emptyset) \) be a graph with given data \( s > 0 \) and \( 0 \neq l \geq 0 \). Let \( \xi, [v_1, \ldots, v_n] \) be an optimal realization of \((E_{\lambda_n})\). If there exists a realization \([\bar{v}_1, \ldots, \bar{v}_n]\) which fulfills the distance constraints together with \(\xi\) but violates the normalization constraint such that \(\sigma := \sum_{i \in N} s_i\|\bar{v}_i\|^2 < 1\), the scaled realization \(\sigma^{-1/2} \cdot [\bar{v}_1, \ldots, \bar{v}_n]\) together with \(\sigma^{-1}\xi\) is feasible. But as \(\sigma^{-1/2} > 1\) all edge lengths are increased in length, hence the old \(\xi\) is not optimal, which is a contradiction.

If \( l = c1 \) with real \( c > 0 \) we may characterize the optimal realization of isolated nodes.

**Theorem 4.7** Let \( G = (N, E \neq \emptyset) \) be a given graph with data \( s > 0 \) and \( 0 \neq l \geq 0 \) and let \( k \in N \). The following statements are equivalent for optimal solutions of \((P_{\lambda_n})\) and \((E_{\lambda_n})\):

(i) \( k \) is isolated in \( G \);
(ii) \( k \) is isolated in the strictly active subgraph \( G_w \);
(iii) \( v_k = 0 \), i.e., \( k \) is embedded in the origin.

**Proof.** [(i) \( \Rightarrow \) (ii)] is a consequence of \( E_w \subseteq E \).

[(ii) \( \Rightarrow \) (iii)] If \( k \) is isolated in the strictly active subgraph, the KKT condition (4.2) reads

\[ \lambda_n s_k v_k = \sum_{i \in E} w_{ik} (v_k - v_i) = 0 \]
for \( k \), thus \( v_k = 0 \).

[(iii) \( \Rightarrow \) (i)] Assume, for contradiction, that \( k \) is not isolated in \( G \). Then

\[ \|v_i - v_k\|^2 = \|v_i\|^2 \geq c^2\xi \]
holds for all \( ik \in E \). Because of Proposition 4.5 this contradicts optimality.
Note that the condition of uniform edge length parameters is essential. In the case of arbitrary nonnegative edge length parameters nodes may be embedded in the origin without being isolated in the strictly active subgraph. Figure 4.2 illustrates an optimal two-dimensional realization of a tetrahedron for \((E_{\lambda_n})\) with data \(s = 1\), \(l_{12} = l_{13} = l_{23} = 1\) and \(l_{14} = l_{24} = l_{34} = 1/\sqrt{3}\). An optimal primal solution is \(\xi = 1, w = \frac{1}{4}1\). Node 4 is embedded in the origin while it is not isolated in the strictly active subgraph.

Because of Theorem 4.7 an arbitrary graph with data \(s > 0\) and \(l = c1\) with real \(c > 0\) has no isolated node if and only if the strictly active subgraph with respect to an optimal edge weighting has no isolated node. Fiedler already proved this result for the special family of bipartite graphs with data \(s = 1\) and \(l = 1\) (see [27], Lemma 3.5). Thus Theorem 4.7 generalizes Fiedler’s lemma twice: the theorem works for arbitrary positive node parameters and for arbitrary graphs with at least one edge.

For bipartite graphs the structure of optimal solutions is particularly simple.

**Theorem 4.8 (Bipartite Graphs)** Let \(G = (N, E \neq \emptyset)\) be bipartite with given data \(s > 0\) and \(0 \neq l \geq 0\). There exists a one-dimensional optimal solution of \((E_{\lambda_n})\).

Moreover, if \(l = c1\) with real \(c > 0\) then for any optimal solution \(\xi\), \(V\) of \((E_{\lambda_n})\) and any optimal \(w\) of \((P_{\lambda_n})\), each non-trivial component of the strictly active subgraph \(G_w\) is embedded in the endpoints of a straight line segment of length \(c\sqrt{\xi}\) that contains the origin in its relative interior.
Proof. Given an optimal $d$-dimensional realization $[v_1,\ldots,v_n]$ with optimal $\xi$ of $(E_{\lambda_n})$ for $G = (A \cup B, E \subseteq \{ij : i \in A, j \in B\})$, consider the one-dimensional realization 

$$v'_i = \begin{cases} -\|v_i\| \cdot h, & i \in A \\ \|v_i\| \cdot h, & i \in B, \end{cases} \tag{4.4}$$

for some $h \in \mathbb{R}^n$ with $\|h\| = 1$. Clearly, the normalization constraint holds and for $ij \in E$ we obtain (use the triangle inequality for the second inequality)

$$l_{ij}^2 \xi \leq \|v_i - v_j\|^2 \leq (\|v_i\| + \|v_j\|)^2 = \|v'_i - v'_j\|^2.$$

So all distance constraints are fulfilled and the new realization with $\xi$ is optimal.

Now consider the case $l = c1$ with real $c > 0$. For $ij \in E_w$ complementarity (4.3) ensures $c^2 \xi = \|v'_i - v'_j\|^2 = \|v_i - v_j\|^2 = (\|v_i\| + \|v_j\|)^2$. This together with Proposition 4.5 and Theorem 4.7 shows that the origin is a strict convex combination of $v_i$ and $v_j$. Continuing this argument along the edges of a spanning tree of each component of $G_w$ completes the proof. 

Figure 4.3 displays a bipartite graph on the left hand side and a corresponding optimal edge weighting for $(P_{\lambda_n})$ with data $s = 1$ and $l = 1$ on the right hand side. As edge $\{4,7\}$ has zero weight, the strictly active subgraph is not connected, it splits into two components. An optimal two- and an optimal one-dimensional realization are given in Figure 4.4. Each component of the strictly active subgraph is embedded in the endpoints of a straight line segment that contains the origin (red circle) in its relative interior. Indeed, the barycenter of each component of the strictly active subgraph is in the origin (cf. Proposition 4.4).

![Figure 4.3: A bipartite graph and an associated optimal edge weighting for $(P_{\lambda_n})$ with data $s = 1$ and $l = 1$. The strictly active subgraph is not connected.](image)

Let us furthermore consider Figure 4.5 which illustrates an optimal realization of the cube graph (see Figure 3.5) with data $s = 1$ and $l = 1$ for $(E_{\lambda_n})$. We notice that, as the strictly active subgraph is connected any optimal solution of this graph must be one-dimensional because of Theorem 4.8. Hence the figure illustrates the unique solution up to congruence.

In the last chapter we have seen, that there is a 3-dimensional optimal realization for $(E_{\lambda_n})$ of the cube graph with the same parameters. So we cannot prove that optimal realizations for $(E_{\lambda_n})$ are “high”-dimensional and those for $(E_{\lambda_2})$ are “low”-dimensional as the example
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Figure 4.4: An optimal two- and an optimal one-dimensional realization of the bipartite graph of Figure 4.3 for $(E_{\lambda n})$ with optimal edge weights, illustrated by gray shades.

Figure 4.5: An optimal one-dimensional realization of the cube graph for $(E_{\lambda n})$ with data $s = 1$ and $l = 1$ (cf. with Figure 3.5 on page 49).

at the beginning of this chapter suggests (cf. page 61). In fact, high-dimensional solutions arise by solution methods of SDPs like central path methods, see [48, 95].

Complete graphs with data $s > 0$ and $l = c1$ with real $c > 0$ have the same optimal realization for $(E_{\lambda n})$ as for the $\lambda_2$-case (cf. Example 3.20).

Example 4.9 (Complete Graphs) For $K_n := (\{1, \ldots, n\}, \{i, j\} : 1 \leq i < j \leq n)$ with data $l = c1$ with real $c > 0$ and arbitrary $s > 0$ we show that the unique optimal realization of $(E_{\lambda n})$ is the regular $(n-1)$-dimensional simplex whose weighted barycenter coincides with the origin: We can handle the normalization constraint of $(E_{\lambda n})$ by Lemma 2.10 and bound it as follows by the use of optimal $\xi > 0$,

$$1 = \sum_{i \in N} s_i \|v_i\|^2 = \bar{s}(N) \|\bar{v}(N)\|^2 + \frac{1}{2s(N)} \sum_{i,j \in N} s_i s_j \|v_i - v_j\|^2 \geq 0 + \frac{1}{2s(N)} \sum_{i \in N} \sum_{j \in N \setminus \{i\}} c^2 \xi s_i s_j \geq \frac{c^2 \xi (\bar{s}(N))^2 - \|s\|^2}{2s(N)}. \tag{4.5}$$

Equality holds if and only if $\bar{v}(N) = 0$ and $\|v_i - v_j\|^2 = c^2 \xi$ for $i, j \in N$ with $i \neq j$.

Note, for use in Example 4.16, that $\|v_i\| = \|v_j\|$ whenever the weights $s_i$ and $s_j$ are equal, because the exchange of two vertices of a regular simplex is a congruence transformation.
We conclude this section with results concerning the symmetry of the underlying graph.

In [27] Fiedler proved that there is a special optimal edge weighting of a graph with data \( s = 1 \) and \( l = 1 \) for \( (P_{\lambda_n}) \) in the sense that edges of the same orbit have same optimal weight (cf. Proposition 3.17). In the next proposition we generalize the result for any data \( s > 0 \) and \( 0 \neq l \geq 0 \). We omit the proof as it is the same argument as in Proposition 3.17: start with an arbitrary optimal solution, apply all automorphisms to this solution resulting in further optimal edge weightings. A convex combination of these solutions yields the required one.

**Proposition 4.10** Given \( G = (N, E \neq \emptyset) \) and data \( s > 0 \), \( 0 \neq l \geq 0 \). There exists an optimal edge weighting of \( (P_{\lambda_n}) \) for which edges of the same orbit under the action of the automorphism group \( \text{Aut}(G, s, l) \) have the same value.

As all edges of an edge transitive graph lie in the same orbit, there is an optimal solution of \( (P_{\lambda_n}) \) for which all edges have the same weight.

**Corollary 4.11 (Edge Transitive Graphs)** Let \( G = (N, E \neq \emptyset) \) be edge transitive and \( s = c_s 1, l = c_l 1 \) with real \( c_s, c_l > 0 \) be given data. There is an optimal solution of \( (P_{\lambda_n}) \) with edge weights \( w_{ij} = \frac{1}{|E|^{1/2}} \) \((ij \in E)\).

As mentioned in Section 3.3, the cube graph with data \( s = 1 \) and \( l = 1 \) is edge transitive, hence there is an optimal weighting for \( (P_{\lambda_n}) \) with equal weight for all edges.

Using Proposition 4.2 and the previous corollary a map of an optimal realization of edge transitive graphs for \( (E_{\lambda_n}) \) on a one-dimensional subspace proves to be an eigenvector to the maximum eigenvalue of the unweighted Laplacian of the graph or to be the zero vector.

**Corollary 4.12** Let \( G = (N, E \neq \emptyset) \) be an edge transitive graph, \( s = c_s 1, l = c_l 1 \) with real \( c_s, c_l > 0 \) be given data and \( V \) an optimal realization of \( (E_{\lambda_n}) \). For \( h \in \mathbb{R}^n \) the vector \( V^\top h \) is an eigenvector of \( \lambda_{\text{max}}(L(G)) \), unless it is the zero vector.

### 4.3 Sunny-Side Theorem

Structural properties of optimal realizations \([v_1, \ldots, v_n]\) of \( (E_{\lambda_n}) \) are tightly linked to the separator structure of the underlying graph. The first result corresponds to the Separator-Shadow Theorem, Theorem 3.10.
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**Theorem 4.13 (Sunny-Side)** Given a graph $G = (N, E \neq \emptyset)$, data $s > 0$, $0 \neq l \geq 0$, an optimal solution $\xi, V = [v_1, \ldots, v_n]$ of $(E_{\lambda_n})$, and two disjoint nonempty subsets $A$ and $S$ of $N$ such that each edge of the corresponding active subgraph $G_{V, \xi, l}$ leaving $A$ ends in $S$. Then the barycenter $\bar{v}(A)$ is contained in $S := \text{aff}(V_S) - \text{cone}(V_S)$.

To avoid similar and familiar calculations in the proof of Theorem 4.13, we first collect some easy properties of distances during rotation around an affine subspace of $\mathbb{R}^n$.

**Lemma 4.14** Let $b, u \in \mathbb{R}^n$, with $u \perp b$, $\|u\| = 1$, $\|b\| = 1$, $\beta, \nu \in \mathbb{R}$ and put

$$\mathcal{H} := \{x \in \mathbb{R}^n : b^T x = \beta, u^T x = \nu\}.$$  

Let $p_{\mathcal{H}}(x) = x + (\beta - b^T x)b + (\nu - u^T x)u$ be the projection of $x$ onto $\mathcal{H}$.

Then $x \in \mathbb{R}^n$ may be written as

$$x = p_{\mathcal{H}}(x) + \|x - p_{\mathcal{H}}(x)\|(b \cos \alpha_x + u \sin \alpha_x), \quad (4.6)$$

with an appropriate $\alpha_x \in [0, 2\pi)$.

Let $\varphi(x, \gamma) := p_{\mathcal{H}}(x) + \|x - p_{\mathcal{H}}(x)\|(b \cos(\alpha_x + \gamma) + u \sin(\alpha_x + \gamma))$, for $\gamma \in [-\pi, \pi)$.

Then

1. $\|\varphi(x, \gamma) - y\|^2 = \|x - y\|^2$, for all $x \in \mathbb{R}^n, y \in \mathcal{H}$;
2. $\|\varphi(x, \gamma) - \varphi(y, \gamma)\|^2 = \|x - y\|^2$, for all $x, y \in \mathbb{R}^n$;
3. $\|\varphi(x, \gamma) - y\|^2 = \|x - y\|^2 + 2\|x - p_{\mathcal{H}}(x)\|\|y - p_{\mathcal{H}}(y)\|(\cos(\alpha_x - \alpha_y) - \cos(\alpha_x - \alpha_y + \gamma))$, for all $x, y \in \mathbb{R}^n$;
4. $\|\varphi(x, \gamma) - x\|^2 = 2\|x - p_{\mathcal{H}}(x)\|^2(1 - \cos \gamma)$, for all $x \in \mathbb{R}^n$.

**Proof.** Because $x$, $p_{\mathcal{H}}(x)$ and $x - (u^T x - \nu)u$ build a right angle triangle, equation (4.6) follows (compare Figure 4.6).

1. Follows because we rotate around $\mathcal{H}$.
2. As we use the same rotation angle $\gamma$ for $x$ and $y$ the statement is correct.
3. We use (4.6) with an appropriate angle $\alpha_y$ for $y$.

Let $d_x := \|x - p_H(x)\| = \|(\nu - u^\top x)u + (\beta - b^\top x)b\| (d_y$ respectively) and observe that

$$d_x^2 = (\beta - b^\top x)^2 + (\nu - u^\top x)^2$$

(4.7)

and

$$(x - y)^\top b = (\beta - b^\top y) - (\beta - b^\top x),$$

$$(x - y)^\top u = (\nu - u^\top y) - (\nu - u^\top x)$$

(4.8)

hold. Then

$$\|\varphi(x, \gamma) - y\|^2$$

$$= \|x - y + (\beta - b^\top x)b + (\nu - u^\top x)u + d_x (b \cos(\alpha_x + \gamma) + u \sin(\alpha_x + \gamma))\|^2.$$  (4.9)

To expand the squared norm (4.9) we firstly calculate the single parts. Using (4.7) and $\sin^2 \alpha + \cos^2 \alpha = 1$ the quadratic terms read

$$\|A\|^2 + \|B\|^2 + \|C\|^2 = \|x - y\|^2 + 2d_x^2.$$

With (4.7), (4.8) and $u^\top b = 0$, the mixed terms are

$$2A^\top B = 2(\beta - b^\top x)(\beta - b^\top y) + 2(\nu - u^\top x)(\nu - u^\top y) - 2d_x^2,$$

$$2B^\top C = 2(\beta - b^\top x)d_x \cos(\alpha_x + \gamma) + 2(\nu - u^\top x)d_x \sin(\alpha_x + \gamma),$$

$$2A^\top C = 2(\beta - b^\top y)d_x \cos(\alpha_x + \gamma) + 2(\nu - u^\top y)d_x \sin(\alpha_x + \gamma) - 2B^\top C.$$
Therefore and with
\[ (\beta - b^\top x) = -d_x \cos \alpha_x, \]
\[ (\nu - u^\top x) = -d_x \sin \alpha_x \]
for \( x \) and \( y \) respectively, the proof is complete because
\[ \|\varphi(x, \gamma) - y\|^2 = \|x - y\|^2 + 2(\beta - b^\top x)(\beta - b^\top y) + 2(\nu - u^\top x)(\nu - u^\top y) \]
\[ + 2(\beta - b^\top y)d_x \cos(\alpha_x + \gamma) + 2(\nu - u^\top y)d_x \sin(\alpha_x + \gamma) \]
\[ = \|x - y\|^2 + 2d_x d_y(\cos(\alpha_x + \gamma) \cos \alpha_y + \sin(\alpha_x + \gamma) \sin \alpha_y) \]
\[ - 2d_x d_y(\cos(\alpha_x + \gamma) \cos \alpha_y + \sin(\alpha_x + \gamma) \sin \alpha_y) \]
\[ = \|x - y\|^2 + 2d_x d_y(\cos(\alpha_x - \alpha_y) - \cos(\alpha_x - \alpha_y + \gamma)). \]

4. Follows from 3.

We consider the normalization constraint of \((E_{\lambda_n})\) for the situation of Theorem 4.13. In consequence of Lemma 2.10, the equality of (2.5) and (2.8), the sum may be grouped in the parts of \( N = A \cup S \cup B \) with \( B := N \setminus (A \cup S) \) and the distances of the barycenters:

\[
\sum_{i \in N} s_i \|v_i\|^2 = \sum_{i \in A} s_i \|v_i - \bar{v}(A)\|^2 + \sum_{i \in S} s_i \|v_i - \bar{v}(S)\|^2 + \sum_{i \in B} s_i \|v_i - \bar{v}(B)\|^2
\]
\[
+ \frac{\bar{s}(A)\bar{s}(S)}{\bar{s}(N)} \|\bar{v}(A) - \bar{v}(S)\|^2 + \frac{\bar{s}(A)\bar{s}(B)}{\bar{s}(N)} \|\bar{v}(A) - \bar{v}(B)\|^2
\]
\[
+ \frac{\bar{s}(B)\bar{s}(S)}{\bar{s}(N)} \|\bar{v}(B) - \bar{v}(S)\|^2 + \bar{s}(N) \|\bar{v}(N)\|^2. \tag{4.10}
\]

The proof of Theorem 4.13 will be indirect. Given an optimal realization that does not satisfy the statement of the theorem, we improve it by rotation around the affine hull of the separator \( S \).

**Proof.** Let \( \xi, [v_1, \ldots, v_n] \) be an optimal solution of \((E_{\lambda_n})\). If \( B := N \setminus (A \cup S) = \emptyset \) then Lemma 2.10, equation (2.4), and Proposition 4.4 imply \( \bar{v}(A) = -\frac{\bar{s}(S)}{\bar{s}(A)} \bar{v}(S) \) and therefore

\[ \bar{v}(A) = \bar{v}(S) - \left(1 + \frac{\bar{s}(S)}{\bar{s}(A)}\right) \bar{v}(S) \in S. \]

Thus we assume \( B \neq \emptyset \) and we assume for contradiction \( \bar{v}(A) \notin S \).

For simplification we use the following notation: for an affine subspace \( \mathcal{H} \) and \( v_i \ (i \in N) \) let \( \alpha_i \) be the corresponding angle of Lemma 4.14 and \( d_i := \|v_i - p_{\mathcal{H}}(v_i)\| \). Let \( \bar{v}_J := \bar{v}(J) \)
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and \( \bar{s}_J := \bar{s}(J) \) (\( J \in \{A, B, S, N\} \)) denote the barycenters and corresponding weights of the specified subgraphs and \( \bar{\alpha}_J \) and \( \bar{d}_J \) denote the corresponding angles and distances.

Let \( \mathcal{L} := \text{lin}(V_S \cup \{\bar{v}_A\}) \) be the linear hull of \( V_S \) unified with the barycenter \( \bar{v}_A \). Then \( V_S \subseteq \mathcal{L} \) and \( \mathbb{R}^n \setminus \mathcal{L} \neq \emptyset \) because of Proposition 4.4. Let \( p_0 \) denote the projection of the origin onto \( \text{aff}(V_S) \).

The proof works as follows: We will choose appropriate \( b \) and \( u \in \mathbb{R}^n \), with \( \|b\| = 1, \|u\| = 1 \) and \( b \perp u \). Then we consider the affine subspace \( \mathcal{H} := \{x \in \mathbb{R}^n : b^T x = \|p_0\|, u^T x = 0\} \).

We find a different realization \( \varphi(v_i, \gamma) \), with \( i \in N \), by rotating \( v_i \) for \( i \in A \), around \( \mathcal{H} \) with rotation angle \( \gamma \), to be determined below, via

\[
\varphi(v_i, \gamma) := \begin{cases} 
  p_{\mathcal{H}}(v_i) + d_i [b \cos(\alpha_i + \gamma) + u \sin(\alpha_i + \gamma)], & i \in A \\
  v_i, & \text{otherwise.}
\end{cases}
\] (4.11)

For \( \text{aff}(V_S) \subseteq \mathcal{H} \), the distance constraints of the new realization (together with \( \xi \)) hold again because of Lemma 4.14: distances within \( A \) and distances to the separator nodes are maintained. Only distances of edges \( \{ij \in E \setminus E_{V,\xi,t} : i \in A, j \in B, v_j \notin \mathcal{H}\} \) change. By the definition of \( G_{V,\xi,t} \) we then have

\[
\|v_i - v_j\|^2 = l_{ij}^2 \xi + \epsilon_{ij} > l_{ij}^2 \xi
\]

and

\[
\|\varphi(v_i, \gamma) - v_j\|^2 = \|v_i - v_j\|^2 + 2d_id_j [\cos(\alpha_i - \alpha_j) - \cos(\alpha_i - \alpha_j + \gamma)] \\
= l_{ij}^2 \xi + \epsilon_{ij} + 2d_id_j [\cos(\alpha_i - \alpha_j) - \cos(\alpha_i - \alpha_j + \gamma)] \\
> l_{ij}^2 \xi
\]

for appropriate \( |\gamma| > 0 \) small enough.

For \( |\gamma| > 0 \) small enough, the normalization constraint is violated. More precisely we will prove that the sum of weighted squared norms is decreased, i.e., \( \sum_{i \in N} s_i \|\varphi(v_i, \gamma)\|^2 < 1 \) which contradicts optimality of the initial realization by Remark 4.6.

Consequently in the following it suffices to specify \( b \) and \( u \) and to calculate the normalization constraint.

Before we go on with the proof let us observe

\[
\bar{s}_N^2 \|\varphi(\bar{v}_N, \gamma)\|^2 = \|\bar{s}_A \varphi(\bar{v}_A, \gamma) + \bar{s}_B \bar{v}_B + \bar{s}_S \bar{v}_S\|^2 = \|\bar{s}_A \varphi(\bar{v}_A, \gamma) - \bar{s}_A \bar{v}_A\|^2
= 2\bar{d}_A^2 \bar{s}_A^2 (1 - \cos \gamma),
\] (4.12)

using \( \bar{v}_N = 0 \), thus \( \bar{s}_A \bar{v}_A = -\bar{s}_B \bar{v}_B - \bar{s}_S \bar{v}_S \) for optimal realizations and using Lemma 4.14.

For choosing an appropriate affine subspace \( \mathcal{H} \) we have to consider the two cases that the origin is not contained in the affine hull of the separator and the second that it is contained.
Case 1: $p_0 \neq 0$. We choose $b := \frac{p_0}{\|p_0\|}$.

For $u \perp b$ and because of $\bar{v}_N = 0$ and (4.6)

$$0 = \bar{s}_A b^\top \bar{v}_A + \bar{s}_B b^\top \bar{v}_B + \bar{s}_S b^\top \bar{v}_S = \bar{s}_N \|p_0\| + \bar{s}_A \bar{d}_A \cos \bar{\alpha}_A + \bar{s}_B \bar{d}_B \cos \bar{\alpha}_B \tag{4.13}$$

thus

$$\cos \bar{\alpha}_B = -\frac{\bar{s}_N \|p_0\|}{\bar{s}_B \bar{d}_B} - \frac{\bar{s}_A \bar{d}_A \cos \bar{\alpha}_A}{\bar{s}_B \bar{d}_B} \tag{4.14}$$

holds.

In specifying $u$ we have to consider the two cases $\text{lin}(V_S) \neq \mathcal{L}$ and $\text{lin}(V_S) = \mathcal{L}$. We illustrate the cases in Figure 4.7.

Figure 4.7: Case 1, where $p_0 \neq 0$. On one hand $\text{lin}(S) \neq \mathcal{L}$ and on the other hand $\text{lin}(S) = \mathcal{L}$.

First suppose $\text{lin}(V_S) \neq \mathcal{L}$. Choose $u \in \mathcal{L}$, with $u \perp \text{lin}(V_S)$ and $\|u\| = 1$. Then $\text{aff}(V_S) \subseteq \mathcal{H}$ and the realization $\varphi(v_i, \gamma)$ ($i \in N$) of (4.11), fulfills the distance constraints for appropriate $\gamma$, as already discussed.

Next we consider $\gamma$ in more detail for the purpose of calculating the normalization constraint of $\varphi(v_i, \gamma)$ for $i \in N$.

As $\bar{v}_A \notin \mathcal{S}$ and the barycenter of the graph is in the origin we get

$$\bar{v}_B \notin \text{lin}(V_S) \quad \text{(because $\bar{v}_A \notin \text{lin}(V_S)$ by $\mathcal{L} \neq \text{lin}(V_S)$)} \quad \text{and} \quad \bar{v}_B \in \mathcal{L} \quad \text{(because $\bar{v}_A \in \mathcal{L}$)}.$$

Thus

$$\begin{aligned}
&\quad \begin{cases}
\frac{1}{\bar{s}_N} (\bar{s}_A \bar{v}_A + \bar{s}_B \bar{v}_B + \bar{s}_S \bar{v}_S) = \frac{\bar{s}_A}{\bar{s}_N} u^\top \bar{v}_A + \frac{\bar{s}_B}{\bar{s}_N} u^\top \bar{v}_B = 0 \quad \text{(4.15)}
\end{cases} \\
&= 0
\end{aligned}$$
and because of (4.6) and (4.15) we obtain

\[ 0 = \bar{s}_A u^\top \bar{v}_A + \bar{s}_B u^\top \bar{v}_B = \bar{s}_A \bar{d}_A \sin \bar{\alpha}_A + \bar{s}_B \bar{d}_B \sin \bar{\alpha}_B \iff \sin \bar{\alpha}_B = -\frac{\bar{s}_A \bar{d}_A}{\bar{s}_B \bar{d}_B} \sin \bar{\alpha}_A. \]  \hspace{1cm} (4.16)

Because \( \bar{v}_A \notin \text{lin}(V_S) \) we have \( \bar{\alpha}_A \notin \{0, \pi\} \) and by the former equation

\[ (\bar{\alpha}_A \in (0, \pi) \Rightarrow \bar{\alpha}_B \in (\pi, 2\pi)) \text{ or } (\bar{\alpha}_A \in (\pi, 2\pi) \Rightarrow \bar{\alpha}_B \in (0, \pi)). \]

We choose

\[ \gamma > 0, \text{ for } \bar{\alpha}_A \in (0, \pi) \]
\[ \gamma < 0, \text{ otherwise}. \]  \hspace{1cm} (4.17)

Now we are able to consider the normalization constraint of \( \varphi(v_i, \gamma) \) for \( i \in N \). For this we use the representation (4.10). Because of Lemma 4.14 only two terms change: the distance of the barycenters of \( A \) and \( B \) and the squared norm of the new realization’s barycenter.

\[ \| \varphi(\bar{v}_A, \gamma) - \bar{v}_B \|^2 \]
\[ = \| \bar{v}_A - \bar{v}_B \|^2 + 2 \bar{d}_A \bar{d}_B (\cos(\bar{\alpha}_A - \bar{\alpha}_B) - \cos(\bar{\alpha}_A - \bar{\alpha}_B + \gamma)) \]
\[ = \| \bar{v}_A - \bar{v}_B \|^2 + 2 \bar{d}_A \bar{d}_B [\cos \bar{\alpha}_B (\cos \bar{\alpha}_A - \cos(\bar{\alpha}_A + \gamma)) + \sin \bar{\alpha}_B (\sin \bar{\alpha}_A - \sin(\bar{\alpha}_A + \gamma))]. \]

With (4.14) and (4.16) we get

\[ \| \varphi(\bar{v}_A, \gamma) - \bar{v}_B \|^2 + \| \varphi(\bar{v}_N, \gamma) \|^2 \]
\[ = \| \bar{v}_A - \bar{v}_B \|^2 + \frac{2 \bar{d}_A}{\bar{s}_B} \left[ \bar{s}_N \| p_0 \| \left[ \cos(\bar{\alpha}_A + \gamma) - \cos \bar{\alpha}_A \right] \right. \]
\[ - \bar{s}_A \bar{d}_A \left[ \cos \bar{\alpha}_A (\cos \bar{\alpha}_A - \cos(\bar{\alpha}_A + \gamma)) + \sin \bar{\alpha}_A (\sin \bar{\alpha}_A - \sin(\bar{\alpha}_A + \gamma)) \right] \]
\[ = \| \bar{v}_A - \bar{v}_B \|^2 + \frac{2 \bar{d}_A}{\bar{s}_B} \left[ \bar{s}_N \| p_0 \| \left[ \cos(\bar{\alpha}_A + \gamma) - \cos \bar{\alpha}_A \right] + \bar{s}_A \bar{d}_A \left[ \cos \gamma - 1 \right] \right]. \]

Thus, with \( \bar{s}_N = \bar{s}_A + \bar{s}_B + \bar{s}_s, (4.12), (4.17) \) and \( |\gamma| \) small enough this results in

\[ \| \varphi(\bar{v}_A, \gamma) - \bar{v}_B \|^2 + \| \varphi(\bar{v}_N, \gamma) \|^2 \]
\[ = \| \bar{v}_A - \bar{v}_B \|^2 + \frac{2 \bar{d}_A \bar{s}_N \| p_0 \|}{\bar{s}_B} \left[ \cos(\bar{\alpha}_A + \gamma) - \cos \bar{\alpha}_A \right] + \left( \frac{2 \bar{d}_A^2 \bar{s}_A}{\bar{s}_B} - \frac{2 \bar{d}_A^2 \bar{s}_A^2}{\bar{s}_B^2} \right) \left[ \cos \gamma - 1 \right] \]
\[ = \| \bar{v}_A - \bar{v}_B \|^2 + \frac{2 \bar{d}_A \bar{s}_N \| p_0 \|}{\bar{s}_B} \left[ \cos(\bar{\alpha}_A + \gamma) - \cos \bar{\alpha}_A \right] + 2 \bar{d}_A^2 \bar{s}_A \left( \frac{\bar{s}_N^2 - \bar{s}_A \bar{s}_B}{\bar{s}_B \bar{s}_N^2} \right) \left[ \cos \gamma - 1 \right] \]
\[ < \| \bar{v}_A - \bar{v}_B \|^2 \]

Hence \( \sigma = \sum_{i \in N} s_i \| \varphi(v_i, \gamma) \|^2 < 1 \) which contradicts optimality of \( v_i \) (\( i \in N \)) by Remark 4.6.
Now consider the case \( \text{lin}(V_S) = \mathcal{L} \). Let \( u \in \mathbb{R}^n \setminus \mathcal{L} \) with \( u \perp \{v_1, \ldots, v_n\} \) and \( \|u\| = 1 \).

Then \( \text{aff}(V_S) \subseteq \mathcal{H} \) and the realization \( \varphi(v_i, \gamma) \) \((i \in N)\) of (4.11) satisfies the distance constraints for \( |\gamma| \) small enough.

As the graph’s barycenter is in the origin we have \( \bar{v}_B \in \mathcal{S} \) but \( \bar{v}_B \notin \text{aff}(V_S) \) because \( \bar{v}_A \notin \mathcal{S} \).

In the normalization constraint again the distance of the two barycenters of \( A \) and \( B \) and the squared norm of the realization’s barycenter change. By \( \bar{v}_B \in \mathcal{S} \) and the special choice of \( u \)

\[
\bar{\alpha}_A = 0, \quad \bar{\alpha}_B = \pi \quad \Rightarrow \quad \bar{\alpha}_A - \bar{\alpha}_B = -\pi.
\]

Thus, by Lemma 4.14,

\[
\| \varphi(\bar{v}_A, \gamma) - \bar{v}_B \|^2 \\
= \| \bar{v}_A - \bar{v}_B \|^2 + 2\bar{d}_A\bar{d}_B(\cos(\bar{\alpha}_A - \bar{\alpha}_B) - \cos(\bar{\alpha}_A - \bar{\alpha}_B + \gamma)) \\
= \| \bar{v}_A - \bar{v}_B \|^2 + 2\bar{d}_A\bar{d}_B(\cos \gamma - 1)
\]

and, using (4.13) and \( \bar{\alpha}_A = 0, \bar{\alpha}_B = \pi \),

\[
\bar{s}_A\bar{d}_A = \bar{s}_B\bar{d}_B - \bar{s}_N\|p_0\|
\]

we get with (4.12)

\[
\| \varphi(\bar{v}_A, \gamma) - \bar{v}_B \|^2 + \| \varphi(\bar{v}_N, \gamma) \|^2 \\
= \| \bar{v}_A - \bar{v}_B \|^2 + \left( 2\bar{d}_A\bar{d}_B - \frac{2\bar{d}_A^2\bar{s}_A^2}{\bar{s}_N^2} \right)(\cos \gamma - 1) \\
= \| \bar{v}_A - \bar{v}_B \|^2 + \frac{2\bar{d}_A}{\bar{s}_N^2}(\bar{d}_B\bar{s}_N^2 - \bar{d}_A\bar{s}_A^2)(\cos \gamma - 1) \\
= \| \bar{v}_A - \bar{v}_B \|^2 + \frac{2\bar{d}_A}{\bar{s}_N^2}(\bar{d}_B\bar{s}_N^2 - \bar{d}_A\bar{s}_A^2 + \bar{s}_A\bar{s}_N\|p_0\|)(\cos \gamma - 1) \\
< \| \bar{v}_A - \bar{v}_B \|^2
\]

Therefore, as before, \( \sigma = \sum_{i \in N} s_i\|\varphi(v_i, \gamma)\|^2 < 1 \).

**Case 2:** \( p_0 = 0 \). Compare Figure 4.8. As the barycenter of the graph is in the origin, \( \bar{v}_B \notin \mathcal{S} \).

Let \( \bar{p}_A \) be the projection of \( \bar{v}_A \) onto the affine hull of \( V_S \). Let \( b := \frac{\bar{p}_A}{\|\bar{p}_A\|}, \ u \in \mathbb{R}^n, \ u \perp \{v_1, \ldots, v_n\}, \|u\| = 1 \). Then \( \text{aff}(V_S) \subseteq \mathcal{H} \). Thus for \( |\gamma| > 0 \) small enough the realization \( \varphi(v_i, \gamma) \) of (4.11) fulfills the distance constraints.

Because of the special choice of \( u \) and \( b \) we obtain \( \bar{\alpha}_I \in \{0, \pi\} \) \((I \in \{A, B\})\) and \( \bar{\alpha}_A \neq \bar{\alpha}_B \) (the barycenters lie on different sides of the affine hull).
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With Lemma 4.14 we obtain
\[
\|\varphi(\vec{v}_A, \gamma) - \vec{v}_B\|^2 \\
= \|\vec{v}_A - \vec{v}_B\|^2 + 2\bar{d}_A\bar{d}_B(\cos(\bar{\alpha}_A - \bar{\alpha}_B) - \cos(\bar{\alpha}_A - \bar{\alpha}_B + \gamma)) \\
= \|\vec{v}_A - \vec{v}_B\|^2 + 2\bar{d}_A\bar{d}_B(\cos \gamma - 1),
\]
thus, using (4.12),
\[
\|\varphi(\vec{v}_A, \gamma) - \vec{v}_B\|^2 + \|\varphi(\vec{v}_N, \gamma)\|^2 < \|\vec{v}_A - \vec{v}_B\|^2
\]
like in the previous case. Again \( \sigma = \sum_{i \in N} s_i\|\varphi(v_i, \gamma)\|^2 < 1. \)

In order to motivate the name “sunny side” denote the projection of the origin onto \( \text{aff}(V_S) \) by \( p_0 \), then
\[
\text{aff}(V_S) - \text{cone}(V_S) = \{v - \alpha p_0 : v \in \text{aff}(V_S), \alpha \geq 0\}.
\]
If \( 0 \notin \text{aff}(V_S) \) then this is the half space in \( \text{lin}(V_S) \) containing the origin.

If the origin is viewed as the sun, then the barycenter of \( V_A \) lies in the sunny half space with respect to the affine hull of \( V_S \), where \( S \) separates \( A \) from the - possibly empty - rest of the graph. Thus Theorem 4.13 characterizes a folding property of optimal realizations of \( (E_{\lambda_n}). \)

For example, consider the graph of the left hand side of Figure 4.9 with data \( s = 1 \) and \( l = 1 \). The node set \( S = \{3, 4\} \) forms a separator leading to the components \( A = \{1, 2\} \) (marked in blue) and \( B = \{5, 6\} \) (marked in green). An optimal two-dimensional realization is given on the right hand side of Figure 4.9. The red circle displays the origin, the dotted line displays the affine hull of the separator. Indeed, the barycenters \( \vec{v}(A) \) and \( \vec{v}(B) \) of both components \( A \) and \( B \), respectively, lie on the sunny side of the separator’s affine hull.

While the Separator-Shadow Theorem, Theorem 3.10, ensures that every single node of at least one of the separated node sets lies in the shadow of the convex hull of the separator, the current theorem is limited to the barycenter of the node sets but holds for all separated node sets at the same time.

Figure 4.8: Case 2, where \( p_0 = 0 \).
Figure 4.9: In an optimal realization, not all nodes need to lie on the sunny side of the separator.

It is not possible to extend the result to all nodes. This is also illustrated in Figure 4.9. In this optimal realization the nodes 1 and 6 are not in $\text{aff}(V_S) - \text{cone}(V_S)$, hence both components have one node on the sunny side and one node in the shadow of the separator's affine hull.

### 4.4 Tree-Width Bound

Depending on the separator structure of the graph, there always exist optimal realizations of rather small dimension. The next result depends on the tree-width of a graph and is an analogous result for $(E_{\lambda_n})$ to Theorem 3.14 for $(E_{\lambda_2})$. In general, it is $NP$-complete to determine the tree-width, but any valid tree-decomposition provides an upper bound.

**Theorem 4.15 (Tree-Width Bound)** For each graph $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$ there exists an optimal realization of $(E_{\lambda_n})$ of dimension at most 1 if $\text{tw}(G) = 1$ and $\text{tw}(G) + 1$ otherwise.

**Proof.** We will prove the tree-width theorem algorithmically by implicitly exploiting the property of any tree-decomposition $(T, \mathcal{N} = (N_t)_{t \in T})$ that for adjacent nodes $t$ and $t'$ in $T$ the node set $N_t \cap N_{t'}$ is a separator of $G$ (see Lemma 2.17).

Graphs with $\text{tw}(G) = 1$ are trees. For these the theorem follows from Theorem 4.8. So we may assume $\text{tw}(G) > 1$. 
Given any tree-decomposition \((T, \mathcal{N} = (N_t)_{t \in T})\) of \(G\) and an optimal realization \(V = [v_1, \ldots, v_n]\) and optimal \(\xi\) of \((\mathcal{E}_N, \mu)\), put \(\mathcal{L}_t := \text{lin}(V_{N_t})\) and let
\[
d^* := \max\{\dim \mathcal{L}_t : t \in T\}
\]
denote the maximum dimension spanned by any bag \(N_t\). Let \(t^* \in T\) be a node, for which \(d^*\) is attained. Starting from \(V\) we show how to construct an optimal realization \(V' = [v'_1, \ldots, v'_n]\) with \(v'_i \in \mathcal{L}_{t^*}\) for \(i \in N\). Because \(\dim \mathcal{L}_{t^*} \leq |N_{t^*}|\), the dimension of the new realization is bounded by the width of the tree-decomposition plus one. As there is a tree-decomposition of width \(\text{tw}(G)\) this proves the theorem.

Consider \(t^*\) as the root of the tree \(T\). Let \(\hat{t} \in T\) be a node with \(\mathcal{L}_\hat{t} \not\subset \mathcal{L}_{t^*}\), but \(\mathcal{L}_t \subset \mathcal{L}_{t^*}\) for all other \(t\) on the tree-path from \(\hat{t}\) to \(t^*\) (if no such \(\hat{t}\) exists, then \(v_i \in \mathcal{L}_{t^*}\) for all \(i \in N\) and we are done). Let \(\hat{T} \subset T\) denote the set of all successors \(t' \in T\) for which \(\hat{t}\) is on the tree-path from \(t'\) to \(t^*\) (so \(\hat{t} \in \hat{T}\)), put \(\hat{N} := \bigcup_{t \in \hat{T}} N_t\) and \(\bar{N} := \bigcup_{t \in \hat{T} \setminus \hat{t}} N_t\). It suffices to transform \(V\) to an optimal realization \(V' = [v'_1, \ldots, v'_n]\) with \(v'_i = v_i\) for \(i \in \bar{N}\), \(v'_i \in \mathcal{L}_{t^*}\) for \(i \in N_{\bar{N}}\) and \(\dim \text{lin}(V'_{N_t}) = \dim \mathcal{L}_t\) for \(t \in T\), because then this step can be repeated inductively until there is no node \(t \in T\) with \(\mathcal{L}_t \not\subset \mathcal{L}_{t^*}\).

Next let \(p \in T\) be the \((\text{predecessor})\) node adjacent to \(\hat{t}\) on the tree-path from \(\hat{t}\) to \(t^*\). By assumption, \(\mathcal{L}_p \subset \mathcal{L}_{t^*}\) and \(d := \dim \mathcal{L}_t \leq d^*\). The points of \(S := N_{\bar{N}} \cap N_p\) span a (possibly empty) common subspace \(S := \text{lin}(V_S) \subset \mathcal{L}_{t^*} \cap \mathcal{L}_t\) whose dimension is denoted by \(d_S\). Choose an orthonormal basis \(\{e_1, \ldots, e_{d_S}\}\) of \(S\), extend it to an orthonormal basis of \(\mathcal{L}_{t^*}\) by \(\{e_1, \ldots, e_{d_S}, \ldots, e_d\}\) and then to an orthonormal basis of \(\mathbb{R}^n\) by \(\{e_1, \ldots, e_{d_S}, \ldots, e_d, \ldots, e_n\}\). Likewise, extend \(\{e_1, \ldots, e_{d_S}\}\) to an orthonormal basis of \(\mathcal{L}_t\) by \(\{e_1, \ldots, e_{d_S}, f_{d_S+1}, \ldots, f_d\}\) and this again to an orthonormal basis of \(\mathbb{R}^n\) by \(\{e_1, \ldots, e_{d_S}, f_{d_S+1}, \ldots, f_d, \ldots, f_n\}\). Using the orthogonal matrices \(P := [e_1, \ldots, e_n]\) and \(\bar{P} := [e_1, \ldots, e_{d_S}, f_{d_S+1}, \ldots, f_n]\), the new realization is defined by
\[
v'_i := \begin{cases} v_i & \text{for } i \in N \setminus \bar{N}, \\ \bar{P}\bar{P}^\top v_i & \text{for } i \in \bar{N}. \end{cases}
\]

Note that by construction, \(v'_i = v_i\) for \(i \in S\) and \(v'_i \in \mathcal{L}_{t^*}\) for \(i \in N_{\bar{N}}\). Due to property 3 of Definition 2.16 we have \(S = \bar{N} \cap \bar{N}\). Therefore \(v'_i = v_i\) for \(i \in \bar{N}\). If \(t \in T \setminus \hat{T}\) then \(N_t \subseteq \bar{N}\) and so \(\|v'_i - v'_j\| = \|v_i - v_j\|\) for all \(\{i, j\} \subseteq N_t\). For \(t \in \hat{T}\) there holds \(N_t \subseteq \bar{N}\), so \(\|v'_i - v'_j\| = \|\bar{P} \bar{P}^\top (v_i - v_j)\| = \|v_i - v_j\|\) for all \(\{i, j\} \subseteq N_t\). By property 2 of Definition 2.16, for each \(ij \in E\) there is a \(t \in T\) with \(ij \in N_t\), thus \(V'\) is feasible. Furthermore, \(\|v'_i\| = \|v_i\|\) for \(i \in N\), so the new realization is again optimal. Let \(\mathcal{L}'_{t} := \text{lin}(V'_{N_t})\) for \(t \in T\), then we see that \(\mathcal{L}'_{t} = \mathcal{L}_t\) for \(t \in T \setminus \hat{T}\) and (in slight abuse of notation) \(\mathcal{L}'_{t} = \bar{P}\bar{P}^\top \mathcal{L}_t\) for \(t \in \hat{T}\), so \(\dim \mathcal{L}'_{t} = \dim \mathcal{L}_t\) for \(t \in T\), which completes the proof.

Note, that on the one hand the tree-width bound of Theorem 4.15 may be arbitrarily bad. For example consider the \(n \times n\) grid which is a bipartite graph on \(n^2\) nodes. Its tree-width equals \(n\) (see [80]). While the tree-width bound ensures the existence of an
optimal \((n + 1)\)-dimensional realization there exists an optimal one-dimensional one by Theorem 4.8.

On the other hand the tree-width bound may not be improved in general. By the following example we present a family of graphs for which the bound of Theorem 4.15 is tight.

**Example 4.16 (Graphs With Tight Dimension Bound)** To each node of \(K_d\) append an additional node and consider the complement of this graph, i.e., set \(D := \{1, \ldots, d\}\), \(N := \{1, \ldots, 2d\}\), and

\[
G(d) := (N, \{ij: i, j \in D, i \neq j\} \cup \{ij: i \in D, j \in N \setminus (D \cup \{d+i\})\}).
\]

Let \(s = 1\) and \(l = 1\).

By construction \(G(d)\) has tree-width \(\text{tw}(G(d)) = d - 1\). For \(d > 2\) there is a unique optimal solution \(\xi, [v_1, \ldots, v_n]\) of \((E_{\lambda_n})\) (up to congruence) and its dimension is \(d\). In order to prove this, set \(N_i := \{d+i\} \cup D \setminus \{i\}\) for \(i \in D\) and introduce weights \(s'_j := \frac{1}{d-1}\) for \(j \in D\) and \(s'_j := 1\) for \(j \in N \setminus D\).

We first bound the normalization constraint using (4.5) of Example 4.9 on each weighted sub sum for \(i \in D\),

\[
1 = \sum_{k \in N} \|v_k\|^2 = \sum_{i \in D} \sum_{j \in N_i} s'_j \|v_j\|^2 \geq \sum_{i \in D} \frac{\xi}{2s'(N_i)} \left(s'(N_i)^2 - \sum_{j \in N_i} s'_j^2\right) = \xi d \frac{3d - 4}{4(d - 1)}.
\]

By Example 4.9, equality holds if and only if

\[
\forall i \in D: \sum_{j \in N_i} s'_j v_j = 0 \land \forall j, k \in N_i, j \neq k: \|v_j - v_k\|^2 = \xi
\]

and therefore we put \(\xi = \frac{4(d-1)}{d(3d-4)}\) and show that it can be attained.

Such a realization can be constructed and it is uniquely determined up to congruence, because

1. \(\|v_i\| = \|v_j\|\) for \(i, j \in D\) by the concluding remark of Example 4.9,
2. \(\|v_i - v_j\|^2 = \xi\) for \(i, j \in D\) with \(i \neq j\), so \(\operatorname{conv}(V_D)\) forms a regular simplex with all vertices having the same distance to the origin (thus for \(D' \subseteq D\), the barycenter \(\bar{v}(D')\) is the projection of \(0\) onto the simplex corresponding to \(D')\),
3. \(v_{d+i} = -\bar{v}(D \setminus \{i\})\) for \(i \in D\) by the choice of \(s'\). Because \(\operatorname{conv}(V_{N_i})\) forms a regular simplex with all edge lengths equal to \(\xi\), this relation allows to compute \(\|v_{d+i}\|\) and \(\|v_i\|\) explicitly, fixing all relative positions uniquely up to congruence. Note, by \(\bar{v}(N_i) = \frac{1}{d}v_{d+i} + \frac{d-1}{d}\bar{v}(D \setminus \{i\})\) we obtain \(\|v_{d+i}\| < \|v_j\|\) \((j \in D)\) and \(\|\bar{v}(D)\| > 0\).
The last fact implies $0 \notin \text{conv}(V_D)$, so the dimension of this realization is $d$.

The case $d = 3$ is illustrated in Figure 4.10. Note, in an optimal 2-dimensional solution all triangles are folded on top of the central triangle, i.e., $v_i = v_{i+3}$ for $i = 1, 2, 3$, the resulting objective value being $\xi = \frac{1}{2}$. The optimal realization, however, (see Figure 4.10 on the right) needs one dimension more and has objective value $\xi = \frac{8}{15}$.

Figure 4.10: Graph with tight dimension bound, for $d = 3$. The optimal solution is not $d - 1$ but $d$-dimensional. See Example 4.16.

Let us have another look at Chapter 3. The Tree-Width Bound of $(E_{\lambda_2}\text{-s})$, Theorem 3.14, is closely linked to the rotational dimension of a graph as it is a bound on the minimal dimension of optimal realizations of $(E_{\lambda_2}\text{-s})$. In Theorem 3.13 it turned out to be a minor monotone graph property.

We want to proceed in a similar way for the maximum eigenvalue and define for a graph $G = (N, E)$ and data $s > 0$ and $l > 0$

$$d_G^{\lambda_{\text{max}}}(s, l) := \min \{\dim \text{lin}(V_N) : V \text{ is optimal for } (E_{\lambda_n})\}$$

with $\dim \emptyset = -1$ by definition. Furthermore let

$$d^{\lambda_{\text{max}}}(G) := \max \left\{d_G^{\lambda_{\text{max}}}(s, l) : s \in \mathbb{R}^{|N|}, \ s > 0, \ l \in \mathbb{R}^{|E|}, \ l > 0 \right\}.$$ 

In contrast to the rotational dimension of a graph $G$, $d^{\lambda_{\text{max}}}(G)$ is not minor monotone:

For a complete graph $K_n$ with $s > 0$ and $l = c1$ for real $c > 0$ we have $d^{\lambda_{\text{max}}}(K_n) = n - 1$ because of Example 4.9. But each $K_n$ is a minor of a bipartite graph (subdivide each edge of $K_n$ exactly once), and by Theorem 4.8, bipartite graphs $G$ have $d^{\lambda_{\text{max}}}(G) = 1$. So, at this time, this parameter seems less promising than the rotational dimension.
4.5 A Scaled Primal-Dual Pair

This section introduces scaled versions of \((P_{\lambda_n})\), \((D_{\lambda_n})\) and \((E_{\lambda_n})\) similar to the scaled programs \((P_{\lambda_2}-s)\), \((D_{\lambda_2}-s)\) and \((E_{\lambda_2}-s)\) in Chapter 3. They enable slightly different interpretations and other views on the problems which may help to get better geometric intuition.

As already mentioned the optimal value of \((P_{\lambda_n})\), thus all feasible \(\lambda_n\) are strictly greater than zero. Dividing all constraints by \(\lambda_n\) and considering new variables \(\hat{w}_{ij} := \frac{w_{ij}}{\lambda_n}\) we eliminate \(\lambda_n\) from \((P_{\lambda_n})\):

\[
\begin{align*}
\text{minimize} & \quad \lambda_n \\
\text{subject to} & \quad I - \sum_{ij \in E} \hat{w}_{ij} D E_{ij} D \succeq 0, \\
& \quad \sum_{ij \in E} l_{ij}^2 \hat{w}_{ij} = \frac{1}{\lambda_n}, \\
& \quad \lambda_n \in \mathbb{R}, \quad \hat{w} \geq 0.
\end{align*}
\]

Replacing the objective function by the second constraint we arrive at the scaled primal program

\[
\begin{align*}
\text{maximize} & \quad \sum_{ij \in E} l_{ij}^2 \hat{w}_{ij} \\
\text{subject to} & \quad I - \sum_{ij \in E} \hat{w}_{ij} D E_{ij} D \succeq 0, \\
& \quad \hat{w} \geq 0.
\end{align*}
\]

\((P_{\lambda_n}-s)\)

The semidefinite dual of \((P_{\lambda_n}-s)\) reads

\[
\begin{align*}
\text{minimize} & \quad \langle I, \hat{Y} \rangle \\
\text{subject to} & \quad \langle DE_{ij} D, \hat{Y} \rangle \geq l_{ij}^2 (ij \in E), \\
& \quad \hat{Y} \succeq 0.
\end{align*}
\]

\((D_{\lambda_n}-s)\)

Using again the Gram representation \(D \hat{Y} D = \hat{V}^\top \hat{V} \) with \(\hat{V} = [\hat{v}_1, \ldots, \hat{v}_n]\) we get a graph realization (embedding) problem

\[
\begin{align*}
\text{minimize} & \quad \sum_{i \in N} s_i \|\hat{v}_i\|^2 \\
\text{subject to} & \quad \|\hat{v}_i - \hat{v}_j\|^2 \geq l_{ij}^2 (ij \in E), \\
& \quad \hat{v}_i \in \mathbb{R}^n (i \in N).
\end{align*}
\]

\((E_{\lambda_n}-s)\)

In \((E_{\lambda_n}-s)\) data \(l_{ij} (ij \in E)\) indeed represents a lower bound on the edge length of edge \(ij\). Optimal realizations satisfy these bounds and have a minimal sum of weighted squared norms. In other words the nodes are embedded as close as possible to the origin but are restricted by the bounds on the edge length.

Note, that the trivial solution \(\hat{w} = 0\) is strictly feasible for \((P_{\lambda_n}-s)\) with respect to the semidefinite constraint. For a feasible dual solution let \(\bar{l} := \max\{l_{ij} : ij \in E\} > 0\) and \(Y_{ii} = s_i \bar{l}^2\) for \(i \in N\) and zero otherwise.
Now strong duality and attainment follow from Corollary 2.15 and the boundedness of the feasible edge weights (cf. proof of Proposition 4.1).

**Proposition 4.17 (Strong Duality)** Let $G = (N, E \neq \emptyset)$ be a graph with given data $s > 0$ and $0 \neq l \geq 0$. Strong duality holds for $(P_{\lambda-n})$ and $(D_{\lambda-n})$ and both programs attain their optimal value.

By the previous discussion it is quite natural that we may compute optimal solutions of $(P_{\lambda-n})$ ($D_{\lambda-n}$) and $(E_{\lambda-n})$ from optimal solutions of $(P_{\lambda-n})$ ($D_{\lambda-n}$) and $(E_{\lambda-n})$ and vice versa.

**Proposition 4.18** Let $G = (N, E \neq \emptyset)$ be a graph with given data $s > 0$ and $0 \neq l \geq 0$. There exist transformations, which map optimal solutions of $(P_{\lambda-n})$, $(D_{\lambda-n})$ and $(E_{\lambda-n})$ to optimal solutions of $(P_{\lambda-n})$, $(D_{\lambda-n})$ and $(E_{\lambda-n})$ with same data $s$ and $l$, and vice versa. In addition, the active and the strictly active subgraphs are the same.

**Proof.** The transformations are listed in Table 4.1. As they are appropriate scalings (with scaling factor $> 0$), feasibility holds and the active and strictly active subgraphs are the same. Optimality follows from strong duality.

<table>
<thead>
<tr>
<th>Optimal solutions</th>
<th>⇒</th>
<th>⇐</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda^<em>_n$, $w^</em>$ of $(P_{\lambda-n})$, $\xi^<em>$, $Y^</em>$ of $(D_{\lambda-n})$, $\xi^<em>$, $v^</em><em>i$ ($i \in N$) of $(E</em>{\lambda-n})$, $\hat{w}^<em>$ of $(P_{\lambda-n})$, $\hat{Y}^</em>$ of $(D_{\lambda-n})$, $\hat{v}^*<em>i$ ($i \in N$) of $(E</em>{\lambda-n})$.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(P_{\lambda-n}) \Leftrightarrow (P_{\lambda-n})$</td>
<td>$\hat{w}<em>{ij} = \frac{w</em>{ij}^<em>}{\lambda_n^</em>}$ ($ij \in E$)</td>
<td>$\lambda_n = \frac{1}{\sum_{ij \in E} \hat{w}<em>{ij}^*}$, $w</em>{ij} = \frac{\hat{w}<em>{ij}^*}{\sum</em>{ij \in E} \hat{w}_{ij}^*}$ ($ij \in E$)</td>
</tr>
<tr>
<td>$(D_{\lambda-n}) \Leftrightarrow (D_{\lambda-n})$</td>
<td>$\hat{Y} = \frac{1}{\xi^<em>}Y^</em>$</td>
<td>$\xi = \frac{1}{\langle I, Y^* \rangle}$, $Y = \frac{1}{\langle I, Y^* \rangle}\hat{Y}^*$</td>
</tr>
<tr>
<td>$(E_{\lambda-n}) \Leftrightarrow (E_{\lambda-n})$</td>
<td>$\hat{v}_i = \frac{1}{\sqrt{\xi^<em>}}v^</em>_i$ ($i \in N$)</td>
<td>$\xi = \sum_{i \in N} s_i |v^<em><em>i|^2$, $v_i = \frac{1}{\sum</em>{i \in N} s_i |v^</em>_i|^2} \hat{v}^*_i$ ($ij \in E$)</td>
</tr>
</tbody>
</table>

Table 4.1: Transformations of optimal solutions of $(P_{\lambda-n})$, $(D_{\lambda-n})$ and $(E_{\lambda-n})$ on optimal solutions of $(P_{\lambda-n})$, $(D_{\lambda-n})$ and $(E_{\lambda-n})$ and vice versa.
Let us consider an optimal realization of a graph for \((E_{\lambda_n}s)\) with given data. Because of propositions 4.4 and 4.18 its barycenter is in the origin. If we move this realization in \(\mathbb{R}^n\), its structure is still the same, \(e.g.,\) the distances of every two nodes have not changed.

In fact, we may reformulate the graph realization problem independent from the position of a realization's barycenter by reformulating the objective function.

Because of Lemma 2.10 the objective function may be bounded by

\[
\sum_{i \in \mathcal{N}} s_i \|v_i\|^2 = \bar{s}(N)\|\bar{v}(N)\|^2 + \sum_{i \in \mathcal{N}} s_i \|v_i - \bar{v}(N)\|^2 \geq \frac{1}{2\bar{s}(N)} \sum_{i,j \in \mathcal{N}} s_i s_j \|v_i - v_j\|^2.
\]

Equality holds if the barycenter of the realization coincides with the origin. Since the bound does not depend on the absolute positions of the embedded nodes, the minimum of the bound is also the minimum of the objective function. Hence, considering the problem

\[
\begin{align*}
\text{minimize} & \quad \sum_{i,j \in \mathcal{N}} s_i s_j \|v_i - v_j\|^2 \\
\text{subject to} & \quad \|v_i - v_j\|^2 \geq l^2_{ij} \quad (i,j \in E), \\
& \quad v_i \in \mathbb{R}^n \quad (i \in \mathcal{N}),
\end{align*}
\]

we obtain the following result.

**Proposition 4.19** Each optimal solution of \((E_{\lambda_n}s)\) is an optimal solution of \((E_{\lambda_n}b)\) with the same active subgraph.

For \(s = 1\) the objective function of \((E_{\lambda_n}b)\) is also known as the variance of the data \(v_i\) (see, \(e.g.,\) [35, 94]), it appears in statistics (see, \(e.g.,\) [58]) and as the moment of inertia of rotating rigid bodies in physics (see, \(e.g.,\) [22]).

### 4.6 Variable Edge Length Parameters

Like in the \(\lambda_2\) case, Proposition 4.2 states that optimal realizations are maps of eigenvectors to the minimal maximum eigenvalue of the corresponding optimal weighted Laplacian. For edge transitive graphs they are even maps of the eigenvectors to the maximum eigenvalue of the Laplacian itself (see Corollary 4.12).

Based on the scaled graph realization problem \((E_{\lambda_n}s)\) with node parameter \(s = 1\) we formulate a program with variable edge length parameters, such that optimal realizations are maps of the eigenvectors to the maximum eigenvalue of the unweighted Laplacian.

Therefore we replace the squared edge length parameters \(l^2_{ij}\) by real variables \(d_{ij}\) \((i,j \in E)\) and insert an additional normalization constraint into the graph realization formulation.
Graph $G = (N, E \neq \emptyset)$.

<table>
<thead>
<tr>
<th>primal</th>
<th>dual</th>
</tr>
</thead>
<tbody>
<tr>
<td>max $\rho$ s.t. $\sum_{ij \in E} w_{ij} E_{ij} \preceq I$, $\rho - w_{ij} = 0$ $(ij \in E)$, $w \geq 0$, $\rho \geq 0$</td>
<td>min $\langle I, Y \rangle$ s.t. $\sum_{ij \in E} d_{ij} \geq 1$, $\langle E_{ij}, Y \rangle \geq d_{ij}$ $(ij \in E)$, $d_{ij} \in \mathbb{R}$ $(ij \in E)$, $Y \succeq 0$</td>
</tr>
</tbody>
</table>

Table 4.2: Primal, dual and graph realization formulation with variable edge length parameters.

The so obtained graph realization program and the corresponding dual and primal problems are listed in Table 4.2.

For $(P_{\lambda_n}-l)$ and $(D_{\lambda_n}-l)$ strong duality holds.

Proposition 4.20 (Strong Duality) Let $G = (N, E \neq \emptyset)$ be a graph. Strong duality holds for $(P_{\lambda_n}-l)$ and $(D_{\lambda_n}-l)$ and both programs attain their optimal value.

Proof. A strictly feasible solution of $(P_{\lambda_n}-l)$ with respect to the semidefinite constraint is $(\tilde{w} = 0, \tilde{\rho} = 0)$. Thus strong duality follows by Corollary 2.15. Furthermore $Y = I$ and $d = 1$ is a feasible dual solution, thus both feasible sets are not empty and a finite optimal value as well as the attainment of a dual optimal solution follow. As in addition the feasible edge weights are bounded also the primal program attains its optimal solution.

We observe that the optimal value is strictly greater than zero, because $d = 0$ is not feasible for $(E_{\lambda_n}-l)$ thus at least one edge must have positive length. Due to $w = \rho 1$ in
an optimal solution all edge weights are strictly positive. Thus complementarity requires  \( \|v_i - v_j\|^2 = d_{ij} \) for \( ij \in E \) from optimal graph realizations and corresponding distance variables.

In analogy to Section 3.4, optimal realizations of \((E_{\lambda_n} - l)\) may be interpreted as maps of eigenvectors to \( \lambda_{\text{max}}(L(G)) \) and eigenvectors to \( \lambda_{\text{max}}(L(G)) \) yield optimal realizations. While the proofs of the corresponding theorems are similar to these of theorems 3.22 and 3.23 we add them for the sake of completeness.

**Theorem 4.21** Given a connected graph \( G = (N, E \neq \emptyset) \), let \( V = [v_1, \ldots, v_n] \) be an optimal solution of \((E_{\lambda_n} - l)\). Then

\[
\sum_{i \in N} \|v_i\|^2 = \frac{1}{\lambda_{\text{max}}(L(G))}
\]

and for \( h \in \mathbb{R}^n \) the vector \( V^\top h \) is an eigenvector of \( \lambda_{\text{max}}(L(G)) \), unless it is the zero vector.

**Proof.** Because of strong duality the optimal primal equals the optimal dual value, i.e., \( \sum_{i \in N} \|v_i\|^2 = \rho \). The semidefinite constraint of \((P_{\lambda_n} - l)\) then equals \( \frac{1}{\rho} I - L \succeq 0 \) using \( \rho > 0 \). As \( \rho \) is maximal, \( \rho = \sum_{i \in N} \|v_i\|^2 = \frac{1}{\lambda_{\text{max}}(L)} \) follows (see the comments about the semidefinite constraint (3.3) on page 37).

By semidefinite complementarity and an eigenvalue decomposition \( P \Omega P^\top \) of \( \frac{1}{\rho} I - L \) with eigenvalues \( \omega_i \geq 0 \) \((i = 1, \ldots, n)\) we obtain

\[
0 = \left\langle V^\top V, \frac{1}{\rho} I - L \right\rangle = \left\langle V^\top V, P \Omega P^\top \right\rangle = \left\langle I, V P \Omega P^\top V^\top \right\rangle = \sum_{i=1}^n \omega_i (Vp_i)^\top Vp_i,
\]

thus either \( \omega_i = 0 \) or \( Vp_i = 0 \) for \( i \in N \). It follows that

\[
\left( \frac{1}{\rho} I - L \right) V^\top = P \Omega (VP)^\top = P[\omega_1 Vp_1, \ldots, \omega_n Vp_n] = 0
\]

which proves, that the columns of \( V^\top \) are contained in the eigenspace of \( \lambda_{\text{max}}(L) = \frac{1}{\rho} \). \( \blacksquare \)

**Theorem 4.22** Given a connected graph \( G = (N, E \neq \emptyset) \), let \( v \in \mathbb{R}^n, \|v\| = 1 \), be an eigenvector to \( \lambda_{\text{max}}(L(G)) \). An optimal solution of \((E_{\lambda_n} - l)\) is

\[
Y = \frac{1}{\lambda_{\text{max}}(L(G))} vv^\top \quad \text{and} \quad d_{ij} = \frac{1}{\lambda_{\text{max}}(L(G))} ([v]_i - [v]_j)^2 \quad \text{for} \quad ij \in E.
\]
4.6. VARIABLE EDGE LENGTH PARAMETERS

**Proof.** For \(ij \in E\),

\[
\langle E_{ij}, Y \rangle = \frac{1}{\lambda_{\max}(L)} v^\top E_{ij} v = \frac{1}{\lambda_{\max}(L)} ([v]_i - [v]_j)^2 = d_{ij},
\]

thus \(\sum_{ij \in E} d_{ij} = \frac{1}{\lambda_{\max}(L)} v^\top L v = 1\). As \(\langle I, Y \rangle = \frac{1}{\lambda_{\max}(L)}\), optimality follows from Theorem 4.21.

Like in the case of the second smallest eigenvalue an optimal solution of maximum rank to \((D_{\lambda_n^{-1}})\) gives a geometric view of the entire eigenspace of the maximum eigenvalue of the unweighted Laplacian. We obtain a maximum rank solution as follows:

Suppose the columns of \(\hat{V} \in \mathbb{R}^{n \times k}\) with \(\hat{V}^\top \hat{V} = I_k\) span the eigenspace to \(\lambda_{\max}(L(G))\), then the convex combination

\[
Y = \frac{1}{k\lambda_{\max}(L(G))} \hat{V} \hat{V}^\top \text{ with } d_{ij} = \langle E_{ij}, Y \rangle \text{ for } ij \in E
\]

(4.18)

is a corresponding maximum rank solution of \((D_{\lambda_n^{-1}})\) and its \(k\)-dimensional realization \((E_{\lambda_n^{-1}})\) is given by the columns of

\[
V = \frac{1}{\sqrt{k\lambda_{\max}(L(G))}} \hat{V}^\top.
\]

Let us close this chapter with the example graph of Figure 3.1. Because the maximum eigenvalue of the graph’s Laplacian is a simple one, any optimal realization with respect to \((E_{\lambda_n^{-1}})\) has to be one-dimensional. An optimal realization is illustrated in Figure 4.11. The order of the nodes is given below the realization of the graph.

![Figure 4.11: A one-dimensional optimal realization of the graph of Figure 3.1 for \((E_{\lambda_n^{-1}})\).](image-url)
We encourage the reader to compare the optimal one-dimensional realization with respect to \((E_{\lambda_2}-l)\) of Figure 3.6 on page 51 with the optimal realization with respect to \((E_{\lambda_n}-l)\) of Figure 4.11.
Chapter 5

Minimizing the Difference of Maximum and Second Smallest Eigenvalue

After we have presented connections of the extremal eigenvalues of the Laplacian to graph properties in the previous chapters, we are now interested in the interplay of both. Furthermore we want to establish relations to the single problems. For this purpose in this chapter we will optimize both eigenvalues at the same time. More precisely, for a graph $G = (N, E \neq \emptyset)$ let $s \in \mathbb{R}^{|N|}$, $s > 0$ be node weights, $l \in \mathbb{R}^{|E|}$, $0 \neq l \geq 0$ specify edge lengths and put $D := \text{diag}(s^{-1/2}_1, \ldots, s^{-1/2}_n)$. The program

$$\min \left\{ \lambda_{\max}(DL_wD) - \lambda_2(DL_wD) : \sum_{ij \in E} l^2_{ij}w_{ij} = 1, \ w \geq 0 \right\}$$

(5.1)

is in some sense a combination of $(P_{\lambda_2})$ and $(P_{\lambda_n})$, i.e., we minimize the maximum eigenvalue and maximize the second smallest eigenvalue of the graph’s Laplacian at the same time resulting in a common edge weighting.

In this chapter we start with formulating the problem (5.1) as primal-dual pair of semidefinite programs and a graph realization problem and present some considerations about strong duality. Connections of optimal realizations to the eigenspaces of the corresponding eigenvalues of the optimal weighted Laplacian are established. The problem of maximizing the difference of extremal Laplacian eigenvalues under the same constraints is shortly analyzed.

The second section is devoted to basic properties and examples. In particular, we identify complete graphs to be the only ones which have optimal value zero. We start to consider the connectedness of the graph resulting from the optimal weighted Laplacian and optimal
solutions of its components. Furthermore the realization’s barycenters and upper bounds on the vector lengths are presented.

In the third section we discuss relations between the single programs of chapters 3 and 4 and the coupled problem. Properties of the realizations are concluded concerning the separator structure of the graph, as the Sunny-Side Theorem (Corollary 5.16), Separator-Shadow Theorem (Corollary 5.19) and Tree-Width Bounds on the realization’s dimensions (corollaries 5.17 and 5.20). We consider isolated nodes and try to develop some intuition why the graph of an optimal weighted Laplacian may decompose into more components than the original graph.

In Section 5.4 we pay attention to bipartite graphs and optimal solutions which take the graph’s symmetry into account.

In the next section we establish scaled programs. Based on them we additionally want to optimize over the edge length parameters in the last section. Optimal realizations turn out to be maps of the eigenvectors to the extremal eigenvalues of the graph’s (unweighted) Laplacian and optimal realizations may be obtained from eigenvectors to the extremal eigenvalues. Finally relations between the corresponding single programs of chapters 3 and 4 and the coupled problem are determined.

The theory presented in this chapter is joint work with Frank Göring and Christoph Helmberg and is mainly taken verbatim from [37]. For a more detailed and illustrative presentation we include a lot of additional examples and figures and present some of the proofs in more detail. Unfortunately [37] contains a lot of faults that we have eliminated in this thesis (a revised version of [37] is already submitted to a journal). We want to highlight the last section of this chapter. While the programs and results concerning the eigenspace of the Laplacian are taken from [37], in this thesis we present a slightly different derivation, a detailed analysis of strong duality and in particular connections of optimal realizations of the single programs to the coupled one, see Theorem 5.46.

5.1 Primal-Dual Formulation

Like in chapters 3 and 4 matrix inequalities yield bounds on the second smallest and the maximum eigenvalue of a weighted Laplacian. Thus the constraints of the semidefinite formulation of (5.1) are just a union of the constraints of the single programs \((P_{\lambda_2})\) and \((P_{\lambda_n})\)

\[
\begin{align*}
\text{minimize} & \quad \lambda_n - \lambda_2 \\
\text{subject to} & \quad \sum_{ij \in E} w_{ij} DE_{ij} D + \mu D^{-1} 11^T D^{-1} - \lambda_2 I \succeq 0, \\
& \quad \lambda_n I - \sum_{ij \in E} w_{ij} DE_{ij} D \succeq 0, \\
& \quad \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \\
& \quad \lambda_2, \lambda_n, \mu \in \mathbb{R}, \ w \geq 0.
\end{align*}
\]
5.1. PRIMAL-DUAL FORMULATION

Recall the free variable $\mu$ just serves to shift the zero eigenvalue of $DL_{\mu}D$.

The feasible set of $(P_{\lambda_2})$ is not empty as the graph’s edge set is not empty and $l \neq 0$. In particular $(\lambda_2 < 0, \lambda_n, \mu \geq 0, \bar{w})$ is strictly feasible with respect to the semidefinite constraints whenever $\sum_{ij \in E} l_{ij}^2 \bar{w}_{ij} = 1$ and $\lambda_n > \sum_{ij \in E} \bar{w}_{ij}(s_i^{-1} + s_j^{-1})$.

The Lagrangian dual of $(P_{\lambda_n - \lambda_2})$ reads

\[
\begin{align*}
\text{maximize} & \quad \xi \\
\text{subject to} & \quad \langle I, X \rangle = 1, \\
& \quad \langle I, Y \rangle = 1, \\
& \quad (D^{-1}11^T D^{-1}, X) = 0, \\
& \quad (DE_{ij} D, Y) - (DE_{ij} D, X) - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \quad \xi \in \mathbb{R}, \ X, Y \succeq 0.
\end{align*}
\]

Again the feasible set is not empty: we construct a feasible $X$ like in Lemma 3.3, i. e., let $N_1 \subset N$ be a nonempty subset of nodes, $N_2 = N \setminus N_1$ (in this case it is independent of $l$) and $h \in \mathbb{R}^n$ with $\|h\| = 1$. Then there exist $\alpha, \beta \in \mathbb{R}$ such that

\[s(N_1)\alpha^2 + \bar{s}(N_2)\beta^2 = 1, \quad (\bar{s}(N_1)\alpha + \bar{s}(N_2)\beta)^2 = 0. \tag{5.2}\]

Thus $X = [u_1, \ldots, u_n]^T [u_1, \ldots, u_n]$ with $u_i = \sqrt{s_i} \alpha h$ ($i \in N_1$) and $u_i = \sqrt{s_i} \beta h$ ($i \in N_2$), $Y = X$ and $\xi = 0$ is feasible.

Expressing in the dual program $(D_{\lambda_n - \lambda_2})$ the semidefinite variables $X = D^{-1}U^T UD^{-1}$ and $Y = D^{-1}V^T VD^{-1}$ by Gram representations $U = [u_1, \ldots, u_n]$ and $V = [v_1, \ldots, v_n]$ we obtain $(E_{\lambda_n - \lambda_2})$ as an equivalent nonconvex quadratic program:

\[
\begin{align*}
\text{maximize} & \quad \xi \\
\text{subject to} & \quad \sum_{i \in N} s_i \|u_i\|^2 = 1, \\
& \quad \sum_{i \in N} s_i \|v_i\|^2 = 1, \\
& \quad \left\| \sum_{i \in N} s_i u_i \right\|^2 = 0, \\
& \quad \|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \quad \xi \in \mathbb{R}, \ u_i, v_i \in \mathbb{R}^n \ (i \in N).
\end{align*}
\]

Interpreting the vectors $u_i$ and $v_i$ ($i \in N$) of any feasible solution of $(E_{\lambda_n - \lambda_2})$ as vector labelings of the nodes $i \in N$, we get two realizations/embeddings $U$ and $V$ of the graph in $\mathbb{R}^n$, one for $\lambda_2$ and one for $\lambda_{\max}$. For these, the node weighted square norms sum up to one (we call this the normalization constraints), the weighted barycenter of $U$ is at the origin (equilibrium constraint; it is convenient to keep the square in view of the KKT conditions (5.3) below) and the difference between the squared edge lengths of the two
realizations is bounded below by the weighted variable $\xi$ \textit{(distance constraints)}. In optimal solutions the minimal weighted difference of the distances over all $ij \in E$ with $l_{ij} > 0$ is as large as possible.

We have seen that strong duality holds for the single problems (see propositions 3.4 and 4.1). Let us verify that it also holds for $(P_{\lambda_n - \lambda_2})$ and $(D_{\lambda_n - \lambda_2})$. In this case it is, however, no problem if some of the $l_{ij}$ are zero.

**Proposition 5.1 (Strong Duality)** \textit{Let $G = (N, E \neq \emptyset)$ be a graph with given data $s > 0$ and $0 \neq l \geq 0$. Strong duality holds for $(P_{\lambda_n - \lambda_2})$ and $(D_{\lambda_n - \lambda_2})$ and both programs attain their optimal value.}

**Proof.** We may rewrite $(D_{\lambda_n - \lambda_2})$ (and also $(P_{\lambda_n - \lambda_2})$) as usual in the form of (2.13), \textit{i.e.}, define

$$Z := \begin{bmatrix} X & 0 \\ 0 & Y \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$$

and adapt the constraints. Then strong duality follows from Corollary 2.15 and the strictly feasible solution $(\tilde{\lambda}_2, \tilde{\lambda}_n, \tilde{\mu}, \tilde{w})$ of $(P_{\lambda_n - \lambda_2})$ with respect to the semidefinite constraints. As both feasible sets are not empty the optimal value is finite, thus the dual attains its optimal solution.

In order to show primal attainment, we prove that for any fixed $\delta > 0$ the assumption $\lambda_{\text{max}}(L_w) - \lambda_2(L_w) < \delta$ implies the boundedness of $w$ (the scaling by $D \succ 0$ may be neglected in these considerations).

For $i, j \in N, i < j$, define vectors

$$q_{ij} = \frac{1}{\sqrt{2}}(e_i - e_j),$$

weighted degrees

$$d^i_w = \sum_{ik \in E} w_{ik}$$

and values

$$\gamma_{ij}^w = q_{ij}^\top L_w q_{ij} = \frac{1}{2}(d^i_w + d^j_w + 2w_{ij})$$

(setting $w_{ij} = 0$ for $ij \notin E$). Note that each $q_{ij}$ is orthogonal to $1$, so by Courant-Fischer

$$\lambda_{\text{max}}(L_w) \geq \max_{ij} \gamma_{ij}^w \geq \min_{ij} \gamma_{ij}^w \geq \lambda_2(L_w).$$

By $\lambda_{\text{max}}(L_w) - \lambda_2(L_w) < \delta$ we obtain $|\gamma_{ij}^w - \gamma_{kh}^w| < \delta$ for any choice of $i, j, k, h \in N$ with $i \neq j, k \neq h$. This allows to conclude $|d^i_w - d^j_w| \leq 4\delta$ for any $i < j$ as we prove next.
For $k \in N \setminus \{i,j\}$,
\[
\begin{align*}
|\gamma_{w}^{ki} - \gamma_{w}^{ij}| < \delta & \quad \Rightarrow \quad |d_{w}^{k} - (d_{w}^{i} + 2w_{ij} - 2w_{ik})| \leq 2\delta, \\
|\gamma_{w}^{kj} - \gamma_{w}^{ij}| < \delta & \quad \Rightarrow \quad |d_{w}^{j} - (d_{w}^{i} + 2w_{ij} - 2w_{jk})| \leq 2\delta \\
& \quad \Rightarrow \quad |(d_{w}^{k} - d_{w}^{j}) - 2(w_{jk} - w_{ik})| \leq 4\delta.
\end{align*}
\]

Using this, $d_{w}^{i} > d_{w}^{j} + 4\delta$ would imply $w_{jk} > w_{ik}$ for all $k \in N \setminus \{i,j\}$ giving rise to the contradicting relation
\[
d_{w}^{i} = \sum_{jk \in E} w_{jk} > \sum_{ik \in E} w_{ik} = d_{w}^{j},
\]
so we obtain $|d_{w}^{i} - d_{w}^{j}| \leq 4\delta$ as claimed. Thus, the inequality $|\gamma_{w}^{ij} - \gamma_{w}^{gh}| < \delta$ yields
\[
|w_{ij} - w_{gh}| \leq 5\delta \quad \text{for } i,j,k,h \in N \text{ with } i \neq j, k \neq h.
\]

Because of $l \neq 0$ there is an $ij \in E$ with $l_{ij} > 0$ and $w_{ij} \leq l_{ij}^{-2}$ by feasibility, so all $w_{hk}$ remain bounded whenever $\lambda_{n}(L_{w}) - \lambda_{2}(L_{w}) \leq \delta$ for some fixed $\delta > 0$. 

One might wonder, whether requiring $l > 0$ would not lead to more elegant formulations, after all the effect on the optimal value is small by Proposition 5.1. However, we will see in Theorem 5.4 below that $\xi = 0$ in $(E_{\lambda_{n} - \lambda_{2}})$ if and only if $G$ is complete. In consequence, if $l > 0$ and $G$ is not complete we might lose characteristic optimal solutions in $(E_{\lambda_{n} - \lambda_{2}})$, because if $G$ is not complete the distance constraint would not allow $v_{i} = v_{j}$ for any $ij \in E$.

Let us again consider the graph of Figure 3.1 with node and edge parameters equal to one. An optimal edge weighting of the graph for $(P_{\lambda_{n} - \lambda_{2}})$ is given by gray shades in Figure 5.1. Optimal realizations for $(D_{\lambda_{n} - \lambda_{2}})$ are illustrated in Figure 5.2: the left picture

![Figure 5.1: Optimal edge weighting of the graph of Figure 3.1 for $(P_{\lambda_{n} - \lambda_{2}})$ with node and edge parameters equal to one.](image-url)
CHAPTER 5. MINIMIZING $\lambda_{\text{MAX}} - \lambda_2$

Figure 5.2: Optimal realizations of the graph of Figure 3.1 for $(E_{\lambda_{n} - \lambda_2})$. The realization on the left corresponds to the second smallest eigenvalue, that on the right corresponds to the maximum eigenvalue.

and the (probably 14-dimensional) realization on the right hand side corresponds to the maximum eigenvalue.

In order to analyze properties of optimal solutions it is sometimes helpful to view optimality conditions from the perspective of the graph realization problem $(E_{\lambda_{n} - \lambda_2})$. Without feasibility and using the Lagrange multipliers $\lambda_2$, $\lambda_n$, $\mu$, and $w_{ij} \geq 0$ of $(P_{\lambda_{n} - \lambda_2})$, its Karush-Kuhn-Tucker conditions read

$$\lambda_2 s_i u_i = \sum_{ij \in E} w_{ij} (u_i - u_j) - \mu s_i \sum_{j \in N} s_j u_j \quad (i \in N),$$  \hspace{1cm} (5.3)

$$\lambda_n s_i v_i = \sum_{ij \in E} w_{ij} (v_i - v_j) \quad (i \in N),$$ \hspace{1cm} (5.4)

$$w_{ij} (\|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi) = 0 \quad (ij \in E).$$ \hspace{1cm} (5.5)

Like in Chapter 4, an interpretation of equations (5.3) and (5.4) via forces is possible. Note, that the last sum of equation (5.3) will cancel out because of feasibility.

Optimal graph realizations $U$ and $V$ also provide a geometric interpretation of extremal eigenvectors of $DL_w D$ for optimal $w$ as stated in the next proposition.

**Proposition 5.2** Let $G = (N, E \neq \emptyset)$ be a graph with given data $s > 0$ and $0 \neq l \geq 0$. Let $(U, V)$ be optimal realizations of $(E_{\lambda_{n} - \lambda_2})$ and $(\lambda_2, \lambda_n, w)$ optimal for $(P_{\lambda_{n} - \lambda_2})$. For any $h \in \mathbb{R}^n$ the scaled projections $D^{-1} U^\top h$ and $D^{-1} V^\top h$ onto the one-dimensional subspace spanned by $h$ yield eigenvectors to $\lambda_2(DL_w D)$ and $\lambda_{\text{MAX}}(DL_w D)$ respectively, unless they are zero vectors.

**Proof.** The proof follows that of Proposition 4.2: the eigenvalue equations of the definition of a matrix eigenvalue with corresponding eigenvector holds by equations (5.3) and (5.4), respectively, and as the last sum of equation (5.3) cancels out by feasibility. 

\[ \square \]
5.2. Basic Properties and Examples

Edges $ij$ with weight $w_{ij} = 0$ are of little relevance in optimal solutions. Therefore we will often restrict considerations to the strictly active and the active subgraph defined next.

**Definition 5.3** Given a graph $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let $U = [u_1, \ldots, u_n]$, $V = [v_1, \ldots, v_n]$ and $\xi$ be an optimal solution of $(E_{\lambda_n - \lambda_2})$ and let $w$ be an optimal solution of $(P_{\lambda_n - \lambda_2})$.

The edge set $E_{U,V,\xi,l} = \{ij \in E : \|v_i - v_j\|^2 - \|u_i - u_j\|^2 = l^2_{ij} \xi\}$ gives rise to the active subgraph $G_{U,V,\xi,l} = (N, E_{U,V,\xi,l})$ of $G$ with respect to $U$, $V$ and $\xi$.

As before, the strictly active subgraph $G_w = (N, E_w)$ of $G$ with respect to $w$ has edge set $E_w = \{ij \in E : w_{ij} > 0\}$.

Before we go into more detail about properties of optimal solutions of $(P_{\lambda_n - \lambda_2})$, $(D_{\lambda_n - \lambda_2})$ and $(E_{\lambda_n - \lambda_2})$ let us think about the direction of optimization. Might it be interesting to analyze

$$\max \left\{ \lambda_{\max}(DL_w D) - \lambda_2(DL_w D) : \sum_{ij \in E} l^2_{ij} w_{ij} = 1, \ w \geq 0 \right\},$$

i. e., to maximize the difference of maximum and second smallest eigenvalue? Well in principle optimal solutions are known. Again we have to consider the two cases that either there exists an edge $\hat{e} \in E$ with $l_{\hat{e}} = 0$ or $l > 0$.

In the first case the optimal value is unbounded. To see this, choose two edges $\hat{e}, \bar{e} \in E$ with $l_{\hat{e}} = 0$ and $l_{\bar{e}} > 0$ and let $w_{\bar{e}} = l_{\bar{e}}^{-2}$, $w_{\hat{e}} \to \infty$ and $w_e = 0$ otherwise. For $n \geq 4$ the edge weighted graph is not connected, thus the second smallest eigenvalue is zero and the maximum eigenvalue goes to infinity because of Weyl’s Theorem, Theorem 2.3. For $n = 3$ the maximum eigenvalue goes to infinity while the second smallest eigenvalue remains finite as $\lambda_2(DL_w D) \leq w_e \lambda_n(De_w D)$.

If $l > 0$ the maximum eigenvalue is bounded by

$$\lambda_n(DL_w D) \leq \max \{l_{ij}^{-2}(s_i^{-1} + s_j^{-1}) : ij \in E\} = l_{kl}^{-2}(s_k^{-1} + s_l^{-1}),$$

for appropriate $k$ and $l$ realizing the maximum and using Weyl’s Theorem. It can be attained, because $w_{kl} = l_{kl}^{-2}$ and $w_{ij} = 0$ otherwise is such a maximizing edge weighting. For $n \geq 3$ the weighted graph is not connected, thus $\lambda_2 = 0$. For $n = 2$ the maximum and second smallest eigenvalue are the same thus the optimal value equals zero.

5.2 Basic Properties and Examples

We start by discussing the special case of optimal value 0.
Theorem 5.4 For any data \( s > 0, \mathbf{0} \neq \mathbf{l} \geq 0 \), problem \((P_{\lambda_n-\lambda_2})\) has optimal value 0 if and only if \( G = K_n \). In this case,

\[
w_{ij} = \frac{s_is_j}{\sum_{k<h} l_{kh}^2 s_k s_h} \quad \text{for} \quad 1 \leq i < j \leq n,
\]
is optimal.

Proof. Any feasible solution \( w \) with \( \lambda_n = \lambda_2 = \lambda \) satisfies \( w \neq \mathbf{0} \) and \( \lambda > 0 \).

Because \( \mu \) only serves to shift the trivial eigenvalue 0 of the Laplacian, we shift it appropriately, i.e., in such a way that all the eigenvalues of \( DL_wD + \mu D^{-1}11^T D^{-1} \) are the same (thus \( \mu > 0 \)). Because of Courant-Fischer this is equivalent to

\[
\lambda I \preceq DL_wD + \mu D^{-1}11^T D^{-1} \preceq \lambda I
\]

which is equivalent to

\[
L_w + \mu D^{-2}11^T D^{-2} = \lambda D^{-2}.
\]

For \( 1 \leq i < j \leq n \) this forces \( w_{ij} = \mu s_i s_j \neq 0 \), therefore the graph must be complete.

Furthermore the \( i \)-th diagonal element must satisfy

\[
\sum_{j \in N, j \neq i} w_{ij} + \mu s_i^2 = \mu s_i \sum_{j \in N} s_j = \lambda s_i,
\]

thus

\[
\mu = \frac{\lambda}{\sum_{i \in N} s_i} = \frac{\lambda}{\|D^{-1}1\|^2}.
\]

The constraint

\[
1 = \sum_{i<j} l_{ij}^2 w_{ij} = \mu \sum_{i<j} l_{ij}^2 s_i s_j = \frac{\lambda}{\|D^{-1}1\|^2} \sum_{i<j} l_{ij}^2 s_i s_j
\]
determines \( \lambda \).

Next we describe some optimal dual realizations for \( G = K_n \).

Example 5.5 (Complete Graphs) Let \( G \) be the complete graph \( K_n \) with given data \( s > 0 \) and \( \mathbf{0} \neq \mathbf{l} \geq 0 \). By Theorem 5.4 and strong duality, any optimal solution \( \xi, U = [u_1, \ldots, u_n] \) and \( V = [v_1, \ldots, v_n] \) of \((E_{\lambda_n-\lambda_2})\) fulfills \( \xi = 0 \). Because all \( w_{ij} \) are positive, complementarity implies \( \|u_i - u_j\| = \|v_i - v_j\| \) for all \( i, j \in N \).
An optimal $d$-dimensional realization of $(D_{\lambda_n - \lambda_2})$ $(1 \leq d \leq n - 1)$ is given by taking $M \subseteq N$, where $|M| = d + 1$ and

$$\xi = 0, \quad X_{kl} = Y_{kl} = \begin{cases} \bar{s}(M \setminus \{k\}) & \text{for } k, l \in M, \ k = l, \\ -\sqrt{s_{kl}} & \text{for } k, l \in M, \ k \neq l, \\ 0 & \text{otherwise} \end{cases}$$

(5.6)

Note, the $n - d - 1$ nodes of $N \setminus M$ are embedded in the origin.

For illustration, Figure 5.3 shows a one-, a two- and a three-dimensional realization of the tetrahedron with $s = 1$ and $l = 1$ constructed by (5.6) with node sets $M_1 = \{1, 2\}$, $M_2 = \{1, 2, 3\}$ and $M_3 = \{1, 2, 3, 4\}$, respectively.

Figure 5.3: A one-, a two- and a three-dimensional realization of the tetrahedron (see Example 5.5).

If the strictly active subgraph is not connected, the problem almost decomposes into subproblems $(P_{\lambda_n})$ on the components. More precisely, the value of $\lambda_2$ is zero and the minimization of the maximum eigenvalue leads to an identical maximum eigenvalue on each component consisting of at least two nodes. In order to state and prove this result in detail, we denote by $L_{N'}^w$ and $D_{N'}$ the principal submatrix of the weighted Laplacian $L_w$ and of $D$, respectively, with indices $i \in N' \subseteq N$.

**Proposition 5.6** Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let $\lambda_2$, $\lambda_n$, $w$ be optimal for $(P_{\lambda_n - \lambda_2})$ and let the strictly active subgraph $G_w$ consist of $k$ connected components $G_h = (N_h, E_h)$, $h = 1, \ldots, k$. Then

(i) $k > 1$ if and only if $\lambda_2 = 0$,

(ii) there is an optimal $\bar{w} \geq w$ so that for each component $h = 1, \ldots, k$,

$$\lambda_n = \lambda_{\text{max}}(D_{N_h}^l I_{w_h}^n D_{N_h})$$

if and only if $E_h \neq \emptyset$.

**Proof.** (i) was already observed by Fiedler [25], but the argument is short: Suppose $k \geq 2$, then

$$q = D^{-1} \left( \frac{1}{s(N_1)} \sum_{i \in N_1} e_i - \frac{1}{s(N_2)} \sum_{i \in N_2} e_i \right)$$
is an eigenvector to $\lambda_2 = 0$, because $DL_wDq = 0$ and $1^TD^{-1}q = 0$.

Let otherwise $\lambda_2 = 0$ and assume for contradiction that $G$ is connected. Then $L_w$ is irreducible as well as the matrix $2\max\{|L_w|_{ii} : i \in N\}I - L_w$. Moreover the previous matrix is nonnegative and positive definite. Applying Perron-Frobenius yields that the spectral radius of $2\max\{|L_w|_{ii} : i \in N\}I - L_w$ is a simple eigenvalue which is equal to $2\max\{|L_w|_{ii} : i \in N\} - \lambda_1(L_w)$. Thus $\lambda_1(L_w)$ is a simple eigenvalue of $L_w$ which contradicts $\lambda_2(L_w) = 0$ thus $G$ is not connected.

For (ii), we know $\lambda_n > 0$ by Theorem 5.4. Because $L_w$ consists of independent principal submatrices corresponding to the connected components, there is at least one block $N_h$ with $\lambda_n = \lambda_{\max}(D_{N_h}^N L_{w_{N_h}}^N D_{N_h})$ and a $w_{ij} > 0$ with $ij \in E_h$ having $l_{ij} > 0$, otherwise the solution could be improved.

Suppose $E_h = \emptyset$ for some $\bar{h}$, then the component is an isolated node, $|N_h| = 1$, and $0 = L_{w_{N_h}}^N$, so $\lambda_n > \lambda_{\max}(D_{N_h}^N L_{w_{N_h}}^N D_{N_h})$.

Suppose now there is a connected component $(N_h, E_h \neq \emptyset)$ with $\lambda_n > \lambda_{\max}(D_{N_h}^N L_{w_{N_h}}^N D_{N_h})$. If all $l_{ij} = 0$ for $ij \in E_h$, the weights $w_{ij}$ can be increased to some values $\bar{w}_{ij}$ so that $\lambda_n = \lambda_{\max}(D_{N_h}^N L_{w_{N_h}}^N D_{N_h})$ on this component. Otherwise, slightly increasing the weight of a $w_{ij}$ with $l_{ij} > 0$ and $ij \in E_h$ and decreasing the weights of all components with $\lambda_n = \lambda_{\max}(D_{N_h}^N L_{w_{N_h}}^N D_{N_h})$ allows to preserve feasibility and to improve the solution at the same time, so this contradicts optimality.

\begin{remark}
By Proposition 5.6 and its proof, the number of components of the strictly active subgraph with at least one edge is a lower bound on the dimension of the eigenspace corresponding to the maximum eigenvalue $\lambda_n$ of $DL_wD$ for $\bar{w}$ of the proof.
\end{remark}

By summing the KKT conditions (5.4) over all nodes of the graph, or alternatively over the nodes of each connected component, it follows that with respect to optimal $V$ the equilibrium constraint holds automatically for each connected component.

\begin{proposition}
Given $G = (N,E \neq \emptyset)$ and data $s > 0, 0 \neq l \geq 0$, let $\xi$, $U$, $V = [v_1, \ldots, v_n]$ be optimal for $(P_{\lambda_n - \lambda_2})$ and $\lambda_2$, $\lambda_n$, $w$ be optimal for $(P_{\lambda_n - \lambda_2})$. For any connected component $(N_h, E_h)$ of the strictly active subgraph, of the active subgraph, or of the graph itself, the weighted barycenter with respect to $V$ is in the origin, i.e., $\sum_{i \in N_h} s_i v_i = 0$. In particular, nodes $i \in N$ isolated in $G_w$ satisfy $v_i = 0$.
\end{proposition}

Considering the $U$-realization, the barycenter of the entire graph is explicitly forced to lie in the origin. This, however, does not extend to the connected components. In fact, whenever the strictly active subgraph is not connected, the optimal $U$-realizations of each component collapse to single points.
Proposition 5.9 Given $G = (N, E \neq \emptyset)$ and data $s > 0, 0 \neq l \geq 0$, let $U = [u_1, \ldots, u_n]$ be optimal for $(E_{\lambda_n - \lambda_2})$ and $\lambda_2, w$ be optimal for $(P_{\lambda_n - \lambda_2})$. The strictly active subgraph $G_w = (N, E_w)$ is not connected if and only if $u_i = u_j$ for $ij \in E_w$ if and only if $\lambda_2 = 0$.

Proof. The claim follows from semidefinite complementarity

$$\langle X, DL_w D + \mu D^{-1}11^\top D^{-1} - \lambda_2 I \rangle = \sum_{ij \in E} w_{ij} \|u_i - u_j\|^2 - \lambda_2 = 0$$

and Proposition 5.6(i), i.e., $\lambda_2 = 0$ if and only if $G_w$ is not connected. \hfill \Box

If $G$ itself is not connected there exists an optimal one-dimensional $U$ (independent of an optimal $V$). To see this, split the graph into two disjoint node sets such that no edges connect nodes in distinct sets. Each set is mapped onto a separate coordinate so that the normalization constraint and the equilibrium constraint are satisfied.

If $G$ is connected but its strictly active subgraph $G_w$ is not, no optimal one-dimensional realizations $U$ need to exist for a given optimal $V$, because the distance constraints of inactive edges may cause problems. This is illustrated by the following example.

Example 5.10 Consider the graph of Figure 5.4 with data $s = 1$ and $l = 1$. In the optimal solution the edges in the dashed triangle on nodes $\{1, 2, 3\}$ have optimal weight zero, all others $w_{ij} = \frac{1}{9}$ giving $\lambda_2 = 0$ and $\lambda_n = \frac{4}{3} = \xi$. The strictly active subgraph consists of three stars with centers 1, 2 and 3.

Figure 5.4: There may be no one-dimensional realization $U$ even if $G_w$ is not connected.

In an optimal realization $U$, each star is mapped onto one point.

In an optimal $V$ each star is embedded in a one-dimensional subspace with its center at distance $\frac{1}{3}$ from the origin opposite to its three leaves which are embedded on top of each other at distance $\frac{1}{6}$ from the origin, see Corollary 5.16 below. Arranging the three centers in an equilateral triangle with barycenter in the origin results in mutual squared distances $\|v_i - v_j\|^2 = \frac{3}{4}$ for $i, j \in \{12, 13, 23\}$. 
Hence, \(|u_i - u_j|^2 \leq \frac{3}{4} - \frac{4}{9} = \frac{11}{36}\) \((ij \in \{12, 23, 13\})\). This is satisfied, e.g., by embedding the \(u_i\) for \(i = \{1, 2, 3\}\) in an equilateral triangle around the origin with \(|u_i| = \frac{1}{2\sqrt{3}}\), each having its leaves embedded on top of it.

The mentioned optimal realizations are illustrated in Figure 5.5.

![Figure 5.5: Optimal two-dimensional realizations U and V of the graph of Figure 5.4 for \((E_{\lambda_n-\lambda_2})\), cf. Example 5.10.](image)

There is, however, no optimal one-dimensional realization \(u_i = x_i h\) \((i \in N)\) with \(|h| = 1\) and \(x_i \in \mathbb{R}\) \((i \in N)\), because it would have to satisfy the following infeasible system,

- equilibrium constraint \(4x_1 + 4x_2 + 4x_3 = 0\),
- normalization constraint \(4x_1^2 + 4x_2^2 + 4x_3^2 = 1\),
- distance constraints \((x_i - x_j)^2 \leq \frac{11}{36}\) \((ij \in \{12, 23, 13\})\).

The normalization constraint specifies a ball with radius \(\frac{1}{2}\) and the distance constraints specify a polyhedron which lies completely in the ball, so they have no points in common. The equilibrium constraint is just an additional plane through the origin.

Figure 5.6 illustrates the situation after we have eliminated \(x_3\) by the equilibrium constraint. The normalization constraint specifies the red ellipse and the distance constraints the green polyhedron.

The next proposition provides a bound on the length of vectors of optimal realizations of \((E_{\lambda_n-\lambda_2})\).

**Proposition 5.11** Given \(G = (N, E \neq \emptyset)\) and data \(s > 0, 0 \neq l \geq 0, \xi, U = [u_1, \ldots, u_n], V = [v_1, \ldots, v_n]\) be optimal for \((E_{\lambda_n-\lambda_2})\) and put \(\tilde{l} = (\max\{||u_i - u_j||^2 + l_i^2 \xi : ij \in E\})^{1/2}\). Then \(||u_i|| < s_i^{-1/2}\) and \(||v_i|| < \min\{s_i^{-1/2}, \tilde{l}\}\) for \(i \in N\).
5.2. BASIC PROPERTIES AND EXAMPLES

Proof. The bound concerning the $u_i$ is a direct consequence of the normalization and equilibrium constraint. The same argument works for the term $s_i^{-1/2}$ of the bound concerning the $v_i$ using Proposition 5.8.

The proof for $\hat{l}$ follows that of Proposition 4.5, so we only repeat the basic idea: We observe that $\hat{l} > 0$ because $l \neq 0$ and, by Theorem 5.4 and Example 5.5, $\xi > 0$ or $\|u_i - u_j\|^2 > 0$ for at least one $ij \in E$. We suppose for contradiction, that there is a node $k \in N$ with $\|v_k\| = \hat{l} + \epsilon \geq \hat{l}$. Then we may show that there is another feasible realization $V'$ (and $U$) with no smaller objective value having the barycenter of $V'_N$ outside the origin, which contradicts the optimality of $V$ by Proposition 5.8. \hfill \blacksquare

The following example illustrates that the bounds of Proposition 5.11 cannot be improved.

Example 5.12 Let $s = c1$, $l = 1$ with real $c > 0$. For $n > 2$ consider the graph

$$G = (N, E) = (\{1, \ldots, n\}, \{\{2, k\} : k \in N \setminus \{1, 2\}\}),$$

i.e., it consists of two components: an isolated node and a star. Let $h \in \mathbb{R}^n$, $\|h\| = 1$. Optimal realizations of $(P_{\lambda_n-\lambda_2})$ and $(E_{\lambda_n-\lambda_2})$ are given by

$$\lambda_2 = 0, \quad \lambda_n = \frac{n-1}{c(n-2)}, \quad \mu = 0, \quad w_{ij} = \frac{1}{n-2} \quad (ij \in E)$$

and

$$\xi = \frac{n-1}{c(n-2)}, \quad u_i = \begin{cases} \sqrt{\frac{n-1}{cn}} h & \text{for } i = 1, \\ -\sqrt{\frac{1}{cn(n-1)}} h & \text{otherwise,} \end{cases} \quad v_i = \begin{cases} 0 & \text{for } i = 1, \\ \sqrt{\frac{n-2}{c(n-1)}} h & \text{for } i = 2, \\ -\sqrt{\frac{1}{c(n-2)(n-1)}} h & \text{otherwise.} \end{cases}$$

Because $u_i = u_j$ ($ij \in E$) the bounds are $\hat{l} = \sqrt{\xi} > c^{-1/2} = s_i^{-1/2}$ ($i \in N$).

For $n \to \infty$ we obtain $\hat{l} \to c^{-1/2} = s_i^{-1/2}$ ($i \in N$), $\|u_1\| \to c^{-1/2}$ and $\|v_2\| \to c^{-1/2}$. Thus, the bounds cannot be improved.
Remark 5.13  The realizations of complete graphs described in Example 5.5 allow to construct a sequence of problems and solutions with the property that \( \hat{l} \to 0 \) in Proposition 5.11. Indeed, the analysis of the realization yields \( \|v_i\|^2 = \|u_i\|^2 = d^{-1}(s_i^{-1} - \bar{s}(M)^{-1}) \) and \( d^{-1}(s_i^{-1} - \bar{s}(M)^{-1}) < s_i^{-1} \) for \( i \in M \). In addition,

\[
\hat{l}^2 = \max\{0, \|u_i\|^2 (i \in M), \|u_i - u_j\|^2 = d^{-1}(s_i^{-1} + s_j^{-1}) (i, j \in M)\}
\]

For \( s = c1 > 0 \) and \( d > 2 \) we have \( s_i^{-1} = c^{-1} > \hat{l}^2 = 2(dc)^{-1} (i \in N) \) and for, e.g., \( d = n - 1 \) and \( n \to \infty \) we obtain \( \hat{l} \to 0 \).

5.3 Properties Common to \((E_{\lambda_n-\lambda_2})\) and \((E_{\lambda_2})\) or \((E_{\lambda_n})\)

Graph realizations induced by optimal solutions of \((E_{\lambda_2})\) and \((E_{\lambda_n})\) are tightly linked to the separator structure of the graph, see chapters 3 and 4. The aim of this section is to investigate which of the properties of the single problems can be saved for the combined problem \((E_{\lambda_n-\lambda_2})\). The first theorem states that for appropriate choices of \( \xi \) feasible solutions remain feasible. While feasibility is preserved, optimality may be lost.

**Theorem 5.14 (Feasibility)**  Given \( G = (N, E \neq \emptyset) \) and data \( s > 0, l > 0 \), there exist appropriate values for the respective \( \xi \) variables so that feasible realizations \( U \) of \((E_{\lambda_2})\) and \( V \) of \((E_{\lambda_n})\) are feasible realizations \((U, V)\) of \((E_{\lambda_n-\lambda_2})\) and vice versa.

**Proof.**  For feasible solutions \( \xi_2, U \) of \((E_{\lambda_2})\) \((\xi_2 \text{ may be negative})\) and \( \xi_n, V \) of \((E_{\lambda_n})\) the normalization constraints and the equilibrium constraint are satisfied. As \( \xi = \xi_n + \xi_2 \) fulfills the distance constraints, \( \xi, U, V \) is feasible for \((E_{\lambda_n-\lambda_2})\) with data \( s \) and \( l \).

On the other hand let \( \xi, U, V \) be feasible for \((E_{\lambda_n-\lambda_2})\). By choosing

\[
\xi_2 = \min_{ij \in E} \left\{ \xi - \frac{\|v_i - v_j\|^2}{l_{ij}^2} \right\} \text{ and } \xi_n = \min_{ij \in E} \left\{ \frac{\|u_i - u_j\|^2}{l_{ij}^2} + \xi \right\}
\]

\( U, \xi_2 \) is feasible for \((E_{\lambda_2})\) and \( V, \xi_n \) is feasible for \((E_{\lambda_n})\). Indeed, to see this for \((E_{\lambda_2})\), observe that

\[
\sum_{i \in N} s_i \|u_i\|^2 = 1, \quad \sum_{i \in N} s_i u_i = 0
\]

and

\[
-\|u_i - u_j\|^2 - l_{ij}^2 \xi_2 \geq \|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi \geq 0.
\]

For \((E_{\lambda_n})\) we have

\[
\sum_{i \in N} s_i \|v_i\|^2 = 1
\]
and
\[ \|v_i - v_j\|^2 - t_{ij}^2 \xi_n \geq \|v_i - v_j\|^2 - \|u_i - u_j\|^2 - t_{ij}^2 \xi \geq 0. \]

In the previous theorem an \( l_{ij} = 0 \) would only cause difficulties if the feasible solution \( U \) of \((E_{\lambda_N - \lambda_2})\) does not satisfy \( \|u_i - u_j\| = 0 \), because then the corresponding distance constraint of \((E_{\lambda_2})\) cannot be satisfied.

Next we consider optimal realizations. It turns out that optimal realizations \( V \) of \((E_{\lambda_N - \lambda_2})\) for data \( s > 0 \) and \( 0 \neq l \geq 0 \) are optimal for \((E_{\lambda_n})\) for data that are adapted appropriately.

**Theorem 5.15 (Optimal \( V \))** Given \( G = (N, E \neq \emptyset) \) and data \( s > 0 \), \( 0 \neq l \geq 0 \), let \( V \) be an optimal realization of \((E_{\lambda_N - \lambda_2})\). There exist \( 0 \neq \bar{l} \geq 0 \) so that \( V \) is optimal for \((E_{\lambda_n})\) with data \( s \) and \( \bar{l} \). Furthermore, if \( G \) is not complete and \( l > 0 \), also \( \bar{l} > 0 \).

**Proof.** Let \( U, V \) and \( \xi \) be an optimal solution of \((E_{\lambda_n - \lambda_2})\) and \( w \) an optimal solution of \((P_{\lambda_n - \lambda_2})\). Set \( l_{ij}^2 = \|v_i - v_j\|^2 \geq 0 \) (\( ij \in E \)). The proof is given in three steps: first we show \( \bar{l} \neq 0 \), then feasibility and third optimality of \( V \) in \((E_{\lambda_n})\) with data \( s \) and \( \bar{l} \).

In the first step we have to consider two cases: \( G \) is not complete and \( G \) is complete. Let \( G \) be not complete then \( \xi > 0 \) by Theorem 5.4. For each edge \( ij \in E \) with \( l_{ij} > 0 \) (there is at least one by \( 0 \neq l \)) the distance constraint yields \( l_{ij}^2 = \|v_i - v_j\|^2 \geq l_{ij}^2 \xi > 0 \). Thus, if \( l > 0 \), also \( \bar{l} > 0 \). If \( G \) is complete, \( \bar{l} = 0 \) is equivalent to \( v_i = v_j \) (\( i, j \in N \)). The latter, however, is impossible, because the normalization constraint requires \( v_i \neq 0 \) for some \( i \in N \) and by optimality and Proposition 5.8 the barycenter lies in the origin. Hence \( 0 \neq \bar{l} \geq 0 \).

\( V, \bar{\xi} = 1 \) is feasible for \((E_{\lambda_n})\) with data \( s \) and \( \bar{l} \) because of the feasibility of \( V \) for \((E_{\lambda_N - \lambda_2})\) and the special choice of \( \bar{l} \) and \( \bar{\xi} \).

In the last step optimality follows by strong duality, \( i. e. \), we specify a primal feasible solution with the same optimal value as follows. Let \( (\lambda_n, w) \) be optimal for \((P_{\lambda_n - \lambda_2})\). Set \( (\bar{\lambda}_n := 1, \bar{w} := \frac{1}{\lambda_n} w) \). The semidefinite constraint holds because \((\lambda_n, w)\) is feasible for \((P_{\lambda_n - \lambda_2})\). By semidefinite complementarity with respect to \( Y = D^{-1} V^T V D^{-1} \), \( i. e. \),
\[ \langle Y, \lambda_n I - DLw D \rangle = \lambda_n - \sum_{ij \in E} w_{ij} \|v_i - v_j\|^2 = 0, \]

the remaining constraint reads
\[ \sum_{ij \in E} l_{ij}^2 w_{ij} = \frac{1}{\lambda_n} \sum_{ij \in E} \|v_i - v_j\|^2 w_{ij} = 1. \]

Optimality of the primal and dual solutions follows from strong duality.
An immediate consequence is that all structural properties observed in Chapter 4 for optimal solutions of \((E_{\lambda_n})\) also hold for optimal \(V\) of \((E_{\lambda_n-\lambda_2})\) whenever these do not depend on certain constraints being active or strictly active. In particular, we obtain the following two corollaries.

**Corollary 5.16 (Sunny-Side)** Given a graph \(G = (N, E \neq \emptyset)\) and data \(s > 0, 0 \neq l \geq 0\), let \(U, V = [v_1, \ldots, v_n]\) be an optimal solution of \((E_{\lambda_n-\lambda_2})\). For any two disjoint nonempty subsets \(A\) and \(S\) of \(N\) such that each edge of \(G\) leaving \(A\) ends in \(S\), the barycenter

\[
\bar{v}(A) = \frac{1}{\bar{s}(A)} \sum_{i \in A} s_i v_i
\]

is contained in \(S = \text{aff}(V_S) - \text{cone}(V_S)\).

**Proof.** Theorem 5.15 above and Theorem 4.13.

**Corollary 5.17 (Tree-Width Bound)** Given a graph \(G = (N, E \neq \emptyset)\) and data \(s > 0, 0 \neq l \geq 0\), let \(U, V\) be an optimal solution of \((E_{\lambda_n-\lambda_2})\). There exists, for the same \(U\), an optimal solution \(V'\) of \((E_{\lambda_n-\lambda_2})\) of dimension at most 1 if the tree-width of \(G\) is one and of dimension tree-width of \(G\) plus one otherwise.

**Proof.** Theorem 5.15 above and Theorem 4.15, as in its proof the transformations preserve all distances \(\|v_i - v_j\|\) for \(ij \in E\).

There is an almost similar result for \((E_{\lambda_2})\) and optimal \(U\) whenever the strictly active subgraph is connected, i.e., whenever \(\lambda_2(L_w) > 0\) for some optimal \(w\) of \((P_{\lambda_n-\lambda_2})\).

**Theorem 5.18 (Optimal U)** Given \(G = (N, E \neq \emptyset)\) and data \(s > 0, 0 \neq l \geq 0\), let \(U\) be an optimal realization of \((E_{\lambda_n-\lambda_2})\) and suppose there is an optimal \(w\) for \((P_{\lambda_n-\lambda_2})\) resulting in a connected strictly active subgraph \(G_w\). There exist data \(0 \neq \bar{l} \geq 0\) such that each spanning tree of \(G\) has an edge with positive edge length parameter and \(U\) is optimal for \((E_{\lambda_2})\) with data \(s\) and \(\bar{l}\). Moreover the optimal solution of \((P_{\lambda_2})\) is attained.

The proof is almost identical to that of Theorem 5.15, so we refrain from repeating it here. Let us simply remark that if \(\bar{l}\) would cause a zero weighted spanning tree of \(G\), all nodes will be embedded in the same point and so the normalization and the equilibrium constraint cannot hold at the same time, in contradiction to the feasibility of \(U\).

Again, we obtain two corollaries for structural properties observed in Chapter 3.
Corollary 5.19 (Separator-Shadow) Given $G = (N,E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let $U$ be an optimal realization of $(E_{\lambda_n-\lambda_2})$ and suppose there is an optimal $w$ for $(P_{\lambda_n-\lambda_2})$ resulting in a connected strictly active subgraph $G_w$. Let $S$ be a separator in $G_w$, giving rise to a partition $N = S \cup C_1 \cup C_2$ where there is no edge in $E_w$ between $C_1$ and $C_2$. For at least one $C_j$ with $j \in \{1,2\}$

$$\text{conv}\{0,u_i\} \cap \text{conv}\{u_s : s \in S\} \neq \emptyset \quad \forall i \in C_j.$$  \hspace{1cm} (5.8)

In words, the straight line segments $\text{conv}\{0,u_i\}$ of all nodes $i \in C_j$ intersect the convex hull of the points in $S$.

**Proof.** Theorem 5.18 above and Corollary 3.11.

Corollary 5.20 (Tree-Width Bound) Given $G = (N,E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, suppose there is an optimal $w$ for $(P_{\lambda_n-\lambda_2})$ resulting in a connected strictly active subgraph $G_w$. There exists an optimal realization $U$ of $(E_{\lambda_n-\lambda_2})$ of dimension at most the tree-width of $G$ plus one.

**Proof.** Theorem 5.18 above and Corollary 3.15 as in the proof of Theorem 3.14 the transformations preserve all distances $\|u_i - u_j\|$ for $ij \in E$.

The condition of the existence of an optimal $w$ giving rise to a connected strictly active subgraph in Theorem 5.18 is essential. The following Example 5.21 provides an instance of $(E_{\lambda_n-\lambda_2})$ with an optimal $U$ so that $U$ is not the optimal solution of $(E_{\lambda_2})$ for any choice of $s > 0$ and $l \geq 0$.

Example 5.21 Consider the graph $G$ of Figure 5.7 and let $s = 1$ and $l = 1$ be given data. The strictly active subgraph $G_w$ is not connected, because dashed edges 34 and 47 have optimal weight zero.

The plot on the right hand side of Figure 5.7 depicts a two-dimensional optimal realization $U = \{u_1, \ldots, u_9\}$ of $G$ for $(E_{\lambda_n-\lambda_2})$. There, each component is embedded into a separate point, i.e., $u_1 = u_2 = u_3 =: u'_1$, $u_4 = u_5 = u_6 =: u'_2$ and $u_7 = u_8 = u_9 =: u'_3$ with $u'_s \notin \text{conv}\{0,u'_1\}$ and $u'_s \notin \text{conv}\{0,u'_2\}$.

For $(E_{\lambda_2})$ the Separator-Shadow Theorem, Theorem 3.10, holds, as noted above, for all connected graphs with data $s > 0$ and appropriate $l$. Because $S = \{4,5,6\}$ is a separator in $G$ separating $C_1 = \{1,2,3\}$ from $C_2 = \{7,8,9\}$, it requires $\text{conv}\{0,u_i\} \cap \text{conv}\{u_s : s \in S\} \neq \emptyset$ for all $i \in C_j$ for at least one $j \in \{1,2\}$. So there are no choices of data $s > 0$ and $l \geq 0$ rendering $U$ optimal for $(E_{\lambda_2})$. 
CHAPTER 5. MINIMIZING $\lambda_{\text{MAX}} - \lambda_2$

Figure 5.7: Graph $G$ and optimal realization $U$ for $(E_{\lambda_n - \lambda_2})$ with data $s = 1$ and $l = 1$, the strictly active subgraph is not connected, cf. Example 5.21.

On the other hand there exist graphs and data having both, optimal solutions of $(P_{\lambda_n - \lambda_2})$ with positive second smallest eigenvalue and an optimal primal solution with second smallest eigenvalue equal to zero.

Example 5.22 ([30]) Let $G$ be the graph of Figure 5.8 with node parameters $s = 1$ and edge length parameters $l_{12} = l_{36} = l_{45} = 2$ and one otherwise.

![Figure 5.8: The graph of Example 5.22](image)

Feasible realizations of $(E_{\lambda_n - \lambda_2})$ are a two-dimensional one with respect to $\lambda_2$, which builds a regular triangle

$$u_1 = u_2 = -\frac{1}{\sqrt{6}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad u_3 = u_6 = \frac{1}{2\sqrt{6}} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}, \quad u_4 = u_5 = \frac{1}{2\sqrt{6}} \begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix}$$

and a one-dimensional one with respect to $\lambda_n$

$$v_1 = v_3 = v_5 = -\frac{1}{\sqrt{6}}, \quad v_2 = v_4 = v_6 = \frac{1}{\sqrt{6}}$$

with objective value $\xi = \frac{1}{6}$.

For primal solutions let $w_{12} = w_{36} = w_{45} = c$ and the other edges let have weight $\frac{1}{6} - 2c$ for a parameter $c \in \mathbb{R}$ to be determined below. Then the normalization constraint holds. The
5.3. **PROPERTIES COMMON TO** \((E_{\lambda_N-\lambda_2})\) **AND** \((E_{\lambda_2})\) **OR** \((E_{\lambda_N})\)

eigenvalues of the corresponding weighted Laplacian

\[
L_w = \frac{1}{6} \begin{bmatrix}
2 - 18c & -6c & 0 & -1 + 12c & 0 & -1 + 12c \\
-6c & 2 - 18c & -1 + 12c & 0 & -1 + 12c & 0 \\
0 & -1 + 12c & 2 - 18c & -1 + 12c & 0 & -6c \\
-1 + 12c & 0 & -1 + 12c & 2 - 18c & -6c & 0 \\
0 & -1 + 12c & 0 & -6c & 2 - 18c & -1 + 12c \\
-1 + 12c & 0 & -6c & 0 & -1 + 12c & 2 - 18c \\
\end{bmatrix}
\]

are \(\{0, \frac{1}{6}, \frac{1}{6}, \frac{1}{2} - 6c, \frac{1}{3} - 6c, \frac{2}{3} - 6c\}\). Any \(c\) with \(\frac{1}{18} \leq c \leq \frac{1}{12}\) provides a feasible edge weighting with \(\lambda_2 = \frac{1}{2} - 6c\) and \(\lambda_n = \frac{2}{3} - 6c\), thus \(\lambda_n - \lambda_2 = \frac{1}{6} = \xi\). As \(\mu\) serves to shift the zero eigenvalue it suffices to set \(\mu = \lambda_2\). Optimality follows by strong duality.

While the strictly active subgraph is not connected for \(c = \frac{1}{12}\) it is connected for \(\frac{1}{18} \leq c < \frac{1}{12}\).

As an immediate consequence of Proposition 5.9, optimal solutions of \((P_{\lambda_n-\lambda_2})\) are also optimal for \((P_{\lambda_n})\) whenever the strictly active subgraph is not connected.

**Corollary 5.23** Given \(G = (N, E \neq \emptyset)\) and data \(s > 0, 0 \neq l \geq 0\), let \(\xi, U, V\) be optimal for \((E_{\lambda_n-\lambda_2})\) and \(\lambda_2, \lambda_n, \mu\) and \(w\) be optimal for \((P_{\lambda_n-\lambda_2})\). If the strictly active subgraph \(G_w\) is not connected then \(\xi, V\) is optimal for \((E_{\lambda_n})\) and \(\lambda_n, w\) is optimal for \((P_{\lambda_n})\) with data \(s\) and \(l\).

**Remark 5.24** If for a graph \(G = (N, E \neq \emptyset)\) whose strictly active subgraph is not connected, the connected components can be identified in advance, problem \((P_{\lambda_n})\) can be solved by first computing the solution for each single component with the same data (disregarding isolated nodes and components having all edge length parameters equal to zero) and by then combining these to an optimal solution of \(G\) via scaling, see Proposition 5.6. In general, however, it might not be so easy to compose the optimal realizations of each component to a common \(V\) so that a corresponding optimal \(U\) exists.

Isolated nodes are a special case when considering connected components. In Theorem 4.7 it is shown, that in \((E_{\lambda_n})\) with data \(s > 0\) and \(l = c1\) with real \(c > 0\) a node is embedded in the origin if and only if it is isolated in the strictly active subgraph if and only if it is isolated in \(G\) itself.

For \((E_{\lambda_n-\lambda_2})\) Proposition 5.8 states that isolated nodes of \(G_w\) are embedded in the origin in a solution corresponding to \(\lambda_n\). The converse implication is not true in general, see the complete graph of Example 5.5. On the other hand one can find graphs \(G \neq K_n\) and data \(0 \neq l \geq 0\), such that a node \(k \in N\) that is not isolated in the strictly active subgraph is forced to the origin in \(V\).
Example 5.25 Let $G$ be $K_5 \setminus \{24, 35\}$, i.e., the complete graph on five nodes minus (without) the edges 24 and 35. Let $s = 1$ and $l_{1k} = 0$ for $k \in N \setminus \{1\}$ and one otherwise.

An optimal solution of $(E_{\lambda_n - \lambda_2})$ is $\xi = \frac{1}{2}$,
\[
    u_1 = 0, \quad u_2 = \frac{1}{2} e_1, \quad u_3 = \frac{1}{2} e_2, \quad u_4 = -\frac{1}{2} e_1, \quad u_5 = -\frac{1}{2} e_2,
\]
\[
    v_1 = 0, \quad v_2 = v_4 = -\frac{1}{2}, \quad v_3 = v_5 = \frac{1}{2}.
\]

An optimal primal solution is $w = \frac{1}{4} 1$, $\lambda_2 = \mu = \frac{3}{4}$ and $\lambda_n = \frac{5}{4}$.

Because of Theorem 4.7 we conjecture that it is not possible to embed a node into the origin with respect to $V$ whenever $l = c1$ with real $c > 0$ for $G \neq K_n$. For bipartite graphs we are able to prove this, see Theorem 5.32.

Theorem 5.26 (Isolated Nodes - Primal) Let $s > 0$ and $l = c1$, with real $c > 0$ be given data for a graph $G$ with at least one edge and let $w$ be optimal for $(P_{\lambda_n - \lambda_2})$. A node $k \in N$ is isolated in $G$ if and only if $k$ is isolated in the strictly active subgraph $G_w$.

**Proof.** Because $E_w \subseteq E$ a node $k$ is isolated in $G_w$ if it is isolated in $G$. It remains to consider the case of $k$ being isolated in $G_w$. Because $G_w$ is not connected, it suffices to invoke Corollary 5.23 and Theorem 4.7 to complete the proof. \[\blacksquare\]

Again, Theorem 5.26 does not hold for arbitrary $0 \neq l \geq 0$, in general. If we choose appropriate $l$, nodes that are not isolated in $G$ may be isolated in $G_w$.

Example 5.27 Consider the star graph $K_{1,4}$ with five nodes, let node one be the center and let $s = 1$, $l_{12} = 1$, $l_{1k} = \frac{1}{\sqrt{2}}$ for $k = 3, 4, 5$.

An optimal solution of $(E_{\lambda_n - \lambda_2})$ is $\xi = 2$,
\[
    u_1 = u_2 = 0, \quad u_3 = \begin{pmatrix} 0 \\ -\frac{1}{\sqrt{3}} \end{pmatrix}, \quad u_4 = \frac{1}{2} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad u_5 = \frac{1}{2} \begin{pmatrix} -1 \\ \frac{1}{\sqrt{3}} \end{pmatrix},
\]
\[
    v_1 = -\frac{1}{\sqrt{2}}, \quad v_2 = \frac{1}{\sqrt{2}}, \quad v_3 = v_4 = v_5 = 0.
\]

An optimal primal solution is $w_{12} = 1$, $w_{1k} = 0$ for $k = 3, 4, 5$, $\lambda_2 = \mu = 0$ and $\lambda_n = 2$. 
If $G$ is connected, any optimal solution of $(P_{\lambda_2})$ yields a connected strictly active subgraph. So for connected graphs, a nonconnected strictly active subgraph indicates a dominance of $(P_{\lambda_n})$ over $(P_{\lambda_2})$. While the optimal value of $(P_{\lambda_2})$ is related to the connectivity of the graph (cf. Theorem 3.1) $k$-connectivity cannot ensure connectedness of the strictly active subgraph in $(P_{\lambda_n-\lambda_2})$.

**Example 5.28 (k-Edge-Connected Graphs)** For $k \geq 1$, $s = 1$ and $l = 1$ let $G$ be a graph on $12k$ nodes with edge set

\[ E = \{ij : i, j \in \{1, \ldots, 3k\}, i \neq j\} \cup \{ij : i \in \{1 + rk, \ldots, k + rk\}, j \in \{1 + 3k(r + 1), \ldots, 3k + 3k(r + 1)\}, r \in \{0, 1, 2\}\}. \]

So the core of $G$ consists of a complete graph on $3k$ nodes and for each of the core’s three node disjoint subgraphs $K_k$ further $3k$ independent nodes are fully linked to it (see Figure 5.9). Because there are $k$ edge disjoint paths between any two nodes $i, j \in N$, $G$ is $k$-edge-connected.

![Figure 5.9](image-url)

**Figure 5.9:** A $k$-edge-connected graph may have a disconnected strictly active subgraph (see Example 5.28).

Put $\omega = \frac{2}{3(7k^2-k)}$. We prove in the following that an optimal solution with $\lambda_2 = 0$, $\mu = 0$ and $\lambda_n = 4k\omega$ is obtained by setting $w_{ij} = 0$ for edges $ij$ that connect the three $K_k$ (the dashed edges in Figure 5.9) and $w_{ij} = \omega$ for the other edges ($\omega$ normalizes the sum of these weights to 1). Note that the strictly active subgraph $(N, E_w)$ consists of three connected components, so $\lambda_2 = 0$ by Proposition 5.6. In order to see that indeed $\lambda_{\max}(L_w) = 4k\omega$ it suffices to consider the Laplacian block $\bar{L}_w \in \mathbb{R}^{4k \times 4k}$ of a single component. Let the first $k$ columns and rows belong to the complete subgraph $K_k$. Then

\[
x^\top(\lambda_n I - \bar{L}_w)x = \omega x^\top(4kI - \bar{L})x = \omega \left( \sum_{i=1}^{4k} x_i^2 + \sum_{k+1 \leq i < j \leq 4k} (x_i - x_j)^2 \right) \geq 0 \quad \forall x \in \mathbb{R}^{4k}
\]
and \( L_w \geq 0 \) yields feasibility. To show optimality it suffices to construct a feasible dual solution with identical objective value.

By Proposition 5.9, in any optimal \( U \) of \((E_{\lambda} - \lambda_2)\) the nodes of each of the three components are mapped onto a single point. Because of the equilibrium constraint the three points form a regular triangle having its barycenter in the origin. Together with the normalization constraint this yields

\[
\|u_i\|^2 = \frac{1}{12k}, \quad \|u_i - u_j\|^2 = \begin{cases} 
0 & ij \in E_w, \\
\frac{1}{4k} & ij \in E \setminus E_w.
\end{cases}
\]

In an optimal \( V \) of \((E_{\lambda} - \lambda_2)\) each component results in a regular \((k + 1)\)-simplex where the \(3k\) independent nodes are mapped onto a common vertex. We call the straight line segment connecting this special vertex to the barycenter of the remaining \(k\) vertices the height of the simplex. Observe that — due to the \(3k\) nodes assigned to the special vertex — the barycenter of the vertex weighted simplex splits the height into segments of relative length \(1 : 3\). The requirement of identical primal and dual objective values forces the squared distances of the vertices to \(\xi = \lambda_n = 4kw\). The length \(h\) of the height satisfies \(h^2 = \frac{k+1}{2k} \xi\) (recall that in the regular \((k + 1)\)-simplex \(\text{conv}\{e_i \in \mathbb{R}^{k+1} : i = 1, \ldots, k + 1\}\) of edge length \(\sqrt{2}\) the height’s length is \(\|e_{k+1} - \frac{1}{k} \sum_{i=1}^{k} e_i\| = \sqrt{\frac{k+1}{k}}\)). By Proposition 5.8 the barycenter must coincide with the origin, resulting in the distances

\[
\|v_i\|^2 = \begin{cases} 
\frac{25k-7}{8} \omega & i \in \{1, \ldots, 3k\} \\
\frac{k+1}{8} \omega & i \in \{3k + 1, \ldots, 12k\},
\end{cases} \quad \|v_i - v_j\|^2 = 4k\omega \ (ij \in E_w).
\]

Finally, the distance constraints also need to hold for the zero-weighted-edges \(ij \in E \setminus E_w\), so the corresponding distances should be as long as possible. For this, arrange the components heights in a common plane (they intersect in the components barycenters, which is in the origin) so that pairwise they enclose an angle of \(2\pi/3\) and rotate the components around this height such that the affine subspaces spanned by the \(K_k\) are pairwise perpendicular and also perpendicular to the plane spanned by the heights (this is possible, because we do not restrict the dimension of the realization). Then for all edges in \(E \setminus E_w\) one obtains the same length,

\[
\|v_i - v_j\|^2 = \frac{59k - 5}{8} \omega \quad \text{for} \ ij \in E \setminus E_w
\]

and

\[
\|v_i - v_j\|^2 - \|u_i - u_j\|^2 = \frac{19k - 1}{4} \omega > \xi.
\]

Therefore these realizations are feasible and optimality is proven. Note, that the above construction yields a \((3k - 1)\)-dimensional realization.

For \(k = 2\) Figure 5.10 shows the graph, an optimal \(U\) and a three-dimensional projection of an optimal \(V\).
5.3. PROPERTIES COMMON TO \((E_{\lambda_N - \lambda_2})\) AND \((E_{\lambda_2})\) OR \((E_{\lambda_N})\)

Figure 5.10: A 2-connected graph whose strictly active subgraph is disconnected (left), a corresponding optimal \(U\) (center) and a projection of an optimal \(V\) (right).

It seems unlikely that there is a simple structural property characterizing connected graphs whose strictly active subgraph is not connected for \((P_{\lambda_n - \lambda_2})\) or even \((P_{\lambda_N})\). In order to shed some light on the embedding properties underlying the loss of connectedness, consider for some given \(\gamma \geq 0\) the primal dual pair of programs

\[
\begin{align*}
\text{minimize} & \quad \lambda_n - \gamma \lambda_2 \\
\text{subject to} & \quad \sum_{ij \in E} w_{ij} DE_{ij} D + \mu D^{-1}11^T D^{-1} - \lambda_2 I \succeq 0, \\
& \quad \lambda_n I - \sum_{ij \in E} w_{ij} DE_{ij} D \succeq 0, \\
& \quad \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \\
& \quad \lambda_2, \lambda_n, \mu \in \mathbb{R}, \ w \geq 0.
\end{align*}
\]

\((P_{\lambda_n - \gamma \lambda_2})\)

\[
\begin{align*}
\text{maximize} & \quad \xi \\
\text{subject to} & \quad \sum_{i \in N} s_i \|u_i\|^2 = \gamma, \\
& \quad \sum_{i \in N} s_i \|v_i\|^2 = 1, \\
& \quad \left\| \sum_{i \in N} s_i u_i \right\|^2 = 0, \\
& \quad \|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi \geq 0 \ (ij \in E), \\
& \quad \xi \in \mathbb{R}, \ u_i, v_i \in \mathbb{R}^n \ (i \in N).
\end{align*}
\]

\((E_{\lambda_n - \gamma \lambda_2})\)

Note that the set of optimal solutions \(w\) to \((P_{\lambda_n - \gamma \lambda_2})\) is compact by the same arguments leading to Proposition 5.1. Given a connected graph \(G\), whose strictly active subgraph is not connected for \(\gamma = 0\), consider the development of optimal \(U\) in \((E_{\lambda_n - \gamma \lambda_2})\) while increasing \(\gamma\) until the strictly active subgraph \(G_{w,\gamma}\) becomes connected. At first \(G_{w,\gamma}\) consists of components \(G^h_{w,\gamma} = (N^h_{w,\gamma}, E^h_{w,\gamma})\) and, by Proposition 5.9, each node \(i\) of component \(h\) is embedded in a point \(\bar{u}_h\), i.e., \(u_i = \bar{u}_h\) for \(i \in N^h_{w,\gamma}\). As \(\gamma\) is increased, the values \(\|\bar{u}_h\|\) have to increase due to the normalization constraint for \(U\). By the equilibrium constraints the distances \(\|\bar{u}_h - \bar{u}_{h'}\|\) have to increase for at least two distinct components \(h\) and \(h'\)
that are connected in $G$, so the distance constraint corresponding to an edge connecting the two components will become strictly active eventually, thereby reducing the number of components in the strictly active subgraph until only one connected component remains. This intuitive explanation provides a geometric interpretation for the next result, whose proof is actually much simpler.

**Proposition 5.29** For any connected graph $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$ there is a $\gamma \geq 0$ so that for all optimal $w$ of $(P_{\lambda_n-\gamma \lambda_2})$ with $\gamma > \gamma$ the strictly active subgraph $G_{w, \gamma}$ is connected.

**Proof.** Take some $\overline{w} > 0$ with
\[
\sum_{ij \in E} l_{ij}^2 \overline{w}_{ij} = 1,
\]
then $\lambda_2(L_{\overline{w}}) > 0$ (see the proof of Proposition 5.6(i)) and put
\[
\gamma = \frac{\lambda_{\text{max}}(L_{\overline{w}})}{\lambda_2(L_{\overline{w}})}.
\]
For $\gamma > \gamma$ the value of $(P_{\lambda_n-\gamma \lambda_2})$ is negative for this feasible $\overline{w}$, and because $\lambda_n > 0$ for all feasible $w$ we must have $\lambda_2 > 0$ for all optimal $w$ of $(P_{\lambda_n-\gamma \lambda_2})$. The result now follows from Proposition 5.6 (i).\[\square\]

The size of the smallest such $\gamma(s, l)$ may be interpreted as representing the dominance of $\lambda_n$ over $\lambda_2$ for data $s$ and $l$. Again, it does not seem easy to determine this value on basis of structural properties of the graph.

At the end of this section we give some examples where optimal solutions of the coupled problem $(P_{\lambda_n-\lambda_2})$ coincide with optimal solutions of just one, of both or of none of the single problems $(P_{\lambda_2})$ and $(P_{\lambda_n})$.

**Example 5.30** Let $G$ be a graph consisting of two cycles of length $k$ and additional edges $\{ij : j = k + i, j = k + 1 + ((i + 2) \mod k), i = 1, \ldots, k\}$ among them (see Figure 5.11). Let $s = 1$ and $l = 1$. Let $\lambda_2, \lambda_n, \mu, w_{ij} (ij \in E)$ be optimal for $(P_{\lambda_n-\lambda_2})$. For

- $k = 5$ an optimal solution of $(P_{\lambda_n-\lambda_2})$ is optimal for $(P_{\lambda_2})$ and optimal for $(P_{\lambda_n})$ for the same data $s$ and $l$,

- $k = 6$ none of the single problems dominate the solution of $(P_{\lambda_n-\lambda_2})$, i.e., $\lambda_2, \mu, w_{ij} (ij \in E)$ is not optimal for $(P_{\lambda_2})$ and $\lambda_n, w_{ij} (ij \in E)$ is not optimal for $(P_{\lambda_n})$ for the same data $s$ and $l$,
• $k = 7$ an optimal solution of $(P_{\lambda_2})$ dominates that of $(P_{\lambda_n - \lambda_2})$, i.e., $\lambda_2$, $\mu$, $w_{ij}$ $(ij \in E)$ is optimal for $(P_{\lambda_2})$ and $\lambda_n$, $w_{ij}$ $(ij \in E)$ is not optimal for $(P_{\lambda_n})$ for the same data $s$ and $l$.

• $k = 9$ an optimal solution of $(P_{\lambda_n})$ dominates that of $(P_{\lambda_n - \lambda_2})$, i.e., $\lambda_2$, $\mu$, $w_{ij}$ $(ij \in E)$ is not optimal for $(P_{\lambda_2})$ and $\lambda_n$, $w_{ij}$ $(ij \in E)$ is optimal for $(P_{\lambda_n})$ for the same data $s$ and $l$.

\[ \text{Figure 5.11: Graph } G \text{ of Example 5.30 for } k = 6. \]

### 5.4 Special Graph Classes

In Chapter 4 bipartite graphs turned out to play a special role because for these graphs there always exist one-dimensional optimal realizations. It is therefore natural to look at optimal realizations $V$ of $(E_{\lambda_n - \lambda_2})$ for bipartite graphs first. Indeed, the existence of an optimal one-dimensional $V$-realization for bipartite graphs is a direct consequence of Theorem 5.15 above and Theorem 4.8.

**Corollary 5.31** Let $s > 0$ and $0 \neq l \geq 0$ be given data and $G$ a bipartite graph with at least one edge. There is a one-dimensional optimal realization $V$ of $(E_{\lambda_n - \lambda_2})$.

The next theorem is closely related to Proposition 5.8 and Theorem 5.26 and characterizes nodes which are embedded in the origin.

**Theorem 5.32** Let $G$ be a bipartite graph with at least one edge and given data $s > 0$ and $l > 0$. In an optimal realization $V$ of $(E_{\lambda_n - \lambda_2})$ a node is embedded in the origin if and only if it is isolated in the strictly active subgraph.
Proof. Given any optimal realization, with a node embedded in the origin, then it is also embedded in the origin in the corresponding optimal one-dimensional realization constructed in (4.4). Therefore and because of Proposition 5.8 it remains to show that for the optimal one-dimensional realization $V = [v_1, \ldots, v_n] \in \mathbb{R}^{1 \times n}$ of $(E_{\lambda_n - \lambda_2})$ constructed by (4.4) with $h = e_1$ any node $k \in N$ with $v_k = 0$ is isolated in the strictly active subgraph. It suffices to consider, w.l.o.g., $k \in N_2$ with at least one neighbor in $G$. For this $k$ the KKT condition (5.4) reads $0 = \sum_{kj \in E} w_{kj} v_j$. By construction $v_j \geq 0 \ (kj \in E)$ thus the condition requires every single summand to be zero.

Suppose, for contradiction, that there is a neighbor $j$ of $k$ in the strictly active subgraph. Then also $v_j = 0$ and, by complementarity, the distance constraint corresponding to $jk$ is active and reads $-\|u_j - u_k\|^2 - l_{jk}^2 (\lambda_n - \lambda_2) = 0$, thus $\lambda_2 = \lambda_n + l_{jk}^{-2} \|u_j - u_k\|^2$. But $\lambda_2 \geq \lambda_n$ is possible only for complete graphs. The only complete graph that is bipartite is $K_2$ and $v_1 = v_2 = 0$ contradicts the normalization constraint. Thus, $k$ is isolated in the strictly active subgraph.

Note that the restriction concerning data $l$ cannot be dropped. If zero values are allowed there exist bipartite graph instances having a node embedded in the origin without the node being isolated in the strictly active subgraph.

Example 5.33 Consider the graph of Figure 5.12 with node parameters $s = 1$ and edge length parameters $l_{13} = 1$ and zero otherwise.

![Figure 5.12](image)

Figure 5.12: Graph of Example 5.33 with $s = 1$, $l_{13} = 1$ and zero otherwise. As the dashed edges get weight zero in an optimal solution the strictly active subgraph is not connected.

An optimal primal solution is

$$w_{13} = 1, \ w_{23} = w_{34} = 0, \ w_{45} = w_{56} = \frac{2}{3}, \ \lambda_2 = \mu = 0, \ \lambda_n = 2.$$ 

In Figure 5.12 zero-weighted edges are illustrated by dashed lines. So the strictly active subgraph consists of three connected components.

An optimal solution of $(E_{\lambda_n - \lambda_2})$ is $\xi = 2$,

$$u_1 = u_3 = -\frac{1}{3} + \sqrt{\frac{1}{18}}, \ u_2 = -\frac{1}{3} - 2 \sqrt{\frac{1}{18}}, \ u_4 = u_5 = u_6 = \frac{1}{3}.$$
5.4. SPECIAL GRAPH CLASSES

\[ v_1 = -\sqrt{\frac{1}{2}}, \quad v_3 = \sqrt{\frac{1}{2}}, \quad v_2 = v_4 = v_5 = v_6 = 0. \]

While nodes 4, 5 and 6 are not isolated in the strictly active subgraph they are embedded in the origin in the previous \( V \)-realization.

For \( l > 0 \) the only reason for the existence of higher dimensional realizations \( V \) of bipartite graphs are the possibilities to rotate the connected components of the strictly active subgraph.

**Theorem 5.34** Let \( G \) be a bipartite graph with at least one edge and given data \( s > 0 \) and \( l > 0 \). In an optimal realization \( V \) of \( (E_{\lambda_n - \lambda_2}) \) each connected component of the strictly active subgraph is one-dimensional.

**Proof.** Consider an arbitrary optimal solution \( U, V, \xi \) of \( (E_{\lambda_n - \lambda_2}) \), a corresponding (optimal) one-dimensional realization \( V' \) as defined in (4.4) and an optimal solution \( \lambda_2, \lambda_n, w \) of \( (P_{\lambda_n - \lambda_2}) \). For \( ij \in E_w \) complementarity implies

\[ \|u_i - u_j\|^2 + l_{ij}^2 \xi = \|v_i - v_j\|^2 = \|v_i' - v_j'\|^2 = (\|v_i\| + \|v_j\|)^2 = (\|v_i\| + \|v_j\|)^2. \]

Together with Theorem 5.32 this asserts that \( v_i \neq 0 \) and \( v_j \neq 0 \) are linearly dependent. Because a component is connected, all corresponding nodes are linearly dependent. Hence any component of \( G_w \) is one-dimensional.

In the remainder of this section we consider properties of optimal solutions connected to the symmetry of the underlying graph. The first result is closely related to propositions 3.17 and 4.10. It ensures the existence of a special edge weighting, i.e., all edges of the same orbit have the same weight.

**Proposition 5.35** Given \( G = (N, E \neq \emptyset) \) and data \( s > 0, 0 \neq l \geq 0 \). There exists an optimal edge weighting of \( (P_{\lambda_n - \lambda_2}) \) for which edges of the same orbit under the action of the automorphism group \( \text{Aut}(G, s, l) \) have the same value.

As the argumentation follows that of the mentioned theorems we omit the proof but give a short sketch: start with an arbitrary optimal solution, apply all automorphisms to this solution resulting in further optimal edge weightings. A convex combination of these solutions yields the required one.

Proposition 5.35 results in direct consequences for edge transitive graphs.

**Corollary 5.36 (Edge Transitive Graphs)** Let \( G = (N, E) \) be edge transitive with at least one edge and \( s = c_s 1, l = c_l 1 \) with real \( c_s, c_l > 0 \) be given data. There is an optimal solution of \( (P_{\lambda_n - \lambda_2}) \) with edge weights \( w_{ij} = \frac{1}{|E|} \) \( (ij \in E) \).
Corollary 5.37 Let $G = (N, E \neq \emptyset)$ be an edge transitive graph, $s = c_s \mathbf{1}$, $l = c_l \mathbf{1}$ with real $c_s, c_l > 0$ be given data and $U$ and $V$ be optimal realizations for $(E \lambda_n - \lambda_2)$. For $h \in \mathbb{R}^n$ the vectors $U^\top h$ and $V^\top h$ are eigenvectors of $\lambda_2(L(G))$ and $\lambda_n(L(G))$ respectively, unless they are zero vectors.

As there exist edge weights that are optimal for the three programs $(P_{\lambda_2})$, $(P_{\lambda_n})$ and $(P_{\lambda_n - \lambda_2})$ (see corollaries 3.18, 4.11, and 5.36) the combination of both optimal values of $(P_{\lambda_2})$ and $(P_{\lambda_n})$ yields the optimal value of $(P_{\lambda_n - \lambda_2})$.

Corollary 5.38 Let $G = (N, E \neq \emptyset)$ be edge transitive, let $s = c_s \mathbf{1}$ and $l = c_l \mathbf{1}$ with real $c_s, c_l > 0$ be given data. Then optimal $\lambda_2$ of $(P_{\lambda_2})$ and optimal $\lambda_n$ of $(P_{\lambda_n})$ are also optimal in $(P_{\lambda_n - \lambda_2})$.

5.5 A Scaled Primal-Dual Pair

Like in chapters 3 and 4 we may eliminate one variable of $(P_{\lambda_n - \lambda_2})$ and $(D_{\lambda_n - \lambda_2})$, respectively as the feasible sets are specified by inequalities and equations, resulting in corresponding scaled programs.

By Theorem 5.4 the objective value is zero if and only if the graph is complete. So if we do not consider complete graphs, we may divide the constraints of $(P_{\lambda_n - \lambda_2})$ by $\lambda_n - \lambda_2$. Therefore with

$$\hat{\mu} := \frac{\mu}{\lambda_n - \lambda_2}, \quad \hat{w}_{ij} := \frac{w_{ij}}{\lambda_n - \lambda_2} \quad (i,j \in E) \quad \text{and} \quad \hat{\lambda} := \frac{\lambda_n}{\lambda_n - \lambda_2} \quad (5.9)$$

we get $(1 - \hat{\lambda}) = \frac{\lambda_2}{\lambda_n - \lambda_2}$. Replacing the objective function by the left hand side of the equation we arrive at the scaled primal program

maximize $\sum_{ij \in E} l_{ij}^2 \hat{w}_{ij}$
subject to $\sum_{ij \in E} \hat{w}_{ij} D E_{ij} D + \hat{\mu} D^{-1} \mathbf{1} \mathbf{1}^\top D^{-1} - \hat{\lambda} I \succeq -I,$
$\hat{\lambda} I - \sum_{ij \in E} \hat{w}_{ij} D E_{ij} D \succeq 0,$
$\hat{\lambda}, \hat{\mu} \in \mathbb{R}, \hat{w} \geq 0.$

$(P_{\lambda_n - \lambda_2})$

Strictly feasible solutions with respect to the semidefinite constraints of $(P_{\lambda_n - \lambda_2})$ are $0 < \hat{\lambda} < 1$, $\hat{\mu} = 0$ and $\hat{w} = \mathbf{0}$. 
5.5. A SCALED PRIMAL-DUAL PAIR

The semidefinite dual of \((P_{\lambda_n - \lambda_2} - s)\) reads

\[
\begin{align*}
\text{minimize} & \quad \langle I, \hat{X} \rangle \\
\text{subject to} & \quad \langle I, \hat{X} \rangle - \langle I, \hat{Y} \rangle = 0, \\
& \quad \langle (D^{-1}11^\top D^{-1}), \hat{X} \rangle = 0, \quad (D_{\lambda_n - \lambda_2} - s) \\
& \quad \langle DE_{ij}D, \hat{Y} \rangle - \langle DE_{ij}D, \hat{X} \rangle \geq l_{ij}^2 \quad (ij \in E), \\
& \quad \hat{X}, \hat{Y} \succeq 0.
\end{align*}
\]

Observe that by construction the feasible set of \((D_{\lambda_n - \lambda_2} - s)\) is not empty: for a graph with at least one edge that is not the complete graph and given node and edge length parameters Proposition 5.1 ensures attainment of an optimal solution for \((D_{\lambda_n - \lambda_2})\). As the graph is not complete the optimal value is positive by Theorem 5.4. Scaling the solution’s matrices by the reciprocal optimal value of \((D_{\lambda_n - \lambda_2})\) yields a feasible solution for \((D_{\lambda_n - \lambda_2} - s)\). Actually, it is optimal, too, see Proposition 5.40 below and the corresponding transformations.

Because of the strictly feasible solution of \((P_{\lambda_n - \lambda_2} - s)\) with respect to the semidefinite constraint and the feasible solution of \((D_{\lambda_n - \lambda_2} - s)\), strong duality holds and the objective value is finite. Primal attainment follows by construction, i.e., take an optimal solution of \((P_{\lambda_n - \lambda_2})\) and scale it by the optimal value via (5.9). Optimality follows because the functional value is equal to the functional value of the mentioned dual feasible solution.

**Proposition 5.39 (Strong Duality)** Let \(G = (N, E \neq \emptyset)\) be a graph with given data \(s > 0\) and \(0 \neq l \geq 0\) that is not complete. Strong duality holds for \((P_{\lambda_n - \lambda_2} - s)\) and \((D_{\lambda_n - \lambda_2} - s)\) and both programs attain their optimal value.

Finally we obtain the corresponding graph realization formulation of \((D_{\lambda_n - \lambda_2} - s)\) by Gram representations \(D\hat{X}D = \hat{U}^\top \hat{U}\), \(\hat{U} = [\hat{u}_1, \ldots, \hat{u}_n] \in \mathbb{R}^{n \times n}\) and \(D\hat{Y}D = \hat{V}^\top \hat{V}\) with \(\hat{V} = [\hat{v}_1, \ldots, \hat{v}_n] \in \mathbb{R}^{n \times n}\).

\[
\begin{align*}
\text{minimize} & \quad \sum_{i \in N} s_i \|\hat{u}_i\|^2 \\
\text{subject to} & \quad \sum_{i \in N} s_i \|\hat{u}_i\|^2 = \sum_{i \in N} s_i \|\hat{v}_i\|^2, \\
& \quad \sum_{i \in N} s_i \hat{u}_i = 0, \quad (E_{\lambda_n - \lambda_2} - s) \\
& \quad \|\hat{v}_i - \hat{v}_j\|^2 - \|\hat{u}_i - \hat{u}_j\|^2 \geq l_{ij}^2 \quad (ij \in E), \\
& \quad \hat{u}_i, \hat{v}_i \in \mathbb{R}^n \quad (i \in N).
\end{align*}
\]

The graph realization problem \((E_{\lambda_n - \lambda_2} - s)\) searches for two realizations, one for \(\lambda_2\) and one for \(\lambda_{\max}\) such that the sums of weighted squared norms are equal, the weighted barycenter of the \(U\)-realization is in the origin and the difference of squared edge length is bounded below by the corresponding squared edge length parameter. Because of this bound the distance of adjacent nodes with respect to \(V\) is greater than the distance with respect to \(U\) for nonzero edge length parameters.
Let us observe that because of \( l \neq 0 \) some edges must have positive length in \((E_{\lambda_n-\lambda_2}s)\), thus the optimal value is not zero.

For the sake of completeness we formulate the bijection of optimal solutions of the primal (dual, graph realization) program in the next proposition and state the corresponding transformations in Table 5.1.

**Proposition 5.40** Let \( G = (N, E \neq \emptyset) \) be a graph that is not complete with given data \( s > 0 \) and \( 0 \neq l \geq 0 \). There exist transformations, which map optimal solutions of \((P_{\lambda_n-\lambda_2})\), \((D_{\lambda_n-\lambda_2})\) and \((E_{\lambda_n-\lambda_2})\) on optimal solutions of \((P_{\lambda_n-\lambda_2}s)\), \((D_{\lambda_n-\lambda_2}s)\) and \((E_{\lambda_n-\lambda_2}s)\) with same data \( s \) and \( l \), and vice versa. In addition, the active and the strictly active subgraphs are the same.

<table>
<thead>
<tr>
<th>Optimal solutions</th>
<th>((P_{\lambda_n-\lambda_2}) \leftrightarrow (P_{\lambda_n-\lambda_2}s))</th>
<th>((D_{\lambda_n-\lambda_2}) \leftrightarrow (D_{\lambda_n-\lambda_2}s))</th>
<th>((E_{\lambda_n-\lambda_2}) \leftrightarrow (E_{\lambda_n-\lambda_2}s))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda_2, \lambda_n, \mu, w ) of ((P_{\lambda_n-\lambda_2})), ( \xi, X, Y ) of ((D_{\lambda_n-\lambda_2})), ( \xi, u_i, v_i ) (( i \in N )) of ((E_{\lambda_n-\lambda_2})), ( \lambda, \mu, w ) of ((P_{\lambda_n-\lambda_2}s)), ( \hat{X}, \hat{Y} ) of ((D_{\lambda_n-\lambda_2}s)), ( \hat{u}_i, \hat{v}<em>i ) (( i \in N )) of ((E</em>{\lambda_n-\lambda_2}s)).</td>
<td>( \hat{\lambda} = \frac{\lambda^<em>}{\lambda_2 - \lambda_2} ), ( \hat{\mu} = \frac{\mu^</em>}{\lambda_n - \lambda_2} ), ( \hat{w}<em>{ij} = \frac{w</em>{ij}}{\lambda_n - \lambda_2} ) (( ij \in E ))</td>
<td>( \hat{X} = \frac{1}{\xi} X^* ), ( \hat{Y} = \frac{1}{\xi} Y^* ), ( \hat{u}_i = \frac{1}{\sqrt{\xi}} u_i^* ) (( i \in N ))</td>
<td>( \hat{\xi} = \hat{\mu} ), ( \hat{\lambda} = \hat{\mu} ), ( \hat{\mu} ) (( i \in N ))</td>
</tr>
</tbody>
</table>

**Table 5.1**: Transformations of optimal solutions of \((P_{\lambda_n-\lambda_2})\), \((D_{\lambda_n-\lambda_2})\) and \((E_{\lambda_n-\lambda_2})\) on optimal solutions of \((P_{\lambda_n-\lambda_2}s)\), \((D_{\lambda_n-\lambda_2}s)\) and \((E_{\lambda_n-\lambda_2}s)\) and vice versa.

Let us finally denote that we may construct another scaled program by alternatively defining \( \hat{\lambda} := \frac{\lambda^2}{\lambda_n - \lambda_2} \). Then we get \( (1 + \hat{\lambda}) = \frac{\lambda^2}{\lambda_n - \lambda_2} \) and slightly different dual and graph realization programs respectively.
5.6 Variable Edge Length Parameters

As in the previous chapters also for the difference of extremal eigenvalues of the graph Laplacian, optimal realizations are maps of eigenvectors to the maximal second smallest and the minimal maximum eigenvalue of the corresponding optimal weighted Laplacian, respectively (see Proposition 5.2). For edge transitive graphs they are even maps of eigenvectors to the second smallest and maximum eigenvalue of the unweighted Laplacian, respectively (see Corollary 5.37).

Based on the scaled formulation of the graph realization problem \((E_{\lambda_n-\lambda_2^-s})\) with \(s = 1\) we may formulate a program with variable edge length parameters, such that optimal realizations are maps of the eigenvectors to the extremal eigenvalues of the unweighted Laplacian of a noncomplete graph.

Therefore we replace the squared edge length parameters \(l_{ij}^2 (ij \in E)\) by variable “distance slacks” \(d_{ij} \in \mathbb{R}\) so as to allow the distances \(\|u_i - u_j\|\) to exceed \(\|v_i - v_j\|\) in some cases. In order to guarantee boundedness of the graph realization problem we require

\[
\sum_{ij \in E} d_{ij} = 1
\]

so that at least one \(d_{ij}\) is strictly positive. The so obtained graph realization program and the corresponding dual and primal problems are listed in Table 5.2, cf. sections 3.4 and 4.6.

We want to illustrate optimal realizations of \((E_{\lambda_n-\lambda_2^-l})\). In order to compare them with realizations of the single programs we use again the graph of Figure 3.1. On the left hand side of Figure 5.13 an optimal one-dimensional realization with respect to the second smallest eigenvalue and on the right hand side an optimal one-dimensional realization with respect to the maximum eigenvalue is illustrated. The order of the nodes is given below and above the realizations of the graph, respectively. Let us observe that the structures of these realizations seem to be similar to those of the single programs illustrated in figures 3.6 and 4.11.

Strictly feasible solutions of \((P_{\lambda_n-\lambda_2^-l})\) with respect to the semidefinite constraints are \(0 < \hat{\lambda} < 1, \hat{w} = 0, \hat{\rho} = 0\) and \(\hat{\mu} = 0\).

Furthermore the feasible set of \((E_{\lambda_n-\lambda_2^-l})\), thus the feasible set of \((D_{\lambda_n-\lambda_2^-l})\) is not empty by the following example.

**Example 5.41 (Feasible Solution)** As the graph is not complete and as there is at least one edge, there are nodes \(k_1, k_2 \in N\) which are not adjacent, i.e., \(k_1k_2 \notin E\) and \(\{ik_j \in E : i \in N, j = 1, 2\} \neq \emptyset\). In addition \(n > 2\) as \(E \neq \emptyset\) and \(G\) is not complete.
Graph $G = (N, E \neq \emptyset)$, not complete.

<table>
<thead>
<tr>
<th>primal</th>
<th>dual</th>
</tr>
</thead>
<tbody>
<tr>
<td>max $\rho$ s.t. $\sum_{ij \in E} w_{ij} E_{ij} - \lambda I - \mu 11^\top \succeq -I,$ $\lambda I - \sum_{ij \in E} w_{ij} E_{ij} \succeq 0,$ $\rho - w_{ij} = 0$ $(ij \in E),$ $\lambda, \mu, \rho \in \mathbb{R}, w \geq 0.$ $(P_{\lambda_n - \lambda_2 - 1})$</td>
<td>min $\langle I, X \rangle,$ s.t. $\langle I, X \rangle - \langle I, Y \rangle = 0,$ $\langle 11^\top, X \rangle = 0,$ $\langle E_{ij}, Y \rangle - \langle E_{ij}, X \rangle \geq d_{ij}$ $(ij \in E),$ $\sum_{ij \in E} d_{ij} = 1,$ $X, Y \succeq 0,$ $d_{ij} \in \mathbb{R}$ $(ij \in E).$ $(D_{\lambda_n - \lambda_2 - 1})$</td>
</tr>
</tbody>
</table>

| realization | | realization |
| min $\sum_{i \in N} \|u_i\|^2$ s.t. $\sum_{i \in N} \|u_i\|^2 = \sum_{i \in N} \|v_i\|^2$ $\left\| \sum_{i \in N} u_i \right\|^2 = 0,$ $\|v_i - v_j\|^2 - \|u_i - u_j\|^2 \geq d_{ij}$ $(ij \in E),$ $\sum_{ij \in E} d_{ij} = 1,$ $u_i, v_i \in \mathbb{R}^n$ $(i \in N),$ $d_{ij} \in \mathbb{R}$ $(ij \in E).$ $(E_{\lambda_n - \lambda_2 - 1})$ |

Table 5.2: Primal, dual and graph realization formulation with variable edge length parameters.

First we will choose a realization $u_i$ $(i \in N)$, then we construct an appropriate realization $v_i$ $(i \in N)$ and by scaling we ensure feasibility for $(E_{\lambda_n - \lambda_2 - 1}).$

Let $h \in \mathbb{R}^n$ with $\|h\| = 1$ and $u_{k_1} = -h,$ $u_{k_2} = h$ and $u_j = 0$ $(j \in N \setminus \{k_1, k_2\}).$ Then

$$\sum_{i \in N} u_i = 0,$$ $$\sum_{i \in N} \|u_i\|^2 = 2 \quad \text{and} \quad \|u_i - u_j\|^2 = \begin{cases} 1 & i \in \{k_1, k_2\}, j \in N \setminus \{k_1, k_2\} \\ 0 & i, j \in N \setminus \{k_1, k_2\} \end{cases}.$$

Let $v_{k_i} = \alpha h$ $(i = 1, 2)$ and $v_j = \beta h$ $(j \in N \setminus \{k_1, k_2\})$ such that

$$\sum_{i \in N} \|v_i\|^2 = 2\alpha^2 + (n - 2)\beta^2 = 2,$$ $$\|v_{k_i} - v_j\|^2 = (\alpha - \beta)^2 > 1.$$
5.6. VARIABLE EDGE LENGTH PARAMETERS

Figure 5.13: An optimal realization with respect to $\lambda_2$ on the left hand side and an optimal realization with respect to $\lambda_{\text{max}}$ on the right hand side of the graph of Figure 3.1 for $(E_{\lambda_n-\lambda_2^{-1}})$.

If such $\alpha, \beta \in \mathbb{R}$ exist – we will confirm this at the end of the example – set $\hat{d}_{ij} = (\alpha - \beta)^2 - 1$ for $i \in \{k_1, k_2\}$, $j \in N \setminus \{k_1, k_2\}$, $ij \in E$ and zero otherwise resulting in

$$\|v_i - v_j\|^2 - \|u_i - u_j\|^2 = \hat{d}_{ij} \quad \text{for} \quad ij \in E.$$

So far only the normalization constraint of $\hat{d}_{ij}$ ($ij \in E$) may be violated.

To ensure feasibility let

$$\delta^2 := \sum_{ij \in E} \hat{d}_{ij} = \sum_{\substack{ij \in E, \ i \in \{k_1, k_2\}}} ((\alpha - \beta)^2 - 1) > 0.$$

and scale the current solution.

Then $\delta^{-1} u_i$, $\delta^{-1} v_i$ ($i \in N$) and $d_{ij} = \delta^{-2} \hat{d}_{ij}$ for $ij \in E$ is feasible for $(E_{\lambda_n-\lambda_2^{-1}})$.

It remains to show that the system (5.10) and (5.11) is solvable. Figure 5.14 illustrates the situation (cf. Lemma 3.3): Equation (5.10) describes an ellipse (marked in red), the equation $(\alpha - \beta)^2 = 1$ describes two parallel straight lines, thus (5.11) describes all points

$$\{(\alpha, \beta) \in \mathbb{R}^2 : (\alpha - \beta)^2 > 1\} = \{(\alpha, \beta) \in \mathbb{R}^2 : \alpha - \beta > 1\} \cup \{(\alpha, \beta) \in \mathbb{R}^2 : \alpha - \beta < -1\}$$

(marked in green). As the straight lines have common points with the ellipse (e.g. $(1,0)$ and $(-1,0)$ respectively), but are not tangents, there must exist some required $(\alpha, \beta)$.

By the same argument as before strong duality holds for $(P_{\lambda_n-\lambda_2^{-1}})$ and $(D_{\lambda_n-\lambda_2^{-1}})$.

Proposition 5.42 (Strong Duality) Let $G = (N, E \neq \emptyset)$ be a graph that is not complete. Strong duality holds for $(P_{\lambda_n-\lambda_2^{-1}})$ and $(D_{\lambda_n-\lambda_2^{-1}})$ and both programs attain their optimal value.
Figure 5.14: The ellipse (5.10) (red) and inequality (5.11) (green) have points in common.

Remark 5.43 Observe that the optimal value of $(E_{\lambda_n-\lambda_2-1})$ is strictly greater than zero, as at least one $d_{ij}$ is strictly positive. Thus at least one edge must have positive length.

Like in the previous chapters we are able to prove relations of optimal graph realizations of $(E_{\lambda_n-\lambda_2-1})$ to eigenvectors corresponding to $\lambda_2(L(G))$ and $\lambda_{\text{max}}(L(G))$ respectively. As the proofs are similar to these of theorems 3.22 and 3.23 for the $\lambda_2$ solutions and eigenvectors and of theorems 4.21 and 4.22 for the $\lambda_{\text{max}}$ solutions and eigenvectors we omit to repeat them.

Theorem 5.44 Given a connected graph $G = (N, E \neq \emptyset)$ that is not complete, let $U = [u_1, \ldots, u_n], V = [v_1, \ldots, v_n]$ be an optimal solution of $(E_{\lambda_n-\lambda_2-1})$. Then

$$\sum_{i \in N} \|u_i\|^2 = \frac{1}{\lambda_{\text{max}}(L(G)) - \lambda_2(L(G))}$$

and for $h \in \mathbb{R}^n$ the vector $U^\top h$ is an eigenvector of $\lambda_2(L(G))$ and the vector $V^\top h$ is an eigenvector of $\lambda_{\text{max}}(L(G))$, except they are zero vectors.

Theorem 5.45 Given a connected graph $G = (N, E \neq \emptyset)$ that is not complete, let $u \in \mathbb{R}^n, \|u\| = 1$, be an eigenvector of $\lambda_2(L(G))$ and let $v \in \mathbb{R}^n, \|v\| = 1$ be an eigenvector of $\lambda_{\text{max}}(L(G))$. An optimal solution of $(D_{\lambda_n-\lambda_2-1})$ is

$$X = \frac{1}{\lambda_{\text{max}}(L(G)) - \lambda_2(L(G))} uu^\top, \quad Y = \frac{1}{\lambda_{\text{max}}(L(G)) - \lambda_2(L(G))} vv^\top$$

and

$$d_{ij} = \frac{([v]_i - [v]_j)^2 - ([u]_i - [u]_j)^2}{\lambda_{\text{max}}(L(G)) - \lambda_2(L(G))}$$

for $ij \in E$. 
5.6. VARIABLE EDGE LENGTH PARAMETERS

We obtain maximum rank solutions of \((D_{\lambda_n-\lambda_2-1})\) and \((E_{\lambda_n-\lambda_2-1})\) by the same procedure as in sections 3.4 and 4.6: suppose the columns of \(\hat{U} \in \mathbb{R}^{n \times k_1}\) with \(\hat{U}^\top \hat{U} = I_{k_1}\) span the eigenspace to \(\lambda_2(L(G))\) and the columns of \(\hat{V} \in \mathbb{R}^{n \times k_2}\) with \(\hat{V}^\top \hat{V} = I_{k_2}\) span the eigenspace to \(\lambda_{\text{max}}(L(G))\). Then the convex combinations

\[
X = \frac{1}{k_1 \lambda_2(L(G))} \hat{U}^\top, \quad Y = \frac{1}{k_2 \lambda_{\text{max}}(L(G))} \hat{V}^\top
\]

with \(d_{ij} = \langle E_{ij}, Y \rangle - \langle E_{ij}, X \rangle\) for \(ij \in E\) are corresponding maximum rank solutions of \((D_{\lambda_n-\lambda_2-1})\) and their \(k_1\)- and \(k_2\)-dimensional realizations of \((E_{\lambda_n-\lambda_2-1})\) are given by the columns of

\[
U = \frac{1}{\sqrt{k_1 \lambda_2(L(G))}} \hat{U}^\top \quad \text{and} \quad V = \frac{1}{\sqrt{k_2 \lambda_{\text{max}}(L(G))}} \hat{V}^\top,
\]

respectively.

Let us shortly recapitulate some results: Theorem 5.14 ensures that for a graph with given positive node and edge parameters feasible realizations of \((E_{\lambda_2})\) and \((E_{\lambda_n})\) together are feasible for \((E_{\lambda_n-\lambda_2})\) with an appropriate functional value, and \textit{vice versa}. While feasibility is preserved, optimality may be lost.

Furthermore on the one hand we proved that optimal realizations of \((E_{\lambda_2-1})\) are maps of eigenvectors to the second smallest eigenvalue of the unweighted Laplacian, Theorem 3.22, the same holds for optimal \(U\)-realizations of \((E_{\lambda_n-\lambda_2-1})\), Theorem 5.44. On the other hand, an eigenvector of the second smallest eigenvalue of the unweighted Laplacian yields optimal solutions for both programs, theorems 3.23 and 5.45. They differ by a factor. So we may ask whether the set of optimal realizations of \((E_{\lambda_2-1})\) and the set of optimal \(U\)-realizations of \((E_{\lambda_n-\lambda_2-1})\) are equal up to scaling.

Analogous results hold for realizations corresponding to the maximum eigenvalue, thus an analogous question arises.

Indeed, for the primal, dual and graph realization problems with variable edge length parameters optimality is preserved.

\begin{theorem}
Given a connected graph \(G = (N, E \neq \emptyset)\) that is not complete. Let

\[
c_2 = \frac{\lambda_{\text{max}}(L(G)) - \lambda_2(L(G))}{\lambda_2(L(G))} \quad \text{and} \quad c_n = \frac{\lambda_{\text{max}}(L(G)) - \lambda_2(L(G))}{\lambda_{\text{max}}(L(G))}.
\]

For optimal \(\lambda, \mu, \rho, w\) of \((P_{\lambda_n-\lambda_2-1})\), optimal \(X, Y, d\) of \((D_{\lambda_n-\lambda_2-1})\) and optimal \(u_i, v_i\) \((i \in N)\), \(d\) of \((E_{\lambda_n-\lambda_2-1})\),

\[
\tilde{\rho} = c_2 \rho, \quad \tilde{\mu} = c_2 \mu, \quad \tilde{w} = c_2 w \quad \text{is optimal for \((P_{\lambda_2-1})\)},
\]

\[
\tilde{X} = c_2 X, \quad \tilde{d}_{ij} = c_2 \langle E_{ij}, Y \rangle - d_{ij} \quad \text{for \(ij \in E\) is optimal for \((D_{\lambda_2-1})\)} \quad \text{and}
\]

\[
\tilde{u}_i = \sqrt{c_2} u_i \quad \text{for \(i \in N\), \(\tilde{d}_{ij} = c_2 (||v_i - v_j||^2 - d_{ij})\) for \(ij \in E\) is optimal for \((E_{\lambda_2-1})\).}
\]
\end{theorem}
\( \hat{\rho} = c_n \rho, \hat{w} = c_n w \) is optimal for \((P_{\lambda_2} - 1)\),
\(\hat{\varrho} = c_n Y, \hat{d}_{ij} = c_n (\langle E_{ij}, X \rangle + d_{ij}) \) for \(i, j \in E\) is optimal for \((D_{\lambda_2} - 1)\) and
\(\hat{\nu}_i = \sqrt{c_n} v_i \) for \(i \in N\), \(\hat{d}_{ij} = c_n (\|u_i - u_j\|^2 + d_{ij}) \) for \(i, j \in E\) is optimal for \((E_{\lambda_2} - 1)\).

For optimal \(\hat{\rho}, \hat{\mu}, \hat{w}\) of \((P_{\lambda_2} - 1)\), optimal \(\hat{X}, \hat{d}\) of \((D_{\lambda_2} - 1)\), optimal \(\hat{u}_i (i \in N)\), \(\hat{d}\) of \((E_{\lambda_2} - 1)\) and optimal \(\hat{\varrho}, \hat{w}\) of \((P_{\lambda_2} - 1)\), optimal \(\hat{Y}, \hat{d}\) of \((D_{\lambda_2} - 1)\) and optimal \(\hat{\nu}_i (i \in N)\), \(\hat{d}\) of \((E_{\lambda_2} - 1)\),
\(\rho = c_2^{-1} \rho (= c_n^{-1} \hat{\rho}), \lambda = c_n^{-1}, \mu = -c_2^{-1} \hat{\mu}, w = c_2^{-1} \hat{w} (= c_n^{-1} \hat{w})\) is optimal for \((P_{\lambda_2} - 1)\),
\(X = c_2^{-1} \hat{X}, Y = c_n^{-1} \hat{Y}\) and \(d_{ij} = c_n^{-1} \hat{d}_{ij} - c_2^{-1} \hat{d}_{ij}\) for \(i, j \in E\) is optimal for \((D_{\lambda_2} - 1)\)
and
\(u_i = c_2^{-1} \hat{u}_i, v_i = c_n^{-1} \hat{v}_i \) for \(i \in N\) and \(d_{ij} = c_n^{-1} \hat{d}_{ij} - c_2^{-1} \hat{d}_{ij}\) for \(i, j \in E\) is optimal for \((E_{\lambda_2} - 1)\).

Before we will prove Theorem 5.46 we want to summarize some basic properties of optimal solutions of \((P_{\lambda_2} - 1)\) and \((D_{\lambda_2} - 1)\).

**Lemma 5.47** Given a connected graph \(G = (N, E \neq \emptyset)\) that is not complete, let \(X, Y\) and \(d\) be optimal for \((D_{\lambda_2} - 1)\) and \(\lambda, \mu, \rho\) and \(w\) be a corresponding optimal primal solution.

(i) \(\langle E_{ij}, Y \rangle - \langle E_{ij}, X \rangle = d_{ij} \) for all \(i, j \in E\),
(ii) \(\lambda = \frac{\lambda_{\max}(L(G))}{\lambda_{\max}(L(G)) - \lambda_2(L(G))} > 0\), and \(\lambda - 1 = \frac{\lambda_2(L(G))}{\lambda_{\max}(L(G)) - \lambda_2(L(G))} > 0\),
(iii) \(\sum_{i,j \in E} \langle E_{ij}, X \rangle = \lambda - 1\),
(iv) \(\sum_{i,j \in E} \langle E_{ij}, Y \rangle = \lambda\).

**Proof.** (i) Because of strong duality, Proposition 5.42, and the positive optimal value, Remark 5.43, \(w_{ij} = \rho > 0\) follow for all \(i, j \in E\). Complementarity yields the result.

(ii) Strong duality and Theorem 5.44 ensure \(\rho = (\lambda_{\max}(L) - \lambda_2(L))^{-1}\). By the semidefinite inequality constraints of \((P_{\lambda_2} - 1)\) we get
\[
\rho L - \mu 11^T \succeq (\lambda - 1) I \quad \Rightarrow \quad \frac{\lambda_2(L)}{\lambda_{\max}(L) - \lambda_2(L)} \geq \lambda - 1 \quad \Rightarrow \quad \frac{\lambda_{\max}(L)}{\lambda_{\max}(L) - \lambda_2(L)} \geq \lambda
\]
and
\[
\rho L \preceq \lambda I \quad \Rightarrow \quad \frac{\lambda_{\max}(L)}{\lambda_{\max}(L) - \lambda_2(L)} \leq \lambda,
\]
hence the equalities of (ii) follow. As the graph is connected, its edge set is not empty and as it is not complete the values are strictly positive.

(iii) and (iv) Semidefinite complementarity yields
\[
\langle X, (1 - \lambda) I - \mu 11^T + \rho \sum_{i,j \in E} E_{ij} \rangle = \rho (1 - \lambda) + \rho \sum_{i,j \in E} \langle E_{ij}, X \rangle = 0
\]
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thus

$$\sum_{ij \in E} \langle E_{ij}, X \rangle = \lambda - 1$$

and

$$\langle Y, \lambda I - \rho \sum_{ij \in E} E_{ij} \rangle = \rho \lambda - \rho \sum_{ij \in E} \langle E_{ij}, Y \rangle = 0 \Rightarrow \sum_{ij \in E} \langle E_{ij}, Y \rangle = \lambda.$$  \hfill \blacksquare

Let us now prove Theorem 5.46

**Proof.** For the first part of the proof let $\lambda$, $\mu$, $\rho$ and $w$ be optimal for $(P_{\lambda n - \lambda_2^2 - l})$ and $X$, $Y$ and $d$ be optimal for $(D_{\lambda n - \lambda_2^2 - l})$.

Feasibility of $\tilde{\rho}$, $\tilde{\mu}$, $\tilde{w}$ for $(P_{\lambda_2^2 - l})$ follows by feasibility of $\lambda$, $\mu$, $\rho$ and $w$ and by scaling the constraints of $(P_{\lambda n - \lambda_2^2 - l})$ by $c_2 > 0$. Optimality follows from strong duality and theorems 3.22 and 5.44, because $\tilde{\rho} = c_2 \rho = \frac{1}{\lambda_2(L)}$.

Next, we want to verify feasibility and optimality of $\tilde{X}$ and $\tilde{d}$ for $(D_{\lambda_2^2 - l})$. By feasibility of $d$ and Lemma 5.47(ii) and (iv) the normalization constraint holds,

$$\sum_{ij \in E} \tilde{d}_{ij} = c_2 \sum_{ij \in E} (\langle E_{ij}, Y \rangle - d_{ij}) = c_2 (\lambda - 1) = 1.$$  

For an edge $ij \in E$ the distance constraint

$$\langle E_{ij}, \tilde{X} \rangle - \tilde{d}_{ij} = c_2 (\langle E_{ij}, X \rangle - \langle E_{ij}, Y \rangle + d_{ij}) \geq 0$$

holds by complementarity, Lemma 5.47(i). Optimality follows by Theorem 3.22 because the functional value equals

$$\langle I, \tilde{X} \rangle = c_2 \langle I, X \rangle = \frac{c_2}{\lambda_{\max}(L) - \lambda_2(L)} = \frac{1}{\lambda_2(L)},$$

using Theorem 5.44.

The result for $\tilde{U} = [\tilde{u}_1, \ldots, \tilde{u}_n]$, $\tilde{d}_{ij}$ follows by the previous part of the proof as $\tilde{U}^T \tilde{U} = c_2 X'$ and $\|v_i - v_j\|^2 = \langle E_{ij}, Y' \rangle$ for optimal $X'$ and $Y'$ of $(D_{\lambda n - \lambda_2^2 - l})$.

The proofs for optimal solutions for $(P_{\lambda n})$, $(D_{\lambda n})$ and $(E_{\lambda n})$ are similar, so we omit them.

In the second part let $\tilde{\rho}$, $\tilde{\mu}$, $\tilde{w}$ be optimal for $(P_{\lambda_2^2 - l})$, $\tilde{X}$, $\tilde{d}$ be optimal for $(D_{\lambda_2^2 - l})$, $\tilde{u}_i$ ($i \in N$), $\tilde{d}$ be optimal for $(E_{\lambda_2^2 - l})$ and $\tilde{\rho}$, $\tilde{w}$ be optimal for $(P_{\lambda n})$, $\tilde{Y}$, $\tilde{d}$ be optimal for $(D_{\lambda n})$ and $\tilde{u}_i$ ($i \in N$), $\tilde{d}$ be optimal for $(E_{\lambda n})$.  \hfill \blacksquare
Feasibility of $\lambda$, $\mu$, $\rho$ and $w$ follows by feasibility of the solutions of the single problems and by scaling the constraints of $(P_{\lambda_2-1})$ by $c_2^{-1} > 0$ and by scaling the constraints of $(P_{\lambda_n-1})$ by $c_n^{-1} > 0$ respectively. Optimality follows from strong duality and theorems (3.22), (4.21) and (5.44), because $\rho = c_2^{-1} \hat{\rho} = c_n^{-1} \hat{\rho} = \frac{1}{\lambda_{\text{max}}(L) - \lambda_2(L)}$.

The dual solution is feasible because

$$\sum_{ij \in E} d_{ij} = c_n^{-1} \sum_{ij \in E} \hat{d}_{ij} - c_2^{-1} \sum_{ij \in E} \tilde{d}_{ij} = c_n^{-1} - c_2^{-1} = 1,$$

by feasibility of $\tilde{d}$ and $\hat{d}$,

$$\langle E_{ij}, Y \rangle - \langle E_{ij}, X \rangle - d_{ij} = c_n^{-1} \left( \langle E_{ij}, \tilde{Y} \rangle - \hat{d}_{ij} \right) - c_2^{-1} \left( \langle E_{ij}, \tilde{X} \rangle + \tilde{d}_{ij} \right) = 0,$$

by complementarity conditions of $(P_{\lambda_2-1})$ and $(D_{\lambda_2-1})$ (cf. page 52) as well as $(P_{\lambda_n-1})$ and $(D_{\lambda_n-1})$ (cf. page 85).

$$\langle 11^T, X \rangle = c_2^{-1} \langle 11^T, \tilde{X} \rangle = 0$$

because $\tilde{X}$ is feasible for $(D_{\lambda_2-1})$,

$$\langle I, Y \rangle - \langle I, X \rangle = c_n^{-1} \langle I, \tilde{Y} \rangle - c_2^{-1} \langle I, \tilde{X} \rangle = 0$$

using theorems 3.22 and 4.21. Optimality follows by Theorem 5.44 because

$$\langle I, X \rangle = c_2^{-1} \langle I, \tilde{X} \rangle = \frac{1}{\lambda_{\text{max}}(L) - \lambda_2(L)}.$$

Referring to the example graph of Figure 3.1 and the corresponding optimal realizations with respect to $(E_{\lambda_2-1})$, $(E_{\lambda_n-1})$ and $(E_{\lambda_n-\lambda_2-1})$, respectively, the structure of these realizations corresponding to $\lambda_2$ and these corresponding to $\lambda_{\text{max}}$ are indeed very similar. By the previous theorem optimal realizations of $(E_{\lambda_n-\lambda_2-1})$ are scaled optimal realizations of $(E_{\lambda_2-1})$ and $(E_{\lambda_n-1})$ and vice versa.
Chapter 6

Some Open Problems

In this thesis, we considered the extremal eigenvalues of the Laplacian of a graph, thereby summarizing present results of mainly Göring et al. and following their approach to analyze the maximum eigenvalue and the difference of extremal eigenvalues. To get results concerning the eigenspaces of these eigenvalues in connection to structural graph properties we redistributed the edge weights by optimizing the eigenvalues. A semidefinite approach revealed corresponding graph realization problems. Optimal realizations turned out to encode the eigenspaces in some sense because maps onto one-dimensional subspaces are eigenvectors to the considered optimal eigenvalue. Results concerning the separator structure and the existence of optimal realizations of bounded dimension are established.

Certainly, there are remaining open problems and related questions. With an outlook on further research we want to address some of them.

Optimal realizations encoding the whole eigenspace. We explain the problem on $(P_{\lambda_n})$ and $(E_{\lambda_n})$.

Theorem 4.22 and the following explanations state that for a given connected graph on the one hand there are optimal realizations of $(E_{\lambda_n}-1)$ obtained from a maximal set of linearly independent eigenvectors with respect to the maximum eigenvalue of the unweighted Laplacian. On the other hand, projections onto the one-dimensional subspaces spanned by the unit vectors of the canonical basis, yield the same set of eigenvectors, scaled by a factor. That means, such optimal realizations encode the whole eigenspace corresponding to the maximum eigenvalue of the unweighted Laplacian.

For the problem of minimizing the maximum eigenvalue we also know that projections of optimal realizations onto one-dimensional subspaces yield eigenvectors to the optimal weighted Laplacian, Proposition 4.2.
CHAPTER 6. SOME OPEN PROBLEMS

Let $G$ be a given graph with data $s > 0$ and $0 \neq l \geq 0$. Let $\lambda_n, w$ be optimal for $(P_{\lambda_n})$ and let the eigenspace corresponding to $\lambda_{\text{max}}(DL_w D)$ be $k$-dimensional. Is there an optimal realization $V$ of $(E_{\lambda_n})$ and vectors $h_1, \ldots, h_k \in \mathbb{R}^n$ such that $\{V^\top h_1, \ldots, V^\top h_k\}$ is a set of linearly independent eigenvectors with respect to $\lambda_{\text{max}}(DL_w D)$? In other words, are there optimal solutions that are constructed by a maximum set of linearly independent eigenvectors with respect to $\lambda_{\text{max}}(DL_w D)$ in the manner of (4.18)?

In general, the answer to both questions is: no. A path with three edges and data $s = 1$ and $l = 1$ turns out to be a counterexample. An optimal primal solution is

$$w_{12} = w_{34} = \frac{1}{2}, \ w_{23} = 0, \ \lambda_n = 1$$

and an optimal graph realization is given by

$$v_1 = v_3 = -\frac{1}{2}, \ v_2 = v_4 = \frac{1}{2}, \ \xi = 1.$$ 

The realization is unique (up to congruence) because of the constraint $\|v_2 - v_3\|^2 \geq 1$. Projections of that optimal realizations onto one-dimensional subspaces yield one linearly independent eigenvector while the eigenspace corresponding to $\lambda_{\text{max}}(L_w)$ is two-dimensional.

Consider the graph of Figure 4.9 with data $s = 1$ and $l = 1$, the illustrated optimal two dimensional realization and a corresponding primal optimal solution. We observe that the eigenspace corresponding to the maximum eigenvalue of the optimal weighted Laplacian is two-dimensional and that we get two linearly independent eigenvectors by mapping the realization onto the one-dimensional subspaces spanned by the first two unit vectors of the canonical basis. Thus in this case, we have a positive answer.

Does the question’s answer depend on special graph classes and if so, can we identify them? Does it depend on whether the strictly active subgraph is connected or not? What is the influence of the given data?

Analogous questions arise for the problems $(P_{\lambda_2})$, $(E_{\lambda_2})$ and $(P_{\lambda_n - \lambda_2})$, $(E_{\lambda_n - \lambda_2})$.

**Connectedness of the strictly active subgraph in $(P_{\lambda_n - \lambda_2})$.** In Section 5.3 we have traced optimal $V$-realizations of $(E_{\lambda_n - \lambda_2})$ back to optimal realizations of the single problem $(E_{\lambda_n})$ with appropriate data, Theorem 5.15. Thus, structural properties of optimal realizations of the single problem also hold for optimal realizations of the coupled one. Provided that the strictly active subgraph is connected, we may do the same for optimal $U$-realizations, Theorem 5.18. The connectedness of the strictly active subgraph was essential.

We started a discussion about this aspect of nonconnected strictly active subgraphs in the case of a connected graph and already mentioned that it seems unlikely that there is a
simple structural property characterizing that fact. Further research will be necessary to solve this problem.

Also in the case of minimizing the maximum eigenvalue we do not know for which graphs the strictly active subgraph decomposes.

**Family of graphs with tight dimension bounds for** \((E_{\lambda_n} - \lambda_2)\). In dependence on the tree-width of the graph the existence of optimal realizations of bounded dimension is guaranteed for \((E_{\lambda_2})\), \((E_{\lambda_n})\) and \((E_{\lambda_n} - \lambda_2)\) by Corollary 3.15, Theorem 4.15 and corollaries 5.17 and 5.20, respectively. While there are families of graphs for which the tree-width bounds are tight for \((E_{\lambda_2})\) and \((E_{\lambda_n})\), respectively such a family is not observed yet for \((E_{\lambda_n} - \lambda_2)\). In particular, can we find a family of graphs for which both bounds are tight at the same time?

**Graph partitioning.** Graph partitioning problems like graph bisection and MAX-cut are known to be \(NP\)-hard problems. They are tightly linked to the extremal eigenvalues of the Laplacian. Methods known as *spectral partitioning* use the corresponding eigenvectors to generate graph partitions. Of course, these partitions are not optimal in general. Is it possible to find better partitions using information, such as optimal edge weights or the eigenvectors corresponding to the optimized eigenvalues? Are there connections of the considered eigenvalue optimization problems to graph partitioning problems?

**Sum of \(k\)-largest eigenvalues.** The nontrivial eigenvalues of the Laplacian of a graph, i.e., the second smallest and the maximum eigenvalue, are not the only ones that are semidefinite representable by matrix inequalities. The sum of the \(k\)-largest eigenvalues of the Laplacian is a further example. So it would be interesting to apply a similar approach, to get associated semidefinite programs and to analyze the interaction of these eigenvalues and connections of optimal solutions to the graph’s structure.
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Theses

In this dissertation, we consider undirected, simple, finite graphs $G = (N, E)$ with non-empty edge set and given node parameters $s \in \mathbb{R}^{|N|}$, $s > 0$ and edge length parameters $l \in \mathbb{R}^{|E|}$, $0 \neq l \geq 0$. Let $D$ be an $|N| \times |N|$ matrix defined by $D = \text{diag}(s_1^{-1/2}, \ldots, s_n^{-1/2})$.

We discuss three optimization problems whose optimal values depend on the eigenvalues of scaled, edge weighted Laplacian matrices of a graph, such that the edge weights fulfill some additional constraints. Using a semidefinite approach, we generate primal, dual and corresponding graph realization problems and analyze optimal solutions in connection to the graph’s structure.

1. We consider the problem of maximizing the second smallest eigenvalue, i.e.,

$$\max \left\{ \lambda_2(DL_wD) : \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \ w_{ij} \geq 0 \ (ij \in E) \right\}.$$  

By the same approach presented in [2, 3], we reformulate (1) as a pair of primal-dual semidefinite programs and a corresponding graph realization problem. In the latter problem, we search for vectors $u_i \in \mathbb{R}^{|N|}$ ($i \in N$) such that the barycenter is in the origin, a normalization constraint and constraints on the edge lengths hold. We establish strong duality and observe that the attainment of an optimal primal solution may fail if some of the edge length parameters equal zero (strong duality and attainment of optimal solutions for $l > 0$ was already established in [3]).

2. We summarize results, concerning properties of optimal solutions that are already known from [2, 3]: Connections between optimal realizations and the eigenspace corresponding to the optimized second smallest eigenvalue are presented. An unfolding property of optimal realizations with respect to the separator structure of the graph is stated, called the Separator-Shadow Theorem. Furthermore, the existence of optimal realizations of bounded dimension depending on the graph’s tree-width is guaranteed, the tree-width theorem.

As new results we characterize optimal realizations of nonconnected graphs and identify special optimal primal solutions that depend on the graph’s automorphism group, the latter following [1].

3. Based on the realization problem, we additionally optimize over the squared edge length parameters using $s = 1$. The corresponding primal and dual semidefinite
programs satisfy strong duality. For connected graphs maps of optimal realizations onto one-dimensional subspaces turn out to be eigenvectors to the second smallest eigenvalue of the unweighted Laplacian of the graph. Conversely, eigenvectors to the second smallest eigenvalue of the unweighted Laplacian generate optimal realizations.

4. Using the same approach and similar methods we minimize the maximum eigenvalue, \( i.e. \), we consider

\[
\min \left\{ \lambda_{\text{max}}(DL_w D) : \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \ w_{ij} \geq 0 \ (ij \in E) \right\}. \tag{2}
\]

Strong duality holds for the corresponding primal-dual pair of semidefinite programs whose optimal solutions are attained independent of some possible zero edge length parameters.

We prove a close connection of optimal solutions of the related graph realization problem to the eigenspace of the minimal maximum eigenvalue of a corresponding Laplacian.

5. Optimal realizations have some basic properties such as having the barycenter in the origin even though it is not formulated specifically in the optimization problem. Furthermore, there is a bound on the vector lengths and if all of the edge length parameters have the same value, a characterization of nodes that are embedded in the origin is possible.

The existence of a special primal solution, depending on the automorphisms of the graph, is guaranteed.

6. A property that connects the structure of the graph, or rather the graph’s separator structure, to optimal realizations was proven in the Sunny-Side Theorem. It characterizes a folding property of optimal realizations.

We have verified the existence of optimal realizations that have bounded dimension, depending on the tree-width of the graph. Thereby, bipartite graphs take a special position as optimal one-dimensional realizations exist. Also a family of graphs is specified having tight dimension bound, \( i.e. \), the bound is best possible.

7. Additionally, optimizing over the squared edge length parameters in the realization problem having \( s = 1 \), gives rise to a pair of semidefinite primal-dual programs that fulfill strong duality. Also in this case optimal realizations are closely related to the eigenspace of the maximum eigenvalue of the unweighted Laplacian.

8. To analyze the interaction of the second smallest and maximum eigenvalue of the Laplacian we finally consider the difference of both, \( i.e. \),

\[
\min \left\{ \lambda_{\text{max}}(DL_w D) - \lambda_2(DL_w D) : \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \ w_{ij} \geq 0 \ (ij \in E) \right\}. \tag{3}
\]
Strong duality holds for the corresponding primal-dual pair of semidefinite programs whose optimal solutions are attained independent of some possible zero edge length parameters.

The resulting graph realization problem searches for two realizations of the graph in $\mathbb{R}^n$ one corresponding to the second smallest eigenvalue and one corresponding to the maximum eigenvalue. Indeed, also in this case, there is a connection of optimal realizations to the eigenspaces of the corresponding optimal eigenvalues.

9. Some properties, observed for optimal solutions of the single problems from above, may also be observed here. So, optimal realizations corresponding to the second smallest eigenvalue of nonconnected graphs have the same characteristic, i.e., connected components reduce to single points. The barycenter of connected components of optimal realizations corresponding to the maximum eigenvalue lies in the origin. The vector lengths of both optimal realizations are bounded. After all, special optimal primal solutions exist, depending on the automorphisms of the graph.

10. Comparing the feasible sets of the single graph realization problems with the feasible set of the coupled, it becomes obvious that they are somewhat equal. More precisely, a feasible realization of the coupled problem with respect to the second smallest (maximum) eigenvalue is also feasible for the single problem with same data. Then again, feasible realizations of the single problems generate a feasible solution of the coupled one with same data.

While feasibility is preserved, optimality may be lost. In general, optimal solutions of the single problems do not generate an optimal solution of the coupled one. But there exist appropriate data, such that an optimal realization of the coupled problem with respect to the maximum eigenvalue is also optimal for the single problem. If there exists a primal optimal solution with positive second smallest eigenvalue, the same holds for realizations corresponding to that eigenvalue.

Consequently, the Separator-Shadow Theorem (for graphs having positive optimal second smallest eigenvalue), the Sunny-Side Theorem and the bounds on the dimensions also hold. Bipartite graphs take a special position for optimal realizations corresponding to the maximum eigenvalue.

11. Optimizing additionally over the squared edge length parameters yields primal-dual semidefinite programs, fulfilling strong duality. Connections of optimal realizations to the eigenspaces of the extremal eigenvalues of the unweighted Laplacian hold. Indeed, in this case, optimal realizations of the coupled problem are just scaled optimal realizations of the single ones and vice versa. Thus, in this case, optimality is preserved.
Bibliography


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Susanna Reiß