TECHNISCHE UNIVERSITÄT CHEMNITZ

On Graph Embeddings and a new Minor Monotone Graph Parameter associated with the Algebraic Connectivity of a Graph

An der Fakultät für Mathematik
der Technischen Universität Chemnitz eingereichte

D I S S E R T A T I O N

zur Erlangung des akademischen Grades
doctor rerum naturalium (Dr. rer. nat.)

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Tag der Abgabe: 5. Februar 2013
Tag der Verteidigung: 30. Mai 2013

Contents

Chapter 1

Introduction

This dissertation is based on my work [19],[20], jointly with F. Göring and C. Helmberg. It unifies and streamlines the presentations carried out in both articles. Contents of this work that cannot be found there are mainly the connection between Theorem 11 and Lemma 29 leading to a different proof of the Separator-Shadow Theorem, and the application of structural results to trees, see Section 4.4. Although this work does not address latest scientific developments, it aims to be a worthwhile contribution. We start by introducing basic notions of Graph Theory, Linear Algebra and Semidefinite Programming.

1.1 Notations and Preliminaries

Graphs

At some places throughout this work we will also refer to more complicated terms of graph theory. To define all of them precisely is beyond the scope of this work. Instead, we will define intensely used terms here, and refer to the introductory book on graph theory by Diestel [11] otherwise. For example, find the definition of planarity there.

When considering graphs in this work, they are always meant to be simple and undirected (without multiple edges, loops or directed edges). In detail, a *graph* is a pair $G = (N, E)$ consisting of a finite set of *nodes* N and a set of *edges* $E \subseteq \{\{i, j\} : i, j \in N, i \neq j\}$. When there is no danger of confusion we will abbreviate edges $\{i, j\} \in E$ by ij. To the elements of N we may also refer as *vertices*. In order to bind related adjacency matrices to a graph G, we will typically use a node set $N = \{1, 2, \ldots, n\}$.

We call a node $i \in N$ and an edge $e \in E$ *incident* if $i \in e$. We call two nodes $i, j \in N$ *adjacent* if $ij \in E$. For $i \in N$ we call all adjacent nodes $j \in N$, $ij \in E$ *neighbours* of i. With $d_i := |\{j \in N : ij \in E\}|$ we denote the number of all neighbours. We call d_i *valency* or *degree* of i.

A graph $\hat{G} = (\hat{N}, \hat{E})$ is called *subgraph* of $G = (N, E)$ if $\hat{N} \subseteq N$ and $\hat{E} \subseteq E$. We say that $\hat{G}$ is a *proper subgraph* if in addition $\hat{N} \subset N$ or $\hat{E} \subset E$. For $G = (N, E)$ two nodes $i, j \in N$ are called *connected* if there is a sequence $(r_1, r_2, \ldots, r_m)$, $r_k \in N, 1 \leq k \leq m$ of nodes with $r_k r_{k+1} \in E$, $1 \leq k \leq m-1$ and $r_1 = i$, $r_m = j$. A graph is connected if any two of its nodes are connected. A *(connected) component* of $G = (N, E)$ is a connected subgraph which is not a proper subgraph of another connected subgraph of G.

A *separator* is a subset $S \subset N$, whose removal (with all incident edges) increases the number of components. An *articulation* is a separator of cardinality one. A *block* is a (maximal) subgraph that contains no articulation. Maximal means in this context, that it is not properly included in another subgraph without articulation.

An *isomorphism* between two graphs $G = (N, E)$ and $G' = (N', E')$ is a bijection $f : N \to N'$ with $ij \in E \Leftrightarrow f(i)f(j) \in E'$. If an isomorphism exists between two graphs, they are called *isomorphic*. If we refer in the following to *the* graph with a certain property, we do so up to isomorphism.

The *complete graph* on n nodes is the graph $K_n := (N = \{1, \dots, n\}, E = \{ij \subseteq N : i \neq j\})$, i. e. the graph on n nodes, where each pair of nodes is adjacent. The *complete bipartite graph* is the graph $K_{n,m} := (N = \{i_1, \dots, i_n\} \cup \{j_1, \dots, j_m\}, E = \{i_k j_l \subseteq N : 1 \leq k \leq n,\ 1 \leq l \leq m\})$.

The *path* of length $n \geq 1$ is the graph $P_n := (N = \{0, 1, \dots, n\}, E = \{01, 12, 23, \dots, (n-1)n\})$. The *cycle* with $n \geq 3$ nodes is the graph $C_n := (N = \{1, \dots, n\}, E = \{12, 23, \dots, (n-1)n, n1\})$. A *tree* is a connected graph that has no cycle as a subgraph.

As mentioned above we refer to [11] for the introduction of *planar graphs* and related notions such as *face* and *outer face*. An *outerplanar graph* is a planar graph that has a plane embedding such that each node is situated on the boundary of the outer face of this embedding.

Minors

For a graph $G = (N, E)$ we consider three types of operations to obtain a graph $\tilde{G} = (\tilde{N}, \tilde{E})$. The first is the deletion of an isolated node. For this let $i \in N$ be a node with valency $d_i = 0$. Then $\tilde{G} := (N \setminus \{i\}, E)$ is the desired graph. The second operation is the deletion of an edge $e \in E$. In this case $\tilde{G} := (N, E \setminus \{e\})$ is the requested graph. The third operation is the contraction of an edge. Let $i, j \in N$ and $ij \in E$. Now, $\tilde{G}$ arises from deleting the nodes i and j (and the respective edge ij) and replacing them by a new node r, and connecting it to all remaining nodes that were adjacent to i or j. I. e. let $N_1 \subseteq N$ be the set of all nodes that are adjacent to i and N_2 be the set of all nodes that are adjacent to j. Then $\tilde{G} := (N \setminus \{i, j\} \cup \{r\}, (E \setminus \{pq : p \in \{i, j\}, q \in N_1 \cup N_2\}) \cup \{rq : q \in (N_1 \cup N_2) \setminus \{i, j\}\})$ is the graph we wanted to construct.

A graph M is called *minor* of G and we write $M \preceq G$ if there is a sequence of graphs $(G_1, G_2, \dots, G_m)$ with $G_1 = G$, $G_m = M$ and for $1 \leq k \leq m-1$ the graph G_{k+1} is obtained from G_k by one of the three operations. The sequence of graphs may have a cardinality of one, in this case $M = G$. As two of these sequences may be chained together we have transitivity of the $\preceq$ relation. Furthermore, the sum of the number of nodes and the number of edges decreases when these operations are applied. Hence, $\preceq$ is anitsymmetric and forms a partial order on the set of graphs.

We recall the following result of Robertson and Seymour, also known as Wagner's conjecture.

Theorem 1 (cf. [39]) *Every (infinite) sequence* $(G_k)_{k\geq 0}$ *of graphs contains two graphs* G_{k_1}, G_{k_2}, $k_1 \leq k_2$ *where* G_{k_1} *is isomorphic to a minor of* G_{k_2}.

Let $\mathcal{G}$ be a class of graphs that is closed under taking minors, that is with $G \in \mathcal{G}$ also every minor of G belongs to $\mathcal{G}$. We consider the set-theoretic complement $\bar{\mathcal{G}}$. Let $\mathcal{F} \subseteq \bar{\mathcal{G}}$ be the set of all graphs that have no minor in $\bar{\mathcal{G}}$. Since $\mathcal{G}$ is closed under taking minors it may also be characterized in terms of $\mathcal{F}$:

$$\mathcal{G} = \{G : F \not\preceq G,\ \forall F \in \mathcal{F}\}.$$

Theorem 1 now yields that $\mathcal{F}$ is a finite set. Each property a graph may or may not have induces a class $\mathcal{G}$ of all graphs that fulfill this property. If this class is closed under taking minors we call the graph property to be *minor monotone*. On the other hand we define

$$\mathrm{Forb}_{\preceq}(G_1, \ldots, G_m) := \{G : G_k \not\preceq G,\ 1 \leq k \leq m\}.$$

We call the graphs $G_1, \ldots, G_m$ *forbidden minors* for the so characterized class of graphs $\mathrm{Forb}_{\preceq}(G_1, \ldots, G_m)$. With this notation we may sum up and give examples:

Theorem 2 (cf. [11]) *For each minor monotone graph property exists a finite list of graphs* $G_1, \ldots, G_m$ *such that the set of all graphs that fulfill the property is* $\mathrm{Forb}_{\preceq}(G_1, \ldots, G_m)$.

Furthermore, the following classes of graphs are closed under taking minors and characterized by the respective lists of forbidden minors.

(i) The class of graphs, that have no edges, is $\mathrm{Forb}_{\preceq}(K_2)$.

(ii) The class of graphs, that are a disjoint union of paths, is $\mathrm{Forb}_{\preceq}(K_3, K_{1,3})$.

(iii) The class of outerplanar graphs is $\mathrm{Forb}_{\preceq}(K_4, K_{2,3})$.

(iv) The class of planar graphs is $\mathrm{Forb}_{\preceq}(K_5, K_{3,3})$.

The assertions of (i) and (ii) are easy to verify. The characterization of planar graphs is known as Wagner's theorem, and can be found in Diestel [11] for example. The characterization of outerplanar graphs is also given in Diestel, but within an excercise.

Graphs and linear algebra

All vectors and matrices in this work are real valued. The vector $e = (1, \ldots, 1)^T$ is the vector of all ones of appropriate length. For the sake of convenience we refer to the elements of a matrix $A \in \mathbb{R}^{n\times n}$ as A_{ij}, $1 \leq i, j \leq n$. (We only consider quadratic matrices). The vector $diag(A) := (A_{11}, \ldots, A_{nn})$ denotes the main diagonal of A. For a vector $v \in \mathbb{R}^n$ the matrix $Diag(v)$ is the matrix with $diag(Diag(v)) = v$ and $Diag(v)_{ij} = 0$, $i \neq j$. The inner product with respect to matrices $A, B \in \mathbb{R}^{n \times n}$ is defined as

$$\langle A, B \rangle := \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij}.$$

Note that a quadratic form may also be written as

$$x^T A x = \langle A, xx^T \rangle.$$

With $N = \{1, \ldots, n\}$ we can assign vectors to the set of nodes. E.g., let X be an arbitrary set. Then we might consider vectors $v \in X^n$ and refer to them as *node weights* or node weightings, resp. Each number v_i is meant to be the assigned weight to node $i \in N$. To make the intent of using a vector as node weights clear, we will write X^N instead of X^n. In a similar way we will consider *edge weights* and refer to them as elements of X^E.

Furthermore we will consider matrices $A \in \mathbb{R}^{n \times n}$. They can be interpreted as combinations of node and edge weights. Thus, an element A_{ii}, $i \in N$ refers to a node weight of i, and A_{ij}, $i \neq j$ refers to an edge weight if $ij \in E$. For $ij \neq E$ it has no special meaning, often $A_{ij} = 0$ in this case. Similarly we indicate that a matrix is related to a graph by writing $A \in \mathbb{R}^{N \times N}$.

The set $\mathbb{R}^N_+ := \{v \in \mathbb{R}^N : v_i \geq 0,\ i \in N\}$ denotes all nonnegative node weightings and $\mathbb{R}^N_{++} := \{v \in \mathbb{R}^N : v_i > 0,\ i \in N\}$ all positive node weightings. Likewise we will use the same notation for $\mathbb{Z}^N, Z^N_+, Z^N_{++}$ and $\mathbb{Q}^N, \mathbb{Q}^N_+, \mathbb{Q}^N_{++}$. Similarly, $\mathbb{R}^E_+ := \{v \in \mathbb{R}^E : v_i \geq 0,\ i \in E\}$ and $\mathbb{R}^E_{++} := \{v \in \mathbb{R}^E : v_i > 0,\ i \in E\}$.

Now, let $w \in \mathbb{R}^E_+$ be a nonnegative edge weighting. Later we will use all edges of $G = (N, E)$ where the corresponding entry of w is positive. We will call all these edges $\text{supp}_{++}(w) := \{e \in E : w_e > 0\}$ *positive support* of w. Accordingly the *positive support graph* is the graph $G[\text{supp}_{++}(w)] := (N, \text{supp}_{++}(w))$.

Furthermore we will represent the structure of graphs by symmetric matrices. We recall the fact that these have a real-valued sprectrum and an orthonormal basis of eigenvectors. We will observe correlations between spectral properties and structural properties of the underlying graph. For this we will exploit the following basic matrix theorems. The first is a variant of the Courant-Fischer Theorem.

Theorem 3 (cf. [24], section 4.2) *Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix with eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ and corresponding eigenvectors $y_1, \ldots, y_n$. Then*

$$\lambda_i = \min_{\|x\|=1,\, x \perp y_1, \ldots, x \perp y_{i-1}} x^T A x, \quad \textit{for all } 1 \leq i \leq n.$$

Let $A \in \mathbb{R}^{n \times n}$ be a matrix and $\rho(A) = \max\{|\lambda| : \lambda \text{ is eigenvalue of } A\}$ its spectral radius. A is called *irreducible* if either $n = 1$ and $A \neq 0$, or $n \geq 2$ and there is no permutation matrix $P \in \mathbb{R}^{n \times n}$ and square matrices B and D such that $P^T A P = \begin{bmatrix} B & C \\ 0 & D \end{bmatrix}$.

Theorem 4 (Perron-Frobenius, cf. [24], Theorem 8.4.4) *Let $A \in \mathbb{R}^{n \times n}$ be an irreducible and nonnegative matrix. Then*

1. *$\rho(A) > 0$,*
2. *$\rho(A)$ is an eigenvalue of A,*
3. *There is a positive vector x such that $Ax = \rho(A)x$, and*
4. *$\rho(A)$ is an algebraically (and hence geometrically) simple eigenvalue of A.*

Semidefinite Programming

We will give only a very brief introduction to semidefinite programs. See [21] for further information, particularly with regard to application of semidefinite programming in combinatorial optimization.

A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is called *positive semidefinite* if $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n$. A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is said to be *positive definite* if $x^T Ax > 0$ for all $x \in \mathbb{R}^n \setminus \{0\}$. We denote the fact that a matrix A is positive semidefinite by $A \succeq 0$. (There will be no confusion with the minor relation of graphs due to the different mathematical objects.) Positive definite matrices are denoted by $A \succ 0$.

The set of all matrices $A \succeq 0$ forms a cone in the space of symmetric matrices. This is closed under taking nonnegative linear combinations. A semidefinite program is a linear program over the cone of positive semidefinite matrices:

$$\begin{array}{rl} \text{minimize} & \langle C, X \rangle , \\ \text{subject to} & \langle A_i, X \rangle = b_i,\ 1 \leq i \leq m, \\ & X \succeq 0. \end{array} \tag{1.1}$$

To derive its Lagrangian dual we lift the primal equality constraints into the objective by means of Lagrangian multipliers $y_1, \ldots, y_m \in \mathbb{R}$. The primal program reads

$$\inf_{X \succeq 0} \sup_{y_1,\ldots,y_m \in \mathbb{R}} \langle C, X \rangle + \sum_{i=1}^{m} y_i (b_i - \langle A_i, X \rangle).$$

With $b = (b_1, \ldots, b_m)^T$ and $y = (y_1, \ldots, y_m)^T$ we get the dual by interchanging infimum and supremum:

$$\sup_{y_1,\ldots,y_m \in \mathbb{R}} \inf_{X \succeq 0} \langle b, y \rangle + \left\langle X, C - \sum_{i=1}^{m} y_i A_i \right\rangle .$$

We will not discuss the unbounded (degenerated) cases here. In order for the outer supremum to be finite the inner infimum over $X \succeq 0$ must remain finite for some $\hat{y} \in \mathbb{R}^m$. This requires $C - \sum_{i=1}^{m} \hat{y}_i A_i \succeq 0$. See [21] for details. We reformulate this condition by introducing a positive semidefinite slack matrix Z and obtain the standard formulation of the dual semidefinite program:

$$\begin{array}{rl} \text{maximize} & \langle b, y\rangle\,, \\ \text{subject to} & \sum_{i=1}^m y_i A_i + Z = C, \\ & y \in \mathbb{R}^m,\ Z \succeq 0. \end{array} \tag{1.2}$$

We call a matrix X *strictly feasible* for (1.1) if it is feasible for (1.1) and satisfies $X \succ 0$. We call a pair (y, Z) *strictly feasible* for (1.2) if it is feasible for (1.2) and satisfies $Z \succ 0$. If for at least one of the problems (1.1) and (1.2) exists a strictly feasible solution, then strong duality holds:

Theorem 5 (cf. [21], Corollary 2.2.6) *Let*

$$p^* := \inf\{\langle C, X\rangle : \langle A_i, X\rangle = b_i,\ 1 \le i \le m,\ X \succeq 0\},$$
$$d^* := \sup\{\langle b, y\rangle : \sum_{i=1}^m y_i A_i + Z = C,\ Z \succeq 0\}.$$

(i) If (1.1) *has a strictly feasible solution with p^* finite, then $p^* = d^*$ and this value is attained for* (1.2).

(ii) If (1.2) *has a strictly feasible solution with d^* finite, then $p^* = d^*$ and this value is attained for* (1.1).

(iii) If (1.1) *and* (1.2) *have both strictly feasible solutions, then $p^* = d^*$ is attained for both problems.*

1.2 The Algebraic Connectivity

The Laplacian

The Laplace operator or Laplacian Δ is a fundamental object in the theory of partial differential equations. One example is the wave equation

$$\Delta u = \frac{\partial^2 u}{\partial t^2}\,.$$

For $u : \mathbb{R}^n \to \mathbb{R}$ the operator is defined by $\Delta u := \sum_{i=1}^n \frac{\partial^2 u}{\partial x_i^2}$. The effect of the Laplacian on a function u can be considered numerically by evaluation of u on an equidistant grid $\alpha\mathbb{Z}^n$. The derivatives can be approximated by the central difference formula

$$\frac{\partial^2 u}{\partial x_i^2}(z_1, \ldots, z_n) \approx \frac{u(z_1, \ldots, z_i - \alpha, \ldots, z_n) - 2u(z_1, \ldots, z_n) + u(z_1, \ldots, z_i + \alpha, \ldots, z_n)}{\alpha^2}\,.$$

At a certain point z the obtained discretized Laplacian sums up (up to the factor α^2) the function values at the neighbouring points and subtracts the function value once for each neighbour. At this the neighbourhood consists of all grid points having distance α.

Consider the matrix representation of the discretized operator restricted to a (connected) subset of grid points. With exception of boundary points, rows contain $-2n$ (the number of neighbours) as diagonal elements and entries of value 1 for each neighbour. Extending this concept from grid graphs to general graphs we would expect the Laplace matrix to have the negative valency of a node on the diagonal, and entries of value 1 if and only if the matrix element corresponds to an edge of the graph.

This fits exactly the way the Laplacian of a graph is defined (up to the sign). Let $G = (N := \{1, \ldots, n\}, E)$ denote a (simple) graph. The *Laplacian* $L(G) \in \mathbb{R}^{n \times n}$ is defined to be the matrix having the valencies of the nodes as diagonal elements, $l_{ii} = |N(i)|$, and $l_{ij} = -1$ if and only if $ij \in E$, and $l_{ij} = 0$, otherwise. This means, that each edge $ij \in E$ yields minus ones at matrix elements ij and ji and increases the i-th and j-th diagonal element by 1. This may be expressed by matrices $E_{ij} \in \mathbb{R}^{n \times n}$, with $(E_{ij})_{ii} = (E_{ij})_{jj} = 1$ and $(E_{ij})_{ij} = (E_{ij})_{ji} = -1$ and 0 otherwise. Each matrix E_{ij} represents the edge $ij \in E$, and the Laplacian may be rewritten as

$$L(G) = \sum_{ij \in E} E_{ij} \, .$$

Because the matrices E_{ij} are positive semidefinite, the Laplacian is positive semidefinite as well.

Eigenvalues and algebraic connectivity

The smallest eigenvalue is $\lambda_1(L(G)) = 0$ with eigenvector e. The Laplacian $L(G)$ is irreducible if and only if G is connected. In this case the matrix $(n-1)I - L(G)$ is irreducible as well and nonnegative. The Perron-Frobenius Theorem 4 for matrix $(n-1)I - L(G)$ ensures that its largest eigenvalue $n-1$ is simple and therefore differs from its second largest eigenvalue $n - 1 - \lambda_2(L(G))$. Hence $\lambda_2(L(G)) > 0$.

On the other hand, the dimension of the null eigenspace of $L(G)$ equals to the number of components of G: Let $C_1, \ldots, C_k$ be the components of G. The nodes of G can be ordered in such a way that $L(G)$ is a block diagonal matrix where each block is the Laplacian of a component of G, i.e. $L(G) = \mathrm{Diag}(L(C_1), \ldots, L(C_k))$. Then the null eigenspace of $L(G)$ is given by span $\{(\alpha_1 e_1^T, \ldots, \alpha_k e_k^T)^T : \alpha_1, \ldots, \alpha_k \in \mathbb{R}\}$ where for $i = 1, \ldots, k$ the vector $e_i = (1, \ldots, 1)^T$ is the vector of all ones of appropriate length. Note, that we already used the fact $\lambda_2(L(C_i)) > 0$ for all $1 \leq i \leq k$ because of the connectivity of each component.

Let $G_1 = (N, E_1)$ and $G_2 = (N, E_2)$ be graphs with the same set of nodes but disjoint sets of edges. For $G = (N, E_1 \dot\cup E_2)$ we have $L(G) = L(G_1) + L(G_2)$, and Theorem 3 implies

$$\begin{aligned}\lambda_2(L(G)) &= \min_{\|x\|=1,\, e^T x=0} x^T L(G)x \\ &\geq \min_{\|x\|=1,\, e^T x=0} x^T L(G_1)x + \min_{\|x\|=1,\, e^T x=0} x^T L(G_2)x \\ &= \lambda_2(L(G_1)) + \lambda_2(L(G_2)).\end{aligned}$$

An immediate consequence is that $\lambda_2(L(\cdot))$ is nondecreasing for graphs with the same set of nodes under adding edges. We summarize this in the following theorem:

Theorem 6 (cf. [12]) $\lambda_2(L(G))$ *satisfies the following properties:*

1. $\lambda_2(L(G)) \geq 0$ *and* $\lambda_2(L(G)) > 0$ *if and only if* G *is connected.*
2. *If* $G_1 = (N, E_1)$, $G_2 = (N, E_2)$ *and* $E_1 \subseteq E_2$, *then* $\lambda_2(L(G_1)) \leq \lambda_2(L(G_2))$.
3. *If* $G_1 = (N, E_1)$, $G_2 = (N, E_2)$ *and* $E_1 \cap E_2 = \emptyset$, *then* $\lambda_2(L(G_1)) + \lambda_2(L(G_2)) \leq \lambda_2(L(G))$, *where* $G = (N, E_1 \dot{\cup} E_2)$.

These properties show that $\lambda_2(L(G))$ behaves similarly to different connectivity terms, e.g. edge- or node-connectivity. M. Fiedler suggested in [12] to name it *algebraic connectivity* $a(G)$. Eigenvectors to $a(G)$ are called *Fiedler vectors.*

The absolute algebraic connectivity

Let $G = (N, E)$ be a graph with nonnegative edge weights $w \in \mathbb{R}^E_+$. The *weighted Laplacian* $L(G, w)$ is the (symmetric) matrix having the diagonal elements $l_{ii} = \sum_{j \in N: ij \in E} w_{ij}$, and the off-diagonal elements $l_{ij} = -w_{ij}$ for $ij \in E$ and $l_{ij} = 0$ for $ij \notin E$. Again, the weighted Laplacian may be written with the help of the edge matrices E_{ij} of Section 1.2:

$$L(G, w) = \sum_{ij \in E} w_{ij} E_{ij}.$$

M. Fiedler considered the problem of maximizing $\lambda_2(L(G, w))$ subject to the sum of the edge weights of the graph being the number of edges in [12] and called the resulting value the *absolute algebraic connectivity* $\hat{a}(G)$:

$$\begin{aligned}\hat{a}(G) := \text{maximize} \quad & \lambda_2(L(G, w)), \\ \text{subject to} \quad & \textstyle\sum_{ij \in E} w_{ij} = |E|, \\ & w \geq 0.\end{aligned} \tag{1.3}$$

We generalize this slightly by introducing linear costs for the edge weights. Let these be denoted by $c \in \mathbb{R}^E_{++}$. Additionally, for $d \in \mathbb{R}^N_{++}$ define $D := \operatorname{diag}(d_1, \ldots, d_n)$ and $L_d(G, w) := DL(G, w)D$. The vector d may be interpreted as density of the node set. Its main purpose is to allow the representation of minor operations as it will be seen in

Chapter 5 (d will be needed to delete isolated nodes or contract edges). With this, (1.3) generalizes to:

$$\begin{aligned} \hat{a}(G,c,d) := \text{maximize} \quad & \lambda_2(L_d(G,w)), \\ \text{subject to} \quad & \textstyle\sum_{ij\in E} c_{ij} w_{ij} = |E|, \\ & w \geq 0. \end{aligned} \tag{1.4}$$

The objective function $\lambda_2(L_d(G,\cdot))$ is continuous, and because of $c > 0$ the set of all feasible soutions of (1.4) is bounded. We get:

Observation 7 *Let G be a graph, $d \in \mathbb{R}^N_{++}$ densities of nodes, and $c \in \mathbb{R}^E_{++}$ edge costs. Then the maximal objective value of (1.4) is attained by some w^*, i.e. $\hat{a}(G,c,d) = \lambda_2(L_d(G,w^*)) < \infty$.*

Basic properties

Since $DE_{ij}D$ is positive semidefinite, this also holds for $L_d(G,w) = \sum_{ij\in E} w_{ij} DE_{ij}D$. Its smallest eigenvalue is $\lambda_1(L_d(G,w)) = 0$ with eigenvector $D^{-1}e$. Note that

$$\begin{aligned} x^T L_d(G,w)x &= \sum_{ij\in E} w_{ij} x^T DE_{ij}Dx \\ &= \sum_{ij\in E} w_{ij}(d_i^2 x_i^2 - 2d_i d_j x_i x_j + d_j^2 x_j^2) \\ &= \sum_{ij\in E} w_{ij}(d_i x_i - d_j x_j)^2. \end{aligned}$$

Thus, we obtain from Theorem 3:

$$\lambda_2(L_d(G,w)) = \min_{\substack{\|x\|=1 \\ e^T D^{-1} x = 0}} x^T L_d(G,w)x = \min_{\substack{\|x\|=1 \\ e^T D^{-1} x = 0}} \sum_{ij\in E} w_{ij}(d_i x_i - d_j x_j)^2. \tag{1.5}$$

Again, the behaviour of $\lambda_2(L_d(G,\cdot))$ justifies the name algebraic connectivity as the following generalization of Theorem 6 shows. In the case of $d = e$ it is already known from [14].

Observation 8 *For $d \in \mathbb{R}^N_{++}$ the second smallest eigenvalue $\lambda_2(L_d(G,\cdot))$ satisfies the following properties:*

1. *$\lambda_2(L_d(G,w)) \geq 0$ and $\lambda_2(L_d(G,w)) > 0$ if and only if $G[\mathrm{supp}_{++}(w)]$ is connected.*
2. *$\lambda_2(L_d(G,\alpha w)) = \alpha\lambda_2(L_d(G,w))$ for $\alpha \geq 0$.*
3. *If $w_1, w_2 : N \to \mathbb{R}_+$ and $w_1 \leq w_2$, then $\lambda_2(L_d(G,w_1)) \leq \lambda_2(L_d(G,w_2))$.*
4. *If $w_1, w_2 : N \to \mathbb{R}_+$, then $\lambda_2(L_d(G,w_1)) + \lambda_2(L_d(G,w_2)) \leq \lambda_2(L(G,w_1 + w_2))$.*

Proof. We first prove property 1. Assume that $G[\mathrm{supp}_{++}(w)]$ is connected. In this case the matrix $(n-1)I - L_d(G,w)$ is irreducible and nonnegative. The Perron Frobenius Theorem 4 for this matrix yields that its largest eigenvalue $n-1$ is simple, and therefore differs from the second largest $n-1-\lambda_2(L_d(G,w))$. Hence $\lambda_2(L_d(G,w)) > 0$.

Another way to obtain this is to exploit formula (1.5). Due to the requirement $e^T D^{-1} x = 0$ the vector x has at least one negative entry and at least one positive entry. The corresponding nodes in G are connected in $G[\mathrm{supp}_{++}(w)]$ by a path P. Now

$$\lambda_2(L_d(G,w)) \geq \min_{\substack{\|x\|=1 \\ e^T D^{-1} x = 0}} \sum_{ij \in P} w_{ij}(d_i x_i - d_j x_j)^2 > 0.$$

Assume conversely, that $G[\mathrm{supp}_{++}(w)]$ is divided into components C_1, C_2. Set $x_i := \frac{|C_2|}{d_i}$ for $i \in C_1$ and $x_i := -\frac{|C_1|}{d_i}$ for $i \in C_2$. Then $L_d(G,w)x = 0$ and $e^T D^{-1} x = 0$, so $\lambda_2(L_d(G,w)) = 0$.
Property 2 holds, because:

$$\lambda_2(L(G,\alpha w)) = \lambda_2(\alpha L(G,w)) = \alpha \lambda_2(L(G,w)) \text{ for } \alpha \geq 0\,.$$

Property 3 follows from 4, so this finishes the proof:

$$\begin{aligned}
\lambda_2(L_d(G, w_1 + w_2)) &= \min_{\substack{\|x\|=1 \\ e^T D^{-1} x = 0}} x^T D[L(G,w_1) + L(G,w_2)]Dx \\
&\geq \min_{\substack{\|x\|=1 \\ e^T D^{-1} x = 0}} x^T D L(G,w_1) D x + \min_{\substack{\|x\|=1 \\ e^T D^{-1} x = 0}} x^T D L(G,w_2) D x \\
&= \lambda_2(L_d(G,w_1)) + \lambda_2(L_d(G,w_2)).
\end{aligned}$$

■

En passant we have proved:

Corollary 9 *$\lambda_2(L_d(G,\cdot))$ is a positive homogeneous and concave function on $\mathbb{R}^E_+$.*

Corollary 10 *Let w^* be an optimal solution of (1.4). Then*

$$\hat{a}(G,c,d) > 0 \Leftrightarrow G \text{ is connected} \Leftrightarrow G[\mathrm{supp}_{++}(w^*)] \text{ is connected.}$$

As immediate consequence of Corollary 9 we may relax the sum of weights constraint in (1.4) to obtain the equivalent problem

$$\begin{aligned}
\hat{a}(G,c,d) := \text{maximize} \quad & \lambda_2(L_d(G,w)), \\
\text{subject to} \quad & \textstyle\sum_{ij \in E} c_{ij} w_{ij} \leq |E|, \\
& w \geq 0.
\end{aligned}$$

or may even rewrite it as

$$\begin{aligned}
\tfrac{\hat{a}(G,c,d)}{|E|} = \text{maximize} \quad & \lambda_2(L_d(G,w)), \\
\text{subject to} \quad & \textstyle\sum_{ij \in E} c_{ij} w_{ij} \leq 1, \\
& w \geq 0.
\end{aligned} \tag{1.6}$$

From [13] we recall the following property of Fiedler vectors. It may be understood as a nodal domain theorem. Note, that the existence of $x^{(1)} > 0$ is a consequence of the Perron-Frobenius-Theorem 4.

Theorem 11 (cf. [13], Corollary 2.3) *Let A be an $n \times n$ nonnegative irreducible symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. Let $x^{(1)} > 0$ be an eigenvector corresponding to λ_1 and $x^{(2)}$ an eigenvector corresponding to λ_2. Then for any $\alpha \geq 0$ the submatrix $(a_{ii})_{i \in M_\alpha}$ is irreducible where $M_\alpha = \{i \in \{1, \ldots, n\} : x_i^{(2)} + \alpha x_i^{(1)} \geq 0\}$.*

Let $G = (N, E)$ be a connected graph with nonnegative edge weights $w \in \mathbb{R}_+^E$ so that $G[\mathrm{supp}_{++}(w)]$ is connected. Then the matrix $A = \mu I - L_d(G, w)$ is irreducible and nonnegative for some sufficently large μ. Let x be an eigenvector to $\lambda_2(L_d(G, w))$ and therefore also to the second largest eigenvalue of A. Noting that $D^{-1}e$ is an eigenvector to the largest eigenvalue of A, Theorem 11 applied to A provides:

Corollary 12 *Let $w \in \mathbb{R}_+^E$ be nonnegative edge weights so that $G[\mathrm{supp}_{++}(w)]$ is connected. Then for any eigenvector x to $\lambda_2(L_d(G, w))$ and any $\alpha \geq 0$ the graph $G_\alpha := G[N_\alpha]$ is connected, where $N_\alpha := \{i \in N : x_i + \frac{\alpha}{d_i} \geq 0\}$.*

This corresponds to Theorem 3.3 of [13] and holds in particular for optimal w of program (1.4).

1.3 Two applications

We conclude this introductory chapter with two applications of the algebraic connectivity framework.

Fast mixing Markov processes on a graph

The following is based on an application of the (weighted) Laplacian and the absolute algebraic connecitivity given in [3] and [42]. Consider a symmetric Markov process on a connected graph G. The state space is given by N. Each transition between states $i \in N$ and $j \in N$ is represented by an edge $ij \in E$. If this edge does not exist the transition is not allowed. We denote the probability of this transition by $0 \leq w_{ij} \leq 1$. The probability of switching the state (from $i \in N$ to an arbitrary $j \in N$ with $ij \in E$) has to be less or equal than one, i.e., $\sum_{j \in N : ij \in E} w_{ij} \leq 1$. We will allow the Markov process to retain the current state. For a state $i \in N$ the probability of this event is $1 - \sum_{j \in N : ij \in E} w_{ij}$.

First consider a discrete-time Markov chain. Let $\pi_i(t)$ be the probability that the process is in state $i \in N$ at time $t \in \mathbb{Z}$. Proceeding one step in time this probability increases by the transitions from other states to i and descreases by transitions from i to other states. This is

$$\pi_i(t+1) = \pi_i(t) + \sum_{j \in N : ij \in E} w_{ij} \pi_j(t) - \sum_{j \in N : ij \in E} w_{ij} \pi_i(t).$$

By defining a Laplacian $L(G,w) \in \mathbb{R}^{N\times N}$ by

$$\begin{aligned}(L(G,w))_{ij} &= -w_{ij}, \quad ij \in E\\ (L(G,w))_{ij} &= 0, \quad ij \notin E,\, i \neq j\\ (L(G,w))_{ii} &= \sum_{j\in N: ij\in E} w_{ij},\, i \in N\end{aligned}$$

we may obtain the next distribution of the state $\pi(t) = (\pi_i(t))_{i\in N}$ as

$$\pi(t+1) = (I - L(G,w))\pi(t). \tag{1.7}$$

For $k \in \mathbb{Z}_+$ this leads to

$$\pi(k) = (I - L(G,w))^k \pi(0).$$

Obviously, the uniform distribution $\frac{1}{n}e$ is an equilibrium distribution of the Markov process. If the process is irreducible and aperiodic, it is the unique equilibrium distribution. In this case the sequence of distributions $(\pi(k))_{k\geq 0}$ converges to the equilibrium $\frac{1}{n}e$ as $k \to \infty$. We denote by $\|\cdot\|_{tv}$ the *total variation distance* between two distributions. In terms of this distance and with

$$\lambda(w) := \min\{\lambda_2(L(G,w)), 2 - \lambda_n(L(G,w))\}$$

we can state the following bound on the speed of convergence:

$$\sup_{\pi(0)} \|\pi(k) - \frac{1}{n}e\|_{tv} \leq \frac{1}{2}\sqrt{n}(1-\lambda(w))^k. \tag{1.8}$$

(See [3] for details).

Now one may consider the following optimization problem: For a given graph find an optimal set of transition probabilities such that the Markov chain mixes as fast as possible in terms of the bound given for the total variation distance. This is

$$\begin{array}{rl}\text{maximize} & \lambda(w),\\ \text{subject to} & I - L(G,w) \geq 0.\end{array} \tag{1.9}$$

Note that the constraint ensures that the transition probabilities are nonnegative and that the sum of probabilities of outgoing transitions from a state do not exceed one. Although the objective of (1.9) is similar to the behavior of $\lambda_2(L(G,w))$ and $I - L(G,w) \geq 0$ limits the weights $w \in \mathbb{R}^E$ in some way, the problem is different from (1.6).

This changes if we consider the continuous counterpart and study the related continuous-time Markov chain. (This is discussed in detail in [42].) Again, each edge $ij \in E$ is signed with a real number $0 \leq w_{ij} \leq 1$ which this time gives the transition rate for edge ij. Similar to the considerations above, we get a formula according to (1.7):

$$\frac{d\pi(t)}{dt} = -L(G,w)\pi(t).$$

The solution is given by

$$\pi(t) = e^{-tL(G,w)}\pi(0).$$

Since $L(G,w)e = 0$, the uniform distribution $\frac{1}{n}e$ is again an equilibrium distribution of the Markov process. If $\lambda_2(L(G,w)) > 0$, it is the unique equilibrium distribution. Moreover, $\pi(t) \to \frac{1}{n}e$, $t \to \infty$, and it is also possible to bound the rate of convergence according to (1.8). This time it is determined by $\lambda_2(L(G,w))$:

$$\sup_{\pi(0)} \|\pi(t) - \frac{1}{n}e\|_{tv} \le \frac{1}{2}\sqrt{n}e^{-\lambda_2(L(G,w))t} \,. \tag{1.10}$$

Now, a simple way to obtain a fast mixing Markov process is to bound a weighted sum of the transition rates:

$$\sum_{ij\in E} c_{ij}w_{ij} \le 1, \text{ for a } c \in \mathbb{R}^E_{++} \,.$$

Hence, (1.6) is an appropriate program to find transition rates leading to a fast mixing Markov process on this graph (in terms of the bound given in (1.10)).

Graph bisection

Let $G = (N,E)$ be a graph and $w \in \mathbb{R}^E_+$ nonnegative edge weights. For a subset of nodes $S \subseteq N$ the *cut* $\delta(S) := \{ij \in E : i \in S,\, j \in N \setminus S\}$ is the set of edges with one endpoint in S and the other in $N \setminus S$. The weight of the cut is defined by the total weight of all edges in the cut: $\sum_{ij\in\delta(S)} w_{ij}$. We consider the following program:

$$\begin{aligned} \text{minimize} \quad & \sum_{ij\in\delta(S)} w_{ij}, \\ \text{subject to} \quad & \big||S| - |N \setminus S|\big| \le 1, \\ & S \subseteq N. \end{aligned} \tag{1.11}$$

This is refered to as *minimum equipartitioning problem* and is known to be NP-complete. Applications can be found in the areas of finite element domain decomposition (see [27], [28]) and image partitioning (see [29], [30]), for example. These papers consider approaches to (1.11) based on Fiedler vectors. This works out as follows:

We represent the partitioning of N into S and $N \setminus S$ by an indicator vector $x \in \{-1,1\}^N$ with $x_i = 1$ for $i \in S$ and $x_i = -1$ for $i \in N \setminus S$. With $w_{ii} := \sum_{j:ij\in E} w_{ij}$ we can rewrite the objective as

$$\begin{aligned} \sum_{ij\in\delta(S)} w_{ij} &= \frac{1}{2}\sum_{ij\in E}(1 - x_ix_j)w_{ij} \\ &= \frac{1}{4}(\sum_{i\in N}\underbrace{\sum_{j:ij\in E} w_{ij}}_{=w_{ii}x_i^2} - \sum_{ij\in E} 2w_{ij}x_ix_j) \\ &= \frac{1}{4}x^TL(G,w)x. \end{aligned}$$

Thus, (1.11) may be formulated as

$$\begin{aligned} \text{minimize} \quad & \frac{1}{4}x^T L(G,w)x, \\ \text{subject to} \quad & e^T x \le 1, \\ & x \in \{-1,1\}^N. \end{aligned}$$

Now, we may relax this program by omitting the integral constraints $x_i \in \{-1,1\}$, $i \in N$. Instead we bound the norm of x and replace $e^T x \le 1$ by $e^T x = 0$. This is no longer necessarily a relaxation but serves the purpose to have equally sized partitions (and for an even number of nodes this would have been already satisfied in the intergral problem). Thus by an additional scaling of the objective we come up with

$$\begin{aligned} \text{minimize} \quad & x^T L(G,w)x, \\ \text{subject to} \quad & e^T x = 0, \\ & \|x\| = 1. \end{aligned}$$

By Theorem 3 this is the program that yields $\lambda_2(L(G,w))$ and is solved by the set of Fiedler vectors. Hence, rounding a Fiedler vector of the weighted Laplacian of the underlying graph (together with the weights $w \in \mathbb{R}^E_+$) to a vector in $\{-1,1\}^N$ gives an approximate solution of (1.11).

The most common method to obtain a bisection is to use the median of the components of a Fiedler vector. In [5] it is explored when this is optimal. Some insight as to why nodes with similar "Fiedler values" lie "nearby" in the graph and should probably belong to the same given partition is contained in the following result of Fiedler:

Theorem 13 (cf. [13], Theorem 3.12) *Let G be a connected graph, x a Fiedler vector. Then exactly one of the following two cases occurs:*
Case A. *There is a single block B_0 in G which contains both positively and negatively valuated nodes. Each other block has either nodes with positive valuation only, or nodes with negative valuation only, or nodes with zero valuation only. Every path P starting in B_0 and containing just one node $k \in B_0$ has the property that the values of the articulations contained in P form either an increasing, or decreasing, or a zero sequence along this path according to whether $x_k > 0$, $x_k < 0$ or $x_k = 0$. In the last case all nodes in P have value zero.*
Case B. *No block of G contains both positively and negatively valuated nodes. There exists a single node i which has value zero and has a neighbour with a non-zero valuation. This node is an articulation. Each block contains (with the exception of i) either nodes with positive valuation only, or nodes with negative valuation only, or nodes with zero valuation only. Every path P starting in i has the property that the values at its articulations either increase, and then all values in nodes of P are (with exception of i) positive, or decrease, and then all values (up to that of i) are negative, or all values in nodes of P are equal to zero. Every path containing both positively and negatively valuated nodes passes through i.*

Nevertheless this rounding method may not be sufficient. The work [1] suggests a semidefinite relaxation as alternative approach. We will describe this for a similar problem.

Note, that we may turn (1.11) into a maximization problem. (For all $ij \in E$ replace w_{ij} by $w'_{ij} := C - w_{ij}$ for arbitrarily large C.) Dropping the equipartitioning constraint $\big||S| - |N \setminus S|\big| \leq 1$ yields the program

$$\begin{aligned} \text{maximize} \quad & \sum_{ij \in \delta(S)} w_{ij}, \\ \text{subject to} \quad & S \subseteq N. \end{aligned}$$

This is called *Max-Cut* and it is also NP-complete. Again we may use an indicator vector $x \in \{-1, 1\}^N$ to rewrite the program as

$$\begin{aligned} \text{maximize} \quad & \frac{1}{4} x^T L(G, w) x, \\ \text{subject to} \quad & x \in \{-1, 1\}^N. \end{aligned} \tag{1.12}$$

To get rid of the integrality constraint, consider the matrix xx^T (for a feasible vector x of (1.12)). It is positive semidefinite, has a rank of one, and all main diagonal entries are $(xx^T)_{ii} = x_i^2 = 1$, $i \in N$.

Vice versa, let $X \in \mathbb{R}^{N \times N}$ be a positive semidefinite matrix of rank one. Then there exists a vector $x \in \mathbb{R}^N$ such that the matrix decomposes to $X = xx^T$. If furthermore $X_{ii} = 1$ for all $i \in N$, then $x_i^2 = (xx^T)_{ii} = 1$ and therefore $x_i \in \{-1, 1\}$, $i \in N$.

Hence, as pointed out in [32], we can write (1.12) equivalently as

$$\begin{aligned} \text{maximize} \quad & \frac{1}{4} \langle L(G, w), X \rangle, \\ \text{subject to} \quad & \operatorname{diag}(X) = e, \\ & \operatorname{rank}(X) = 1, \\ & X \succeq 0. \end{aligned}$$

Note, that this is not a semidefinite program, due to the rank one constraint. Leaving out this constraint provides a semidefinte relaxation. Based on this further investigations and algorithmic approaches can be built, see for instance [18] and [21].

1.4 Outline

We have seen so far, that the algebraic connectivity is strongly related to the general graph theoretical term of connectivity. Both, qualitatively as a graph is algebraically connected ($\lambda_2(L(G)) > 0$) if and only if it is connected, and quantitatively as shown by the monotonicity induced by the inclusion of edges.

The difference lies in the fact that the algebraic connectivity yields a more global view on the level of connectedness of the graph, whereas the graph-theoretical connectivity measures the bottleneck of the connectedness. The cardinality of a smallest separating node set determines the graph's connectivity, independent of its structural properties in other parts. The algebraic connectivity is closer to being a mean value of the connectivity along the whole graph.

This perception is confirmed by the consideration of Markov processes on the graph. These model random walks on the node set of the graph along the edges. The probability of being at a certain node converges to the equilibrium distribution over time. As we have seen, the convergence rate is the higher the better connected the graph is in the sense of the algebraic connectivity.

Furthermore we have seen, that the Laplacian and the algebraic connectivity can be exploited in the analysis of graph partitioning problems. Moreover, Fiedler vectors provide good heuristics for solving methods of such problems.

To get a better understanding of these facts, we will use semidefinite programming in order to get deeper insights into the relations between the Laplacian, its second smallest eigenvalue and the underlying graph structure, especially its connectivity. The idea is that by maximizing $\lambda_2(L(G, w))$ the major structure defining properties of the Laplacian come to light.

In Chapter 2 we will translate (1.4) into a semidefinite program. Using Lagrangian duality theory we will derive its dual. The dual can be interpreted as a geometrical embedding problem. The KKT conditions of the dual transform into geometrical constraints as well. The course of this work will mainly be to explore this embedding problem and to figure out implications for the original primal dual setting. Of special interest will be optimal configurations of small dimension for the embedding problem.

For this reason Chapter 3 works out some geometric operations that preserve optimality. The idea behind this rather technical part is to show, that starting from an optimal embedding one can construct another optimal embedding fulfilling a certain dimension bound.

This is finally presented in Chapter 4. It starts with a geometric optimality condition for the embedding problem. Together with the geometric operations this can be extended to show that each graph can be optimally embedded in dimension of tree width of the graph plus one. This can be considered as a first main result of [19].

In Chapter 5 we consider optimal embeddings under variation of the weight parameters of the problem class. The so defined rotational dimension of a graph is a minor monotone graph parameter and can be characterized by a finite list of forbidden minors (for each single value of the parameter). We give these lists for small numbers of the rotational dimension. This is the second main result, published in [20]. Section 5.1 and Section 5.2 are adopted almost verbatim from this article.

We conclude this work by pointing out a surprising relation to another minor monotone graph property, the Colin de Verdière number of a graph.

Note, the optimal embeddings shown in the Figures 2.1, 2.2, 2.3, 4.3, and 4.5 were computed by using SeDuMi [41].

Acknowledgement

I would like to thank my advisor Prof. Dr. Christoph Helmberg for his guidance and valuable comments, my (former) colleagues of the Algorithmic and Discrete Mathematics Group for many lively discussions, and my friends and family for all the motivation.

Chapter 2

The Embedding Problem

2.1 Semidefinite formulation

For a connected graph G we derive a semidefinite formulation of (1.4). For our purposes it is more convenient to handle $\lambda_2(L_d(G,\cdot))$ as a constraint than as the objective. Let w be feasible for (1.4) and let $G[\mathrm{supp}_{++}(w)]$ be connected. Using Observation 8 for $\tilde{w} := \frac{w}{\lambda_2(L_d(G,w))}$ we have

$$\lambda_2(L_d(G,\tilde{w})) = \frac{1}{\lambda_2(L_d(G,w))}\lambda_2(L_d(G,w)) = 1, \text{ and}$$
$$\sum_{ij\in E} c_{ij}\tilde{w}_{ij} = \frac{|E|}{\lambda_2(L_d(G,w))}\ .$$

Thus, if we fix $\lambda_2(L_d(G,w))$ to 1 or require that it is at least 1, a maximizer w^* of (1.4) corresponds to a minimizer $\tilde{w}^*$ of $\sum_{ij\in E} c_{ij}\tilde{w}_{ij}$ via $\tilde{w}^* = \frac{1}{\hat{a}(G,c,d)}w^*$ and vice versa. Hence, the following program is equivalent to (1.4) (as to be explained below):

$$\begin{array}{rl} \frac{|E|}{\hat{a}(G,c,d)} = \text{minimize} & \sum_{ij\in E} c_{ij}w_{ij}, \\ \text{subject to} & \lambda_2(L_d(G,w)) \geq 1, \\ & w \geq 0. \end{array} \tag{2.1}$$

We recall the following fact: Since $c > 0$ the set of all feasible solutions of (1.4) is bounded, and therefore $\lambda_2(L_d(G,\cdot))$ is bounded for this set. Furthermore we may apply Observation 7 to get:

Observation 14 *Given a connected graph G, node densities $d \in \mathbb{R}^N_{++}$ and edge costs $c \in \mathbb{R}^E_{++}$ the problem* (2.1) *attains the minimal objective value (which is finite).*

If $\mathrm{supp}_{++}(w)$ is not connected, the objective of (1.4) is zero. In (2.1) these vectors w are not feasible. Except for this special case the feasible sets and optimizers of (1.4) and (2.1) are the same (up to the scaling above).

Because $\lambda_2(L_d(G,\cdot))$ is a concave function (Corollary 9) we obtain:

Observation 15 (2.1) *is a convex program.*

Next, we will apply graph automorphisms to permute entries of w. Exploiting the convexity of (2.1), we will show that there always exists an optimal solution w^* with equal values $w^*_{e_1} = w^*_{e_2}$ for edges e_1 and e_2 that are mapped by an automorphism (which also preserves the values of d and c). Similar approaches are also common for semidefinite programming in general. The article [31] provides a survey.

Let $\pi : N \to N$ be a graph automorphism on G (this means $\pi(i)\pi(j) \in E$ if and only if $ij \in E$) that preserves densities d_i as well as edge costs c_{ij}, i.e. we have for all $i \in N : d_i = d_{\pi(i)}$ and for all $ij \in E : c_{ij} = c_{\pi(i)\pi(j)}$. We denote the set of all these automorphisms by $\Pi(G)$. We say that edges $ij, rs \in E$ are *automorphic edges* if an automorphism $\pi \in \Pi(G)$ exists with $\{r, s\} = \{\pi(i), \pi(j)\}$. Since $\Pi(G)$ forms a group (with composition as binary operation), the relation of edges to be automorphic is an equivalence relation.

Any feasible solution w of (2.1) maps to a feasible solution $\hat{w}$ of (2.1) with the same objective value when permuted by this automorphism: $\hat{w}_{ij} := w_{\pi(i)\pi(j)}$ for all $ij \in E$. Now, consider an equivalence class of automorphic edges $\{e_1, \ldots, e_k\} \subseteq E$ and a feasible solution w of (2.1). We define $\tilde{w} \in \mathbb{R}^E_+$ by

$$\tilde{w}_{ij} := \frac{1}{|\Pi(G)|} \sum_{\pi \in \Pi(G)} w_{\pi(i)\pi(j)} \quad \text{for all } ij \in E.$$

Then $\tilde{w}$ is a convex combination of feasible solutions of (2.1). By Observation 15 it is also feasible and has an objective value that is less or equal. Moreover $\tilde{w}_{e_1} = \ldots = \tilde{w}_{e_k}$ holds. Hence we get:

Observation 16 *Let G be a graph with densities $d \in \mathbb{R}^N_{++}$ and edge costs $c \in \mathbb{R}^E_{++}$. Then there exists an optimal solution w^* of* (2.1) *so that $w^*_{e_1} = w^*_{e_2}$ for any automorphic edges $e_1, e_2 \in E$.*

We may shift the smallest eigenvalue of the perturbed Laplacian by adding a multiple of the matrix $D^{-1}ee^TD^{-1}$. Since $D^{-1}e$ is perpendicular to all other eigenspaces of $L_d(G, w)$, the other eigenvalues remain unchanged. In this manner it is possible to get access to the second smallest eigenvalue, and we may reformulate (2.1) as a semidefinite program:

$$\begin{array}{rl} \text{minimize} & \sum_{ij \in E} c_{ij} w_{ij}, \\ \text{subject to} & \sum_{ij \in E} w_{ij} D E_{ij} D + \mu D^{-1}ee^TD^{-1} \succeq I, \\ & w \geq 0,\ \mu \text{ free.} \end{array} \tag{2.2}$$

We may apply Observation 14 also to (2.2) to obtain the fact that the optimal value is attained. Introducing a positive semidefinite matrix variable X as Lagrangien multiplier for the definiteness constraint we get the Lagrangien:

$$\begin{aligned} \mathcal{L}(w, \mu, X) &= \sum_{ij \in E} c_{ij} w_{ij} + \left\langle X, I - \sum_{ij \in E} w_{ij} D E_{ij} D - \mu D^{-1}ee^TD^{-1} \right\rangle \\ &= \langle I, X \rangle + \sum_{ij \in E} w_{ij}(c_{ij} - \langle D E_{ij} D, X \rangle) - \mu \left\langle D^{-1}ee^TD^{-1}, X \right\rangle . \end{aligned} \tag{2.3}$$

Now (2.2) is equivalent to

$$\inf_{\substack{w \geq 0 \\ \mu \text{ free}}} \sup_{X \succeq 0} \mathcal{L}(w, \mu, X) \,.$$

The Lagrangian dual is obtained by interchanging inf and sup and reads

$$\begin{array}{rll} \text{maximize} & \langle I, X \rangle \,, & \\ \text{subject to} & \left\langle D^{-1} e e^T D^{-1}, X \right\rangle = 0, & \\ & \langle D E_{ij} D, X \rangle \leq c_{ij} \qquad \text{for } ij \in E, & \\ & X \succeq 0. & \end{array} \tag{2.4}$$

Choosing $w := \frac{1+\varepsilon}{\lambda_2(L_d(G,e))} e$, $\mu := \frac{1+\varepsilon}{\|D^{-1}e\|^2}$ and $\varepsilon > 0$ yields a strictly feasible solution for (2.2). Hence, it fulfills regularity by Slater. Thus, primal and dual optimal values of (2.2) and (2.4) are equal. Since we know that the optimal value of (2.2) is attained and therefore finite, we get the existence of saddle points of the Lagrangian (2.3) as pair of primal and dual optimal solutions. These are characterized by the KKT condtions of (2.2) which contain apart from primal and dual feasiblity the complementary slackness conditions (using Lemma 1.2.3 of [21]):

$$(I - \sum_{ij \in E} w_{ij} D E_{ij} D - \mu D^{-1} e e^T D^{-1}) X = 0, \tag{2.5}$$

$$w_{ij} (c_{ij} - \langle D E_{ij} D, X \rangle) = 0 \qquad \text{for } ij \in E. \tag{2.6}$$

Taking into account the feasibility of X for (2.4) (and again Lemma 1.2.3 of [21]) the condition (2.5) translates to

$$L_d(G, w) X = X. \tag{2.7}$$

2.2 The dual as geometric embedding problem

Each feasible $X \succeq 0$ may be decomposed by a Gram representation $X = (VD^{-1})^T V D^{-1}$ via a matrix $V \in \mathbb{R}^{n \times n}$. We denote the i-th column of V by v_i, i.e., $V = [v_1 \dots v_n]$. Then

$$\begin{aligned} \langle I, X \rangle &= \sum_{i \in N} \frac{1}{d_i^2} \|v_i\|^2, \\ \left\langle D^{-1} e e^T D^{-1}, X \right\rangle &= \left\langle V D^{-2} e, V D^{-2} e \right\rangle = \| \sum_{i \in N} \frac{1}{d_i^2} v_i \|^2, \\ \langle D E_{ij} D, X \rangle &= \|v_i\|^2 + \|v_j\|^2 - 2 \langle v_i, v_j \rangle = \|v_i - v_j\|^2. \end{aligned}$$

With $s_i := \frac{1}{d_i^2}$ and $l_{ij} := \sqrt{c_{ij}}$ the dual (2.4) translates to

$$\begin{array}{rl} \text{maximize} & \sum_{i \in N} s_i \|v_i\|^2, \\ \text{subject to} & \sum_{i \in N} s_i v_i = 0, \\ & \|v_i - v_j\| \leq l_{ij} \qquad \text{for } ij \in E, \\ & v_i \in \mathbb{R}^n \qquad \text{for } i \in N, \end{array} \tag{2.8}$$

and (2.6) is equivalent to

$$w_{ij}(l_{ij} - \|v_i - v_j\|) = 0 \qquad \text{for } ij \in E. \tag{2.9}$$

For $z \in \mathbb{R}^n$ we get $z^T X z = \|VD^{-1}z\|^2 = 0$ if and only if $VD^{-1}z = 0$. Hence, $\text{rank}\,(X) = \text{rank}\,(VD^{-1})$ and $\text{Range}\,(X) = \text{Range}\,(D^{-1}V^T)$. The complementary slackness condition (2.7) simplifies to

$$L_d(G,w)D^{-1}V^T = D^{-1}V^T, \tag{2.10}$$

or respectively

$$L(G,w)V^T = D^{-2}V^T.$$

Evaluating the i-th row of the latter equation yields

$$\sum_{j:ij\in E} w_{ij}(v_i - v_j) = s_i v_i \qquad \text{for } i \in N. \tag{2.11}$$

From $d > 0$ and $c > 0$ we derive $s > 0$ and $l > 0$ for the associated dual parameters. (We will study a relaxed version of the dual problem later on.) We may interpret the data s as significances of the nodes and l as edge lengths. Hence, a solution of problem (2.8) may be interpreted as an embedding of the nodes of the graph in $\mathbb{R}^n$ such that their (weighted) barycenter is at the origin, and the distances of adjacent nodes i and j are bounded by l_{ij}.

Accordingly we refer in the following to (2.8) as embedding problem, and to its optimal solutions as embeddings of the graph G (with data s and l). We denote the constraint $\sum_{i\in N} s_i v_i = 0$ by *equilibrium constraint* and the constraints $\|v_i - v_j\| \le l_{ij}$ for an edge $ij \in E$ by *length constraints*. We may summarize the accomplished results in the following theorem.

Theorem 17 *The programs* (2.1) *and* (2.8) *form a primal dual pair. Feasible solutions w and v_i, $i \in N$ are both optimal if and only if the conditions* (2.9) *and* (2.11) *are satisfied. Moreover for a connected graph $G = (N,E)$ both optimal solutions exist.*

For optimal primal and dual solutions (2.10) *holds, i.e., the vector*

$$[z^T\sqrt{s_1}v_1, \ldots, z^T\sqrt{s_n}v_n]^T$$

is an eigenvector of $L_d(G,w)$ to the second smallest eigenvalue $\lambda_2(L_d(G,w)) = 1$ (equality follows from optimality) for an arbitrary $z \in \mathbb{R}^n \setminus \{0\}$.

If for $ij \in E$ there is an optimal solution w of (2.1) *with $w_{ij} > 0$, then* (2.9) *ensures that in each optimal embedding v_i, $i \in N$ of* (2.8) *the length constraint at this edge is active: $\|v_i - v_j\| = l_{ij}$.*

Later we will make use of the following:

Definition 18 *Let $G = (N,E)$ be a connected graph, $w \ge 0$ be a feasible solution of* (2.1), *$v_i \in \mathbb{R}^N$, $i \in N$, be a feasible solution of* (2.8) *for data $s > 0$, $l > 0$. We call the graph $G_V = (N, E_V := \{ij \in E : \|v_i - v_j\| = l_{ij}\})$* active subgraph of G and data s, l *and the graph $G_w = (N, E_w := \{ij \in E : w_{ij} > 0\})$* strictly active subgraph of G with respect to w.

Theorem 17 asserts that each edge of the strictly active subgraph has tight edge lengths for each optimal embedding. The reverse may not be true. Note, that $E_w \subseteq E_V \subseteq E$ and $L_d(G,w) = L_d(G_w,w)$. Thus, taking into account Corollary 10, we get the following:

Observation 19 *Let $G = (N,E)$ be a connected graph, $w \geq 0$ be an optimal solution of (2.1), $v_i \in \mathbb{R}^N$, $i \in N$ be an optimal solution of (2.8) for data $s > 0$, $l > 0$. Then the active subgraph G_V as well as the strictly active subgraph G_w are connected.*

Note that (2.9) and (2.11) may also be obtained from the KKT conditions of a slightly changed (but equivalent) formulation of (2.8):

$$\begin{array}{rl} \text{maximize} & \sum_{i\in N} s_i\|v_i\|^2, \\ \text{subject to} & (\sum_{i\in N} s_i v_i)^2 = 0, \\ & \|v_i - v_j\|^2 - l_{ij}^2 \leq 0 \qquad \text{for } ij \in E, \\ & v_i \in \mathbb{R}^n \qquad \text{for } i \in N. \end{array}$$

2.3 Physical interpretation and examples

Embeddings suggest the following physical interpretation of optimal primal and dual solutions. Imagine that each node $i \in N$ corresponds to a point mass of size s_i. Edge $ij \in E$ may be thought of as a mass-free cable of length l_{ij}. Now each feasible solution of the embedding problem may be regarded as realization of the graph in $\mathbb{R}^n$ such that its barycenter coincides with 0, and adjacent nodes have a maximal distance of the length of the cable between them.

The embedding of the graph maximizes the (weighted) variance of the realization. This can be seen as a result of a force field acting with force $s_i v_i$ on node i realized in v_i. Each node will move until the net of cables forces the realization to an equilibrium situation. Indeed this force equilibrium is described by the KKT conditions. Thereby w_{ij} fits the force transmitted by the cable between v_i and v_j. Condition (2.9) ensures that these forces are only transmitted through tight cables, and condition (2.11) provides the force equilibrium at each node v_i.

If the embedding is two-dimensional this situation arises by spreading the net on a rotating disk. There should not be any friction between net and disk, and the barycenter of the net should be at the center of rotation. Indeed, if we assume the disk having a constant angular speed of $\omega = 1$, the centralpetal force which ensures, that node i is staying on its orbit around the center, is $s_i v_i$. This has to be exerted by the incident ropes and yields (2.11). Let us look at three examples. For these we set the parameters $d = e$ and $s = e$.

Randomly chosen graph

Figure 2.1 shows a randomly chosen graph on 30 nodes. To determine the edges, we mapped the nodes into $[0,1]^2$ and connected any two of them if the Euclidean distance of their images was less or equal than 0.3 . The edge weights of a computed optimal solution

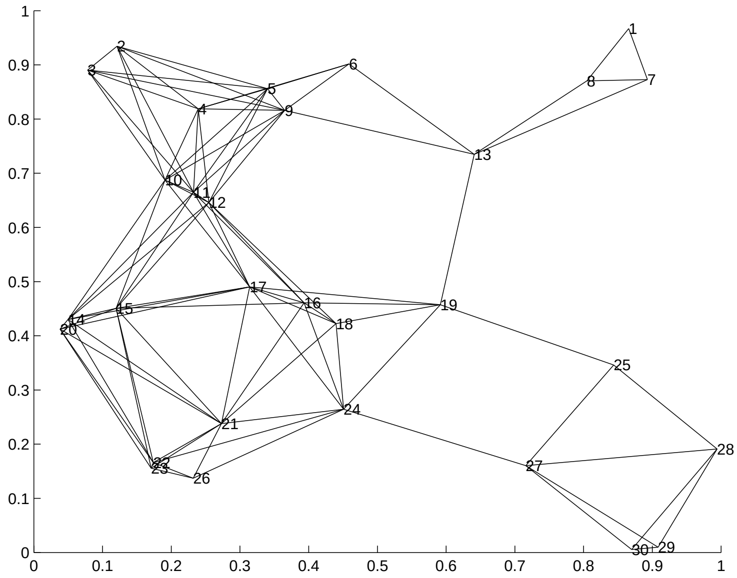

Figure 2.1: Randomly chosen graph on 30 nodes.

of (2.2) of this graph are shown in Figure 2.2. The gray shade, an edge is drawn with, corresponds to the edge weight (white is weight 0, black is maximum weight). A related optimal embedding of (2.8) is shown in Figure 2.3. The small circle in the center of the diagram indicates the origin.

Path on 3 nodes - Use of the KKT conditions

Consider the graph $G = (N, E)$ with $N = \{1, 2, 3\}$ and $E = \{\{1, 2\}, \{1, 3\}\}$. Then the primal program (2.1) substantiates to

$$\begin{array}{rl} \text{minimize} & w_{12} + w_{13}, \\ \text{subject to} & w_{12} + w_{13} - \sqrt{(w_{12} + w_{13})^2 - 3w_{12}w_{13}} \geq 1, \\ & w \geq 0. \end{array}$$

Thus, we have a unique minimizer $w = e$. (Existence of an optimal solution with $w_{12} = w_{13}$ is ensured by Observation 16.) The optimal Laplacian has the following eigenvalues and respective eigenvectors: $\lambda_1 = 0$, $x_1 = e$, $\lambda_2 = 1$, $x_2 = (0, 1, -1)^T$, $\lambda_3 = 3$, $x_3 = (-2, 1, 1)^T$.

The dual reads

$$\begin{array}{rl} \text{maximize} & \|v_1\|^2 + \|v_2\|^2 + \|v_3\|^2, \\ \text{subject to} & v_1 + v_2 + v_3 = 0, \\ & \|v_1 - v_2\| \leq 1, \\ & \|v_1 - v_3\| \leq 1, \\ & v_1, v_2, v_3 \in \mathbb{R}^3. \end{array}$$

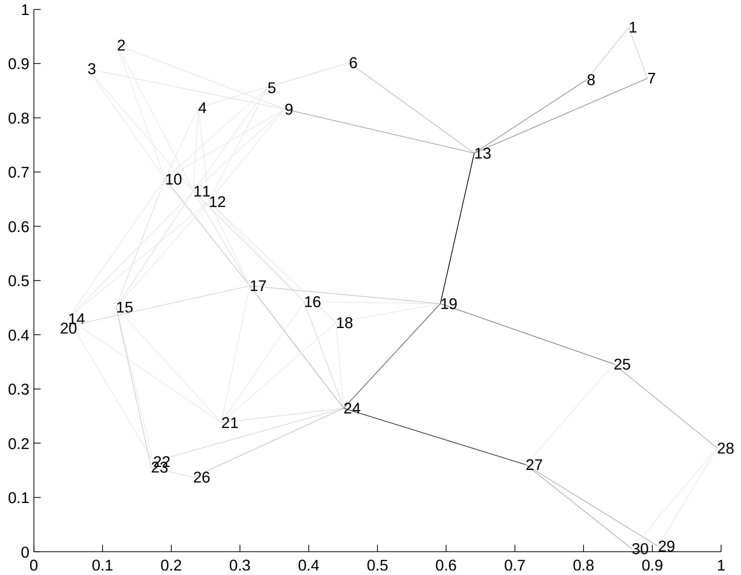

Figure 2.2: Optimal edge weights of the randomly chosen graph.

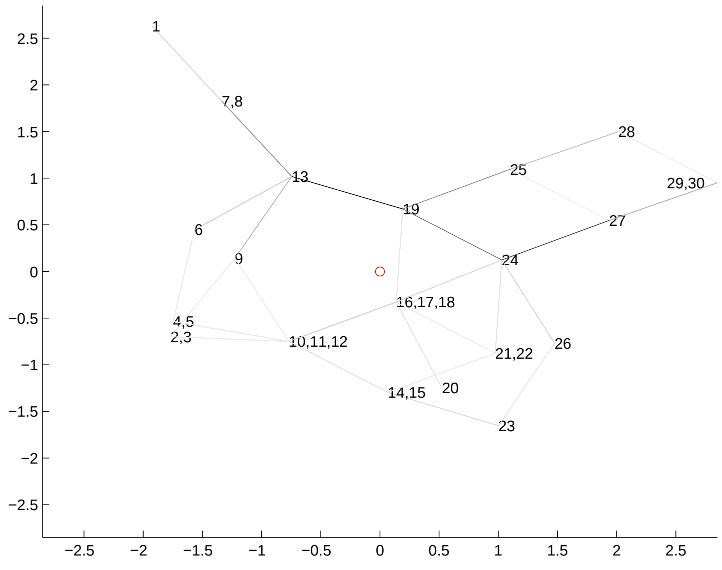

Figure 2.3: Optimal embedding of the randomly chosen graph.

We pretend not to know the primal optimal solution. Then we may use the KKT conditions to solve the embedding problem. Equation (2.9) and Corollary 10 tell us that both edges (cables) are tight. The force equilibrium reads:

$$\begin{aligned}
&v_1 + w_{12}(v_2 - v_1) + w_{13}(v_3 - v_1) = 0,\\
&v_2 + w_{12}(v_1 - v_2) = 0,\\
&v_3 + w_{13}(v_1 - v_3) = 0.
\end{aligned}$$

The equations together enforce the optimal embedding to be one dimensional (second and third row in case $v_1 \neq 0$, first row otherwise). This leaves (up to isomorphism) only two configurations, fulfilling the equilibrium: (coordinates with respect to the affine hull of the embedded nodes) $v_1 = 0, v_2 = -1, v_3 = 1$, $w = e$ and $v_1 = -\frac{1}{3}, v_2 = v_3 = \frac{2}{3}$, $w = \frac{1}{3}e$. The first solution is indeed optimal as can be seen from the feasible primal variable w having the same (optimal) objective value. In accordance with Theorem 17, the vector $(v_1, v_2, v_3)^T = (0, -1, 1)^T$ is eigenvector to the second smallest eigenvalue (equal to one) of the optimal Laplacian.

Consider the second solution. Obviously it is not optimal, but $(-\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ is eigenvector to the eigenvalue 1 of the Laplacian with $w = \frac{1}{3}e$. This is not astonishing as the force equilibrium is equivalent to the eigenvector property (as shown). But since this Laplacian is one third of the optimal Laplacian, the greatest eigenvalue is scaled to one. Thus, the primal constraint $\lambda_2(L_d(G, w)) \geq 1$ is violated.

As seen, considering the KKT conditions without primal feasibility may lead to other eigenspaces. Dual feasibility together with the length condition and force equilibrium alone are not sufficient to obtain structural properties of optimal embeddings.

Star - Low and high dimensional embeddings

For a star $K_{1,n} := (\{0, 1, \ldots, n\}, \{\{0, i\} : i = 1, \ldots, n\})$ with $n \geq 2$ one optimal solution embeds the center node 0 in the origin and all other nodes in the vertices of a regular n-1 dimensional simplex with $\|v_i\| = 1$, $i = 1, \ldots, n$ for an objective value of n (optimality follows from choosing $w_{ij} = 1$ and $\mu = 1$ in (2.2)).

For even $n \geq 2$ a one dimensional optimal embedding is given by assigning the center node 0 to the origin, half the outer nodes to +1 and the other half to -1.

For odd $n \geq 3$ one possibility to find a two dimensional optimal embedding is to put node 0 into the origin, node 1 to $(1, 0)$, even nodes $i \geq 2$ to $(-\frac{1}{n-1}, \sqrt{1 - (\frac{1}{n-1})^2})$ and odd nodes $i \geq 3$ to $(-\frac{1}{n-1}, -\sqrt{1 - (\frac{1}{n-1})^2})$.

2.4 Formulation without fixed barycenter

In this section we will give equivalent formulations of the embedding problem (2.8) that handle partitions of the node set separately. This allows to examine geometrical transformations which affect only a subset of nodes. A similar approach was also utilized in the work [38].

For a subset of nodes $C \subseteq N$ let $\bar{s}_C := \sum_{i \in C} s_i$ be its total significance and $\bar{v}_C := \frac{1}{\bar{s}_C} \sum_{i \in C} s_i v_i$ its (weighted) barycenter. We give a formulation of the embedding problem (2.8) which does not require the barycenter of nodes to be at zero:

$$\begin{array}{rl} \text{maximize} & \sum_{i \in N} s_i \|v_i - \bar{v}_N\|^2, \\ \text{subject to} & \sum_{i \in N} s_i v_i = \bar{s}_N \bar{v}_N, \\ & \|v_i - v_j\| \leq l_{ij} \qquad \text{for } ij \in E, \\ & v_i, \bar{v}_N \in \mathbb{R}^n \qquad \text{for } i \in N. \end{array} \tag{2.12}$$

A solution of (2.12) converts equivalently to a solution v_i', $i \in N$ of (2.8) via $v_i' = v_i - \bar{v}_N$. The next step is to provide a formulation of the objective which does not make use of distances to the barycenter, but only uses distances between the points themselves. For $C \subseteq N$ holds:

$$\begin{aligned} \frac{1}{\bar{s}_C} \sum_{i,j \in C, i<j} s_i s_j \|v_i - v_j\|^2 =& \frac{1}{2\bar{s}_C} \sum_{i,j \in C} s_i s_j \|(v_i - \bar{v}_C) - (v_j - \bar{v}_C)\|^2 \\ =& \frac{1}{\bar{s}_C} \sum_{j \in C} s_j \sum_{i \in C} s_i \|v_i - \bar{v}_C\|^2 \\ & - \frac{1}{\bar{s}_C} \left\langle \underbrace{\sum_{i \in C} s_i v_i - \bar{s}_C \bar{v}_C}_{=0}, \sum_{j \in C} s_j v_j - \bar{s}_C \bar{v}_C \right\rangle \\ =& \sum_{i \in C} s_i \|v_i - \bar{v}_C\|^2. \end{aligned} \tag{2.13}$$

Hence, we get the following equivalent embedding problem. It does not make use of a fixed barycenter:

$$\begin{array}{rl} \text{maximize} & \frac{1}{\bar{s}_N} \sum_{i,j \in N, i<j} s_i s_j \|v_i - v_j\|^2, \\ \text{subject to} & \|v_i - v_j\| \leq l_{ij} \qquad \text{for } ij \in E, \\ & v_i \in \mathbb{R}^n \qquad \text{for } i \in N. \end{array} \tag{2.14}$$

For a partition $C_1 \dot\cup \ldots \dot\cup C_k = N$ of nodes we get:

$$\begin{aligned} \sum_{i \in N} s_i \|v_i - \bar{v}_N\|^2 =& \sum_{l=1}^{k} \sum_{i \in C_l} s_i \|(v_i - \bar{v}_{C_l}) + (\bar{v}_{C_l} - \bar{v}_N)\|^2 \\ =& \sum_{l=1}^{k} \sum_{i \in C_l} s_i \|v_i - \bar{v}_{C_l}\|^2 + \sum_{l=1}^{k} \bar{s}_{C_l} \|\bar{v}_{C_l} - \bar{v}_N\|^2 \\ & + 2 \sum_{l=1}^{k} \left\langle \underbrace{\sum_{i \in C_l} s_i v_i - \bar{s}_{C_l} \bar{v}_{C_l}}_{=0}, \bar{v}_{C_l} - \bar{v}_N \right\rangle. \end{aligned}$$

This provides a two-step formulation of (2.12):

$$\begin{array}{rl} \text{maximize} & \sum_{l=1}^{k} \sum_{i \in C_l} s_i \|v_i - \bar{v}_{C_l}\|^2 + \sum_{l=1}^{k} \bar{s}_{C_l} \|\bar{v}_{C_l} - \bar{v}_N\|^2, \\ \text{subject to} & \sum_{i \in C_l} s_i v_i = \bar{s}_{C_l} \bar{v}_{C_l} \qquad \text{for } 1 \le l \le k, \\ & \sum_{l=1}^{k} \bar{s}_{C_l} \bar{v}_{C_l} = \bar{s}_N \bar{v}_N, \\ & \|v_i - v_j\| \le l_{ij} \qquad \text{for } ij \in E, \\ & v_i, \bar{v}_{C_l}, \bar{v}_N \in \mathbb{R}^n \qquad \text{for } i \in N,\ 1 \le l \le k. \end{array}$$

Using (2.13) for the barycenters, too, we have the equivalent formulation:

$$\begin{array}{rl} \text{maximize} & \sum_{l=1}^{k} \frac{1}{\bar{s}_{C_l}} \sum_{i,j \in C_l,\, i<j} s_i s_j \|v_i - v_j\|^2 \\ & + \frac{1}{\bar{s}_N} \sum_{1 \le l < o \le k} \bar{s}_{C_l} \bar{s}_{C_o} \|\bar{v}_{C_l} - \bar{v}_{C_o}\|^2, \\ \text{subject to} & \sum_{i \in C_l} s_i v_i = \bar{s}_{C_l} \bar{v}_{C_l} \qquad \text{for } 1 \le l \le k, \\ & \|v_i - v_j\| \le l_{ij} \qquad \text{for } ij \in E, \\ & v_i, \bar{v}_{C_l} \in \mathbb{R}^n \qquad \text{for } i \in N,\ 1 \le l \le k. \end{array} \tag{2.15}$$

The objective is decomposed into two levels. Within a partial set C_l, the "low level" sums up the squares of distances of the partial set C_l to the respective barycenter. The "global level" does the same with the barycenters of partial sets (imaginable as super nodes).

This allows to trace the change of the objective easily if we move (or in general map congruently) groups of nodes. For example, this opens another view on the fact that the absolute algebraic connectivity of non-connected graphs is 0. Indeed, let the sets C_l be defined by the components of G. Then these components may be moved arbitrarily far from each other. The objective becomes arbitrarily large which means that there cannot be an optimal $\lambda_2(L_d(G, w^*)) > 0$.

The length condition (2.9) keeps its role of a complementary slackness condition. The force equilibrium may be written as

$$\sum_{j: ij \in E} w_{ij}(v_i - v_j) = s_i(v_i - \bar{v}_N) \qquad \text{for } i \in N.$$

Summing up these equations for all $i \in C_l$ we get new equations that have to be valid in case of optimality (terms within C_l cancel out):

$$\sum_{i \in C_l,\, j \notin C_l,\, ij \in E} w_{ij}(v_i - v_j) = \bar{s}_{C_l}(\bar{v}_{C_l} - \bar{v}_N) \qquad \text{for } 1 \le l \le k.$$

Chapter 3

Geometrical Operations

In this section we will consider geometrical operations which change embeddings (solutions of (2.8)). We will make extensive use of them in the next chapter. Here we will neglect the question whether the solution remains feasible while performing such an operation. When applying the operations later on, we will ensure that the resulting embedding is feasible again. But we will consider the cost function for the operations, and we will be able to describe its change. This will be useful in proofs of optimality or in constructing optimal solutions of low dimension.

Throughout this chapter we use the following notations. The starting point of an operation is an optimal embedding v_i, $i \in N$ of (2.8), where $G = (N, E)$ is the underlying connected (simple) graph. By $S \subset N$ we denote a separator in G, separating G into m connected components and satisfying

$$0 \in \mathcal{S} := \operatorname{conv}\{v_i : i \in S\}.$$

The node sets of the components are denoted by

$$C_j \subset N,\ j \in M := \{1, \ldots, m\}.$$

The operations will not change the embedding with respect to the linear subspace

$$\mathcal{L} := \operatorname{span} \mathcal{S}.$$

The transformations will only affect the projections of the embedded nodes to the orthogonal complement $\mathcal{L}^\perp$. We denote the orthogonal projection of a point $x \in \mathbb{R}^n$ onto $\mathcal{L}^\perp$ by $p_{\mathcal{L}^\perp}(x)$.

3.1 Congruent transformations

First we prove for some given subset C of nodes that transformations represented by orthogonal matrices that do not change the barycenter of the points do not have an affect on the distances between the nodes. These transformations yield congruent point sets.

Observation 20 *Let $Q \in \mathbb{R}^{n \times n}$ be an orthogonal matrix. Given $v_i \in \mathbb{R}^n$, $i \in C \subseteq N$, let $\bar{v}_C := \frac{1}{\bar{s}_C} \sum_{i \in C} s_i v_i$ and set $v_i' := \bar{v}_C + Q(v_i - \bar{v}_C)$. Then the barycenter remains the same,*

$$\frac{1}{\bar{s}_C} \sum_{i \in C} s_i v_i' = \bar{v}_C,$$

and distances do not change,

$$\|v_i' - v_j'\|^2 = \|v_i - v_j\|^2, \text{ for all } i, j \in C.$$

Proof. We compute

$$\begin{aligned} \frac{1}{\bar{s}_C} \sum_{i \in C} s_i v_i' &= \bar{v}_C + \frac{1}{\bar{s}_C} Q \underbrace{(\sum_{i \in C} s_i v_i - \bar{s}_C \bar{v}_C)}_{=0} \\ &= \bar{v}_C, \end{aligned}$$

and

$$\begin{aligned} \|v_i' - v_j'\|^2 &= \|Q(v_i - v_j)\|^2 \\ &= (v_i - v_j)^T \underbrace{Q^T Q}_{=I} (v_i - v_j) \\ &= \|v_i - v_j\|^2. \end{aligned}$$

■

In consequence congruent transformations of this type do not change the objective value of the embedding formulation (2.14) whenever distances to points connected to C do not change. Hence, embedding problem (2.14) is invariant under such congruent transformations with $C = N$.

3.2 Folding a flat halfspace

Later we will often use transformations including folding operations, e.g., rotating nodes out of the subspace of the embedding around an affine subspace. This is only possible if a "free" dimension is available through which the nodes may be rotated. We will show now, that such a dimension always exists. Indeed no feasible solution of the embedding problem (2.8) can be fulldimensional. So there is always space for folding operations.

Observation 21 *Let $v_i \in \mathbb{R}^n$, $i \in N$, be feasible for (2.8). Then there is a vector $h \in \mathbb{R}^n$, $\|h\| = 1$ with $v_i \in \mathcal{H} := \{x \in \mathbb{R}^n : h^T x = 0\}$ for all $i \in N$.*

Proof. Since $\sum_{i \in N} s_i v_i = 0$ the vectors v_i, $i \in N$, are linearly dependent, and therefore $\dim(\operatorname{span}\{v_1, \ldots, v_n\}) \leq n - 1$. ■

Given such a linear subspace

$$\mathcal{H} := \{x \in \mathbb{R}^n : h^T x = 0\},$$

a normalized $b \in \mathcal{H}$, and some $\beta \in \mathbb{R}$, we next describe the operation of rotating the flat half-space

$$\mathcal{B}^- := \{x \in \mathcal{H} : b^T x < \beta\}$$

around the hyperplane

$$\mathcal{B} := \{x \in \mathcal{H} : b^T x = \beta\}$$

of $\mathcal{H}$. Denote by $p_{\mathcal{B}}(x)$ the orthogonal projection of a point $x \in \mathbb{R}^n$ onto $\mathcal{B}$. Due to $\|h\| = \|b\| = 1$ and $h^T b = 0$ it is computed by

$$p_{\mathcal{B}}(x) = x + (\beta - b^T x)b - h^T x h. \tag{3.1}$$

Define now the continuous map $\varphi : \mathcal{H} \times [-\pi, \pi] \to \mathbb{R}^n$ by

$$\varphi(x, \gamma) := \begin{cases} p_{\mathcal{B}}(x) - (\beta - b^T x)[b \cos \gamma + h \sin \gamma] & \text{if } b^T x < \beta, \\ x & \text{if } b^T x \geq \beta. \end{cases} \tag{3.2}$$

It rotates points $x \in \mathcal{B}^-$ around $\mathcal{B}$ by an angle γ, whereas all the other points of $\mathcal{H}$ remain untouched. The radius of the rotation is $\|x - p_{\mathcal{B}}(x)\| = |\beta - b^T x|$. Next we show that distances between "folded" points remain the same. Distances between "folded" points and points not "folded" do not increase. This fact will help to ensure feasiblity later on.

Observation 22 (Folding a Flat Halfspace) *For all $\gamma \in [-\pi, \pi]$ and all $x, y \in \mathcal{H}$,*

(i) $p_{\mathcal{B}}(x) = p_{\mathcal{B}}(\varphi(x, \gamma))$ *and* $\|x - p_{\mathcal{B}}(x)\| = \|\varphi(x, \gamma) - p_{\mathcal{B}}(x)\|$,
(ii) $\|\varphi(x, \gamma) - \varphi(y, \gamma)\| = \|x - y\|$ *if both* $x, y \in \mathcal{B} \cup \mathcal{B}^-$ *or both* $x, y \in \mathcal{H} \setminus \mathcal{B}^-$,
(iii) $\|\varphi(x, \gamma) - \varphi(y, \gamma)\| \leq \|x - y\|$ *for* $x \in \mathcal{B} \cup \mathcal{B}^-$, $y \in \mathcal{H} \setminus \mathcal{B}^-$.

Proof. (i) follows by direct calculation from (3.1).

If $b^T x \geq \beta$ and $b^T y \geq \beta$ the points are not transformed. If $b^T x \leq \beta$ and $b^T y \leq \beta$ both points are subject to the same orthogonal transformation which preserves distances (see Observation 20). This implies (ii).

If, $b^T x < \beta \leq b^T y$, the intersection of the line segment between x and y and $\mathcal{B}$ determines a unique point $z \in \mathcal{B} \cap \operatorname{conv}\{x, y\}$. The triangle inequality and (ii) yield

$$\begin{aligned} \|\varphi(x, \gamma) - y\| &\leq \|\varphi(x, \gamma) - z\| + \|z - y\| \\ &= \|x - z\| + \|z - y\| \\ &= \|x - y\|, \end{aligned}$$

so (iii) holds. ∎

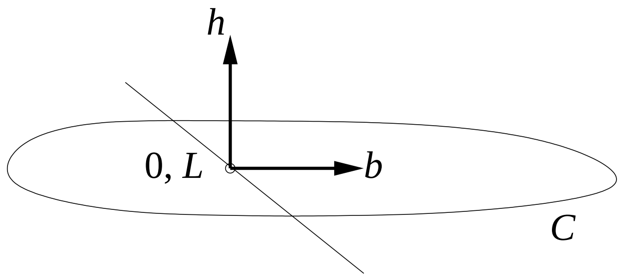

Figure 3.1: Initial setting before the transformation of C in Observations 23-27.

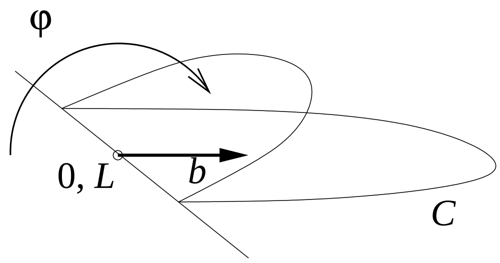

Figure 3.2: φ folds C into the halfspace specified by b (Observation 23).

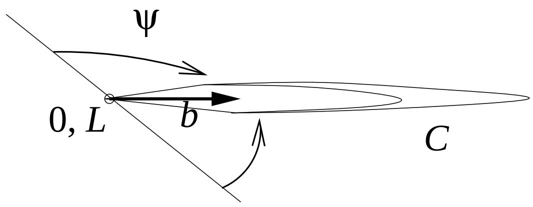

Figure 3.3: ψ collapses C into the flat halfspace spanned by $\mathcal{L}$ and direction b (Observation 25).

3.3 Folding and Collapsing

This section introduces the transformations we will use in Section 4.2. While the results are proved by straight forward calculations with analytical geometry, they are vital for the understanding of what is covered in Section 4.2.

Observation 23 (Transformation Part 1, Folding) *Given $j \in M$ and $b_j \in \mathcal{H} \cap \mathcal{L}^\perp$ with $\|b_j\| = 1$, define $\varphi_i : [0,1] \to \mathbb{R}^n$ for $i \in C_j$ by*

$$\varphi_i(t) := \begin{cases} v_i - (v_i^T b_j)b_j + (v_i^T b_j)[b_j \cos t\pi + h \sin t\pi] & \text{if } v_i^T b_j < 0 \\ v_i & \text{if } v_i^T b_j \geq 0. \end{cases}$$

Then, for $i \in C_j$,
(i) $\varphi_i(0) = v_i$,
(ii) $\varphi_i(1) \in \{x \in \mathcal{H} : b_j^T x \geq 0\}$,
and for all $t \in [0,1]$ it holds that
(iii) $p_{\mathcal{L}}(v_i) = p_{\mathcal{L}}(\varphi_i(t))$ *and* $\|p_{\mathcal{L}^\perp}(v_i)\| = \|p_{\mathcal{L}^\perp}(\varphi_i(t))\|$,
(iv) $\|\varphi_i(t) - v\| = \|v_i - v\|$ *for* $v \in \mathcal{L} \supseteq \{v_s : s \in S\}$,
(v) $\|\varphi_i(t) - \varphi_k(t)\| \leq \|v_i - v_k\|$ *for* $k \in C_j$.

Proof. (i) and (ii) follow from direct calculation and $v_i \in \mathcal{H}$. (iii)-(v) follow from Observation 22(i)-(iii) using $b = b_j$, $\beta = 0$, $\varphi_i(t) = \varphi(v_i, t\pi)$, and the fact that $\mathcal{S} \subseteq \mathcal{L} \subseteq \mathcal{B}$. ∎

Next, we show that the length of the projected cumulated vector increases throughout this first transformation.

Observation 24 *For φ_i, $i \in C_j$ as defined in Observation 23, define $\bar{\varphi}_j : [0,1] \to \mathbb{R}^n$ by*

$$\bar{\varphi}_j(t) := \sum_{i \in C_j} s_i \varphi_i(t).$$

The length $\|p_{\mathcal{L}^\perp}(\bar{\varphi}_j(t))\|$ is nondecreasing in $t \in [0,1]$.

Proof. The choice of b_j ensures $\mathcal{B} := \{x \in \mathcal{H} : b_j^T x = 0\} \supseteq \mathcal{L}$ and $\mathcal{B}^\perp = \text{span}\,\{h, b_j\}$. By definition of the φ_i in Observation 23 we obtain

$$\begin{aligned} \|p_{\mathcal{L}^\perp}(\bar{\varphi}_j(t))\|^2 &= \|p_{\mathcal{L}^\perp}(p_{\mathcal{B}}(\bar{\varphi}_j(0)))\|^2 + \|p_{\mathcal{B}^\perp}(\bar{\varphi}_j(t))\|^2 \\ &= \|p_{\mathcal{L}^\perp}(p_{\mathcal{B}}(\bar{\varphi}_j(0)))\|^2 + \\ &\quad \left\| \sum_{i \in C_j, v_i^T b_j < 0} s_i (v_i^T b_j)[b_j \cos t\pi + h \sin t\pi] + \sum_{i \in C_j, v_i^T b_j \geq 0} s_i (v_i^T b_j) b_j \right\|^2. \end{aligned}$$

As b_j and h are orthogonal it remains to study the monotonicity of

$$\Big[\sum_{i\in C_j, v_i^T b_j<0} s_i v_i^T b_j \cos t\pi + \sum_{i\in C_j, v_i^T b_j\geq 0} s_i v_i^T b_j\Big]^2 + \Big[\sum_{i\in C_j, v_i^T b_j<0} s_i v_i^T b_j \sin t\pi\Big]^2$$

$$= \Big[\sum_{i\in C_j, v_i^T b_j<0} s_i v_i^T b_j\Big]^2 (\cos^2 t\pi + \sin^2 t\pi) + \Big[\sum_{i\in C_j, v_i^T b_j\geq 0} s_i v_i^T b_j\Big]^2 +$$

$$2\underbrace{\Big[\sum_{i\in C_j, v_i^T b_j<0} s_i v_i^T b_j\Big]\Big[\sum_{i\in C_j, v_i^T b_j\geq 0} s_i v_i^T b_j\Big]}_{\leq 0} \cos t\pi \ .$$

The last term is clearly nondecreasing. ■

The collapsing transformation starts from the points $\varphi_i(1)$ and runs as follows.

Observation 25 (Transformation Part 2, Collapsing)
Given the setting of Observation 23 determine for $i \in C_j$ angles $0 \leq \gamma_i \leq \frac{\pi}{2}$ and $q_i \in \mathcal{L}^\perp$, $q_i^T b_j = 0$, $\|q_i\| = 1$ so that $p_{\mathcal{L}^\perp}(\varphi_i(1)) = \|p_{\mathcal{L}^\perp}(\varphi_i(1))\|(q_i \cos\gamma_i + b_j \sin\gamma_i)$, and define $\psi_i : [0,1] \to \mathbb{R}^n$ by

$$\psi_i(t) := p_{\mathcal{L}}(\varphi_i(1)) + \|p_{\mathcal{L}^\perp}(\varphi_i(1))\| \Big[q_i \cos(\gamma_i + t[\frac{\pi}{2} - \gamma_i]) + b_j \sin(\gamma_i + t[\frac{\pi}{2} - \gamma_i])\Big] .$$

Then, for $i \in C_j$,
(i) $\psi_i(0) = \varphi_i(1)$,
(ii) $\psi_i(1) = p_{\mathcal{L}}(v_i) + \|p_{\mathcal{L}^\perp}(v_i)\| b_j \in \mathcal{L} + \{\beta b_j : \beta \geq 0\}$,
and for all $t \in [0,1]$ it holds that
(iii) $p_{\mathcal{L}}(v_i) = p_{\mathcal{L}}(\psi_i(t))$ *and* $\|p_{\mathcal{L}^\perp}(v_i)\| = \|p_{\mathcal{L}^\perp}(\psi_i(t))\|$,
(iv) $\|\psi_i(t) - v\| = \|v_i - v\|$ *for* $v \in \mathcal{L} \supseteq \{v_s : s \in S\}$,
(v) $\|\psi_i(t) - \psi_k(t)\| \leq \|v_i - v_k\|$ *for* $k \in C_j$.

Proof. First note that Observation 23(iii) implies $p_{\mathcal{L}}(v_i) = p_{\mathcal{L}}(\varphi_i(1))$ and $\|p_{\mathcal{L}^\perp}(\varphi_i(1))\| = \|p_{\mathcal{L}^\perp}(v_i)\|$. Now (i) and (ii) follow from direct calculation, and (iii) and (iv) are proved in the same way as (i) and (ii) of Observation 22. It remains to prove (v).

Because of Observation 23(v) it suffices to prove $\|\psi_i(t)-\psi_k(t)\|^2 \leq \|\varphi_i(1)-\varphi_k(1)\|^2$ for $i,k \in C_j$. For this we need to show $\psi_i(t)^T\psi_k(t) \geq \varphi_i(1)^T\varphi_k(1)$ which leads to the condition

$$\begin{aligned} f_{ik}(t) :=& q_i^T q_k \cos(\gamma_i + t[\frac{\pi}{2} - \gamma_i]) \cos(\gamma_k + t[\frac{\pi}{2} - \gamma_k]) \\ &+ \sin(\gamma_i + t[\frac{\pi}{2} - \gamma_i]) \sin(\gamma_k + t[\frac{\pi}{2} - \gamma_k]) \\ \geq& q_i^T q_k \cos\gamma_i \cos\gamma_k + \sin\gamma_i \sin\gamma_k = f_{ik}(0). \end{aligned} \tag{3.3}$$

We prove that $f_{ik}(t)$ is nondecreasing in $t \in [0,1]$. In the case $q_i^T q_k < 0$ both cosine terms in $f_{ik}(t)$ are nonincreasing and the sine terms are nondecreasing. In the remaining case we use the angle addition formulas to find

$$f_{ik}(t) = q_i^T q_k \cos((1-t)[\gamma_i - \gamma_k]) + (1 - q_i^T q_k) \sin(\gamma_i + t[\frac{\pi}{2} - \gamma_i]) \sin(\gamma_k + t[\frac{\pi}{2} - \gamma_k]).$$

But $0 \leq q_i^T q_k \leq 1$ and so the cosine and sine terms are nondecreasing. ■

Again, we continue with showing that during this transformation the length of the projected cumulated vector is nondecreasing.

Observation 26 *For ψ_i, $i \in C_j$ as defined in Observation 25, define $\bar{\psi}_j : [0,1] \to \mathbb{R}^n$ by*

$$\bar{\psi}_j(t) := \sum_{i \in C_j} s_i \psi_i(t).$$

The length $\|p_{\mathcal{L}^\perp}(\bar{\psi}_j(t))\|$ is nondecreasing in $t \in [0,1]$.

Proof. Using the functions f_{ik} introduced in (3.3) and Observation 25(iii) we may write

$$\begin{aligned} \Big\| \sum_{i \in C_j} s_i p_{\mathcal{L}^\perp}(\psi_i(t)) \Big\|^2 &= \sum_{i \in C_j} s_i \|p_{\mathcal{L}^\perp}(\psi_i(t))\|^2 + \sum_{i,k \in C_j, i<k} 2 s_i s_k (p_{\mathcal{L}^\perp}(\psi_i(t)))^T (p_{\mathcal{L}^\perp}(\psi_k(t))) \\ &= \sum_{i \in C_j} s_i \|p_{\mathcal{L}^\perp}(\psi_i(t))\|^2 + \sum_{i,k \in C_j, i<k} s_i \|p_{\mathcal{L}^\perp}(v_i)\| s_k \|p_{\mathcal{L}^\perp}(v_k)\| f_{ik}(t) \end{aligned}$$

and we have shown in the proof of Observation 25 that each $f_{ik}(t)$ is nondecreasing in $t \in [0,1]$. ■

We concatenate both transformations into one and summarize our findings on this collapsing transformation.

Observation 27 (Collapsing Transformation)
Given $j \in M$ and $b_j \in \mathcal{H} \cap \mathcal{L}^\perp$ with $\|b_j\| = 1$, define $u_i : [0,1] \to \mathbb{R}^n$ for $i \in C_j$ by

$$u_i(t) := \begin{cases} \varphi_i(2t) & \text{for } t \in [0, \frac{1}{2}], \\ \psi_i(2[t - \frac{1}{2}]) & \text{for } t \in (\frac{1}{2}, 1], \end{cases} \tag{3.4}$$

with φ_i and ψ_i as given in Observation 23 and Observation 25. Then, for $i \in C_j$,
(i) $u_i(0) = v_i$,
(ii) $u_i(1) = p_{\mathcal{L}}(v_i) + \|p_{\mathcal{L}^\perp}(v_i)\| b_j \in \mathcal{L} + \{\beta b_j : \beta \geq 0\}$,
and for all $t \in [0,1]$ it holds that
(iii) $p_{\mathcal{L}}(v_i) = p_{\mathcal{L}}(u_i(t))$ *and* $\|p_{\mathcal{L}^\perp}(v_i)\| = \|p_{\mathcal{L}^\perp}(u_i(t))\|$,
(iv) $\|u_i(t) - v\| = \|v_i - v\|$ *for* $v \in \mathcal{L} \supseteq \{v_k : k \in S\}$,
(v) $\|u_i(t) - u_k(t)\| \leq \|v_i - v_k\|$ *for* $k \in C_j$.
Furthermore, for

$$\bar{u}_j(t) := \sum_{i \in C_j} s_i u_i(t)$$

the length $\|p_{\mathcal{L}^\perp}(\bar{u}_j(t))\|$ is nondecreasing in $t \in [0,1]$ and $\|p_{\mathcal{L}^\perp}(\bar{u}_j(1))\| = \sum_{i \in C_j} s_i \|p_{\mathcal{L}^\perp}(v_i)\|$.

Proof. The result follows from the Observations 23, 24, 25 and 26. ■

We need yet another transformation in the proof of Theorem 37. It is comparable to closing a fan, see Figure 3.4.

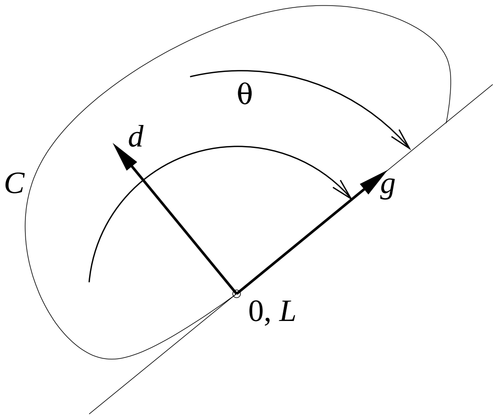

Figure 3.4: θ squeezes C spanned by $\mathcal{L}' + \operatorname{span}\{g\}$ and nonnegative d into the boundary halfspace spanned by $\mathcal{L}$ and nonnegative g. (Observation 28).

Observation 28 (Squeezing Transformation)
Given $C \subseteq N$, a linear subspace $\mathcal{L}' \subseteq \mathbb{R}^n$, vectors $d, g \in \mathcal{L}'^{\perp}$ with $\|d\| = \|g\| = 1$, $d^T g = 0$ and $v_i \in \{x \in \mathcal{L}' + \operatorname{span}\{d, g\} : d^T x \geq 0\}$ for all $i \in C$. For $i \in C$, set $\delta_i' := \|p_{\mathcal{L}'^{\perp}}(v_i)\|$, determine $\gamma_i \in [0, \pi]$ so that $p_{\mathcal{L}'^{\perp}}(v_i) = \delta_i'(g \cos \gamma_i + d \sin \gamma_i)$ and define continuous maps $\theta_i : [0, 1] \to \mathbb{R}^n$

$$\theta_i(t) := p_{\mathcal{L}'}(v_i) + \delta_i' \left[g \cos(\gamma_i - t\gamma_i) + d \sin(\gamma_i - t\gamma_i) \right].$$

Then, for $i \in C$,
(i) $\theta_i(0) = v_i$,
(ii) $\theta_i(1) = p_{\mathcal{L}'}(v_i) + \|p_{\mathcal{L}'^{\perp}}(v_i)\| g$,
and for all $t \in [0, 1]$ it holds that
(iii) $p_{\mathcal{L}'}(v_i) = p_{\mathcal{L}'}(\theta_i(t))$ *and* $\|p_{\mathcal{L}'^{\perp}}(v_i)\| = \|p_{\mathcal{L}'^{\perp}}(\theta_i(t))\|$,
(iv) $\|\theta_i(t) - v\| \leq \|v_i - v\|$ *for* $v \in \mathcal{L}' + \{\beta g : \beta > 0\}$,
(v) $\|\theta_i(t) - \theta_k(t)\| \leq \|v_i - v_k\|$ *for* $k \in C$.
Furthermore, for $\bar{\theta}_C(t) := \sum_{i \in C} s_i \theta_i(t)$,
(vi) $p_{\mathcal{L}'^{\perp}}(\bar{\theta}_C(t)) \in \operatorname{span}\{g\} + \{\beta d : \beta \geq 0\}$ *for* $t \in [0, 1]$,
(vii) $g^T \bar{\theta}_C(t)$ *is strictly increasing in* $t \in [0, 1]$ *if* $\gamma_i \in (0, \pi]$ *and* $\delta_i' > 0$ *for some* $i \in C$,
(viii) $\bar{\theta}_C(1) = \sum_{i \in C} s_i p_{\mathcal{L}'}(v_i) + g \sum_{i \in C} s_i \delta_i'$.

Proof. (i)-(iii) follow from direct calculation and by exploiting the fact that $g, d \in \mathcal{L}'^{\perp}$ are orthonormal vectors. In order to prove (iv), apply the same arguments used in the proofs of Observation 22(ii) and (iii) to $v \in \mathcal{L}'$ and to $v \in \mathcal{L}' + \{\beta g : \beta \geq 0\}$, respectively.

For proving (v), i.e., $\|\theta_i(t) - \theta_k(t)\|^2 \leq \|v_i - v_k\|^2$ for $i, k \in C$, it suffices to show that

$$f_{ik}(t) := \theta_i(t)^T \theta_k(t) \geq v_i^T v_k \overset{\text{(i)}}{=} \theta_i(0)^T \theta_k(0) = f_{ik}(0),$$

or, as $g, d \in \mathcal{L}'^{\perp}$ are orthonormal vectors, that the function

$$f_{ik}(t) = p_{\mathcal{L}'}(v_i)^T p_{\mathcal{L}'}(v_k) + \delta_i' \delta_k' [\cos(\gamma_i - t\gamma_i) \cos(\gamma_k - t\gamma_k) + \sin(\gamma_i - t\gamma_i) \sin(\gamma_k - t\gamma_k)]$$

is nondecreasing in $t \in [0,1]$. By the angle addition formulas and since the cosine is an even function,

$$\cos(\gamma_i - t\gamma_i)\cos(\gamma_k - t\gamma_k) + \sin(\gamma_i - t\gamma_i)\sin(\gamma_k - t\gamma_k) = \cos((1-t)|\gamma_i - \gamma_k|).$$

The right-hand side is nondecreasing and, thus, f_{ik} is nondecreasing.

(vi) and (viii) follow from direct computation and for (vii) it suffices to observe that

$$g^T \bar{\theta}_C(t) = \sum_{i \in C} s_i \delta_i' \cos(\gamma_i - t\gamma_i)$$

is strictly increasing because $\delta_i' \geq 0$ for all $i \in C$ and $\cos(\gamma_i - t\gamma_i)$ is strictly increasing in $t \in [0,1]$ whenever $\gamma_i \in (0, \pi]$. ■

Chapter 4

Structural properties of optimal embeddings

4.1 Separator-Shadow

In this section we will prove a first result on the structure of optimal embeddings. It can be seen as a necessary criterion of optimality. It shows that the structural properties of such embeddings are tightly related to the separator structure of the graph G. This is assumed to be connected throughout the section. In particular let S be a separator of G. That is, $G - S$ consists of $k \geq 2$ nonempty components $C_1, \ldots, C_k$. Let v_i, $i \in N$, be an optimal embedding of (2.8) and suppose that the convex hull $\mathcal{S} := \text{conv}\{v_i : i \in S\}$ of the points corresponding to the nodes of S does not contain the origin. Then all but one component of $G - S$ fulfill the following property: The straight line segment between the origin and each node of the component intersects $\mathcal{S}$.

We may imagine the convex hull of the separator to be a light proof material. It prevents rays from passing through, if we imagine the origin to be a source of light. In this view the result states that the points of all but one component are embedded in the shadow "behind" the convex hull of the separator.

Thus, if all minimal separators are small in size, the Separator-Shadow Theorem suggests that the embedding may be of small dimension or at least that there may exist some small dimensional optimal embedding.

We will formulate this result in an even stronger version for the strictly active subgraph G_w introduced in Definition 18. In case of optimal primal weights w we know from Corollary 10 that G_w is connected if and only if G is connected.

We start with a technical lemma that is central to the proof of the Separator-Shadow Theorem. Given the separator S we consider two subsets C_1 and C_2 of $G - S$. They do not have to be connected itself, i. e. they may contain different components of $G - S$. The only requirement is that there is no edge beween C_1 and C_2 in $G - S$.

Lemma 29 *Given a connected graph $G = (N, E)$ and data $s > 0$, $l > 0$, let the weights $w \geq 0$ and points $v_i \in \mathbb{R}^n$ for $i \in N$ be optimal solutions of* (2.1) *and the embedding problem*

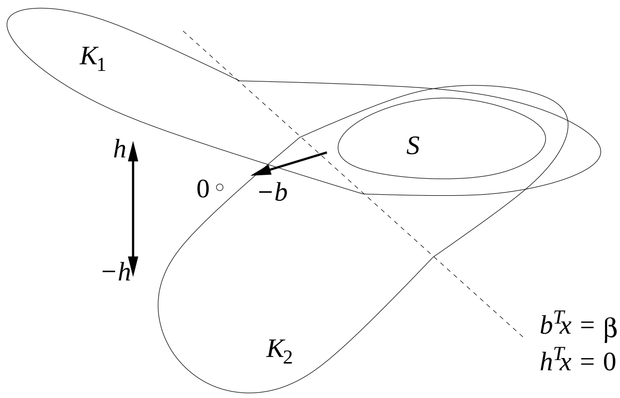

Figure 4.1: Transformation to improve the embedding in Lemma 29, Proof 1.

(2.8), *respectively. Let S be a separator in the strictly active subgraph $G_w = (N, E_w)$ giving rise to a partition $N = S \cup C_1 \cup C_2$ where there is no edge between C_1 and C_2. Suppose there is a normalized $b \in \mathbb{R}^n$ and $\beta > 0$ defining a hyperplane $b^T x = \beta$ within the subspace* $\operatorname{span}\{v_i,\ i \in N\}$ *which separates all points of S from at least one point $\hat{\imath} \in C_1$, namely*

$$b^T v_{\hat{\imath}} \leq \beta < b^T v_i, \text{ for all } i \in S.$$

Then

$$b^T v_i > \beta, \text{ for all } i \in C_2.$$

In words, nodes of at most one component of $G_w - S$ can be separated by such a hyperplane from the points corresponding to S.

We present two independent proofs of this lemma. Actually this leads to two distinct ways of understanding the following Separator-Shadow Theorem. The first proof uses a geometric folding operation that strictly improves solutions that do not satisfy the requirement.

The second proof goes back to the primal side of the framework, the problem of maximizing the second smallest eigenvalue of the Laplacian. It makes use of a result of M. Fiedler. Translated to the dual side it yields the assertion directly.

Proof 1 (illustrated in Figure 4.1). Assume for contradiction that there are nodes in both sets C_1 and C_2 that are separated by the hyperplane $b^T x = \beta$ from the nodes of S. Thus, let for $j \in \{1, 2\}$, $K_j := \{i \in C_j : b^T v_i \leq \beta\} \neq \emptyset$, and $K_3 := N \setminus (K_1 \cup K_2)$. Because $L_d(G, w) = L_d(G_w, w)$ and Theorem 17, the points v_i, $i \in N$, form an optimal embedding of (2.8) for $G_w = (N, E_w)$ with data $s > 0$, $l > 0$, too.

Let $h \in \mathbb{R}^n$, $\|h\| = 1$ be a vector given by Observation 21. Next, consider rotating independently for each $j \in \{1, 2\}$ the points of K_j around the affine subspace

$$\mathcal{B} = \{x \in \mathbb{R}^n : h^T x = 0,\ b^T x = \beta\},$$

as given by (3.2). Because there is no edge between points of K_1 and K_2 and the distances to the remaining points are not increased (see Observation 22) the edge length constraints remain satisfied. We consider the objective of the embedding problem in the form of (2.15). The distances within K_1, K_2 and K_3 remain the same (see Observation 22), thus it suffices to consider the second sum in the cost function of (2.15):

$$\frac{1}{\bar{s}_N}\Bigg(\bar{s}_{K_1}\bar{s}_{K_2}\|\varphi(\bar{v}_{K_1},\delta_1\gamma)-\varphi(\bar{v}_{K_2},\delta_2\gamma)\|^2 \\ +\bar{s}_{K_1}\bar{s}_{K_3}\|\varphi(\bar{v}_{K_1},\delta_1\gamma)-\bar{v}_{K_3}\|^2 \\ +\bar{s}_{K_2}\bar{s}_{K_3}\|\varphi(\bar{v}_{K_2},\delta_2\gamma)-\bar{v}_{K_3}\|^2\Bigg),$$

where we will choose constants $\delta_1 > 0$, $\delta_2 < 0$ so as to ensure that K_1 and K_2 are folded into opposite directions, perhaps at distinct speeds. Let $\mathcal{L} := \operatorname{span}\{b, h\}$. Then there is no movement of points with respect to $\mathcal{L}^\perp$ if γ varies. Thus, we may consider the projection of points onto $\mathcal{L}$:

$$f(\gamma) := \frac{1}{\bar{s}_N}\Bigg(\bar{s}_{K_1}\bar{s}_{K_2}\|p_{\mathcal{L}}(\varphi(\bar{v}_{K_1},\delta_1\gamma)-\varphi(\bar{v}_{K_2},\delta_2\gamma))\|^2 \\ +\bar{s}_{K_1}\bar{s}_{K_3}\|p_{\mathcal{L}}(\varphi(\bar{v}_{K_1},\delta_1\gamma)-\bar{v}_{K_3})\|^2 \\ +\bar{s}_{K_2}\bar{s}_{K_3}\|p_{\mathcal{L}}(\varphi(\bar{v}_{K_2},\delta_2\gamma)-\bar{v}_{K_3})\|^2\Bigg).$$

Note, that $\gamma = 0$ represents the initial setting. In order to finish the proof we will show, that $f(\gamma)$ increases for small $\gamma > 0$.

We may use the law of cosines to express the lenghts. With $r_j := \|\bar{v}_{K_j} - p_{\mathcal{B}}(\bar{v}_{K_j})\|$ for $j = 1, 2, 3$ we have

$$f(\gamma) = \frac{1}{\bar{s}_N}\Bigg(\bar{s}_{K_1}\bar{s}_{K_2}(r_1^2+r_2^2-2r_1r_2\cos((\delta_1-\delta_2)\gamma)) \\ +\bar{s}_{K_1}\bar{s}_{K_3}(r_1^2+r_3^2-2r_1r_3\cos(\pi-\delta_1\gamma)) \\ +\bar{s}_{K_2}\bar{s}_{K_3}(r_2^2+r_3^2-2r_2r_3\cos(\pi+\delta_2\gamma))\Bigg).$$

This gives

$$\begin{aligned} f'(0) &= 0, \\ f''(0) &= \frac{2}{\bar{s}_N}\Big((\delta_1-\delta_2)^2\bar{s}_{K_1}r_1\bar{s}_{K_2}r_2-\delta_1^2\bar{s}_{K_1}r_1\bar{s}_{K_3}r_3-\delta_2^2\bar{s}_{K_2}r_2\bar{s}_{K_3}r_3\Big) \\ &= \frac{2}{\bar{s}_N}\Big(\delta_1^2\bar{s}_{K_1}r_1(\bar{s}_{K_2}r_2-\bar{s}_{K_3}r_3)+\delta_2^2\bar{s}_{K_2}r_2(\bar{s}_{K_1}r_1-\bar{s}_{K_3}r_3)-2\delta_1\delta_2\bar{s}_{K_1}r_1\bar{s}_{K_2}r_2\Big). \end{aligned}$$

Directly from the definition of K_j and $\mathcal{B}$ we conclude

$$\big\langle\bar{v}_{K_j}-p_{\mathcal{B}}(\bar{v}_{K_j}),b\big\rangle = -r_j,\ j=1,2$$

and

$$\langle \bar{v}_{K_3} - p_{\mathcal{B}}(\bar{v}_{K_3}), b \rangle = r_3.$$

Hence, we have

$$-\bar{s}_{K_1} r_1 - \bar{s}_{K_2} r_2 + \bar{s}_{K_3} r_3 = \Bigg\langle \underbrace{\sum_{j=1}^{3} \bar{s}_{K_j} \bar{v}_{K_j}, b}_{=0} \Bigg\rangle - \sum_{j=1}^{3} \bar{s}_{K_j} \underbrace{\langle p_{\mathcal{B}}(\bar{v}_{K_j}), b \rangle}_{=\beta>0}.$$

We get the inequality $\bar{s}_{K_1} r_1 + \bar{s}_{K_2} r_2 > \bar{s}_{K_3} r_3$ and therefore

$$f''(0) > -\frac{2}{\bar{s}_N} (\delta_1 \bar{s}_{K_1} r_1 + \delta_2 \bar{s}_{K_2} r_2)^2.$$

Finally choose δ_1 and δ_2 so that $\delta_1 \bar{s}_{K_1} r_1 + \delta_2 \bar{s}_{K_2} r_2 = 0$ to obtain $f''(0) > 0$. With this choice the objective increases if γ is arbitrarily small. Hence, v_i, $i \in N$ is no optimal embedding of (2.8) for the strictly active subgraph $G_w = (N, E_w)$ with data $s > 0$, $l > 0$. This is a contradiction. ■

Proof 2. From Theorem 17 (choose $z := -b$ and recall that $s_i = \frac{1}{d_i^2}$) we derive that $x := -[\frac{1}{d_1} b^T v_1, \ldots, \frac{1}{d_n} b^T v_n]^T$ is an eigenvector to $\lambda_2(L_d(G_w, w))$. Now we apply Corollary 12 with x and $\alpha := \beta > 0$. Hence, the graph $\tilde{G} = (\tilde{N}, E_w)$ with $\tilde{N} := \{i \in N : b^T v_i \leq \beta\} \ni \{\hat{\imath}\}$ is connected. Since $S \cap \tilde{N} = \emptyset$ the set $\tilde{N}$ cannot contain points of C_2. ■

Now it is possible to prove the Separator-Shadow Theorem. We allow the sets C_1, C_2 and S to be empty, because these cases hold trivially.

Theorem 30 (Separator-Shadow) *Given a connected graph $G = (N, E)$, and data $s > 0$, $l > 0$ let $w \geq 0$ and $v_i \in \mathbb{R}^n$ for $i \in N$ be optimal solutions of* (2.1) *and the embedding problem* (2.8)*, respectively. Let S be a separator in the strictly active subgraph $G_w = (N, E_w)$ giving rise to a partition $N = S \cup C_1 \cup C_2$ where there is no edge between C_1 and C_2. Then, for at least one $j \in \{1, 2\}$:*

$$\operatorname{conv}\{0, v_i\} \cap \operatorname{conv}\{v_s : s \in S\} \neq \emptyset \qquad \forall i \in C_j.$$

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

Proof. If C_1 and C_2 are both nonempty then S is a separator in G. Note that the theorem holds trivially if the origin is contained in the convex hull of the points in S or if one of the sets S, C_1, C_2 is empty (if $S = \emptyset$ then one of C_1 and C_2 must also be empty by the connectedness of G).

Assume, for contradiction, that the theorem is not true. Then, w.l.o.g., there are points v_1, v_2 with $1 \in C_1$, $2 \in C_2$ and $[0, v_1] \cap \mathcal{S} = [0, v_2] \cap \mathcal{S} = \emptyset$ (Note that the set S cannot be empty as C_1 and C_2 are not, and recall $\mathcal{S} = \operatorname{conv}\{v_i : i \in S\}$). By convex separation

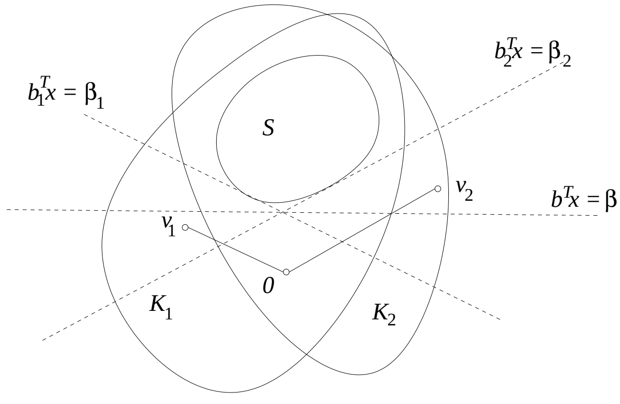

Figure 4.2: Separating hyperplanes of the separator-shadow proof, $K_j := \{v_i : i \in C_j\}$, $j = 1, 2$.

there exist, for $j \in \{1, 2\}$, separating hyperplanes $b_j \in \mathbb{R}^n$ with $\beta_j > 0$ within the subspace spanned by the v_i so that $b_j^T x > \beta_j$ for all $x \in \mathcal{S}$ and $b_j^T x \leq \beta_j$ for all $x \in [0, v_j]$.

Note, there cannot exist $\alpha \in [0, 1]$, $b = \alpha b_1 + (1 - \alpha) b_2$, $\beta = \alpha\beta_1 + (1 - \alpha)\beta_2$ so that $\langle b, v_i \rangle > \beta > 0$ for all $i \in C_1 \cup C_2$, because this hyperplane would separate 0 strictly from $\operatorname{conv}\{v_i : i \in N\}$ and by feasibility of the v_i the origin is a convex combination of the v_i as $\frac{1}{s_N} \sum_{i \in N} s_i v_i = 0$.

Hence, there must exist an $\alpha \in [0, 1]$ so that for $b = \alpha b_1 + (1-\alpha) b_2$, $\beta = \alpha\beta_1 + (1-\alpha)\beta_2$ the halfspace $\mathcal{B}^- = \{x \in \mathcal{H} : b^T x \leq \beta\}$ contains points of both C_1 and C_2. Furthermore $b^T x > \beta$ for all $x \in \mathcal{S}$. (illustrated in Figure 4.2) But this is a contradiction to Lemma 29.
■

In particular, since $E_+ \subseteq E$ we get:

Corollary 31 *Theorem 30 also holds if we replace G_w by G in the assertion.*

4.2 Separators containing the origin

In the case of $0 \in \mathcal{S}$, Theorem 30 is trivially fulfilled and gives no structural information. In this section we will prove two theorems for this kind of separators. These will not formulate necessary conditions for optimal embeddings, but allow to construct optimal embeddings of small dimension.

The idea is as follows: Rotating a point in a plane orthogonal to the subspace $\mathcal{L} := \operatorname{span} \mathcal{S}$ neither changes its distances to points of S nor to $0 \in \mathcal{S}$. Hence, rotating components of $G - S$ in this manner has no influence on the objective value or the length constraints of the embedding problem. We will execute these operations for all components at the same time and coordinate them so that the equilibrium constraint remains valid. Furthermore with those operations distances within each component can only decrease.

The basic operations are explained precisely in Section 3.3. We use the notation introduced there. Let C_j, $j \in M := \{1, \ldots, m\}$ be the components of $G - S$. The first part of the transformation for a fixed $j \in M$ will be the folding given in the Observations 23 and 24. All points of C_j will be rotated arround $\mathcal{L}$ into a direction $b_j \in \mathcal{L}^\perp$. To execute the operation we use an additional dimension $h \in \mathcal{L}^\perp$ according to Observation 21 again. The second part is to collapse the points towards b_j like closing an opened umbrella. This is described in Observations 25 and 26. Both parts concatenated are considered in Observation 27. The resulting continuous transformations $u_i(t)$, $i \in C_j$ parameterized jointly by $t \in [0,1]$ have the property that $u_i(0) = v_i$ and that for $t = 1$ all points $u_i(1)$ lie in the flat halfspace $\mathcal{L} + \{\beta b_j : \beta \geq 0\}$. Furthermore the weighted norm $\delta_j(t) := \bar{s}_{C_j} \|p_{\mathcal{L}^\perp}(\bar{u}_j(t))\|$ of the barycenter $\bar{u}_j(t) := \frac{1}{\bar{s}_{C_j}} \sum_{i \in C_j} s_i u_i(t)$ is monotonically increasing, reaching its maximum in $\delta_j := \bar{s}_{C_j} \|p_{\mathcal{L}^\perp}(\bar{u}_j(1))\| = \sum_{i \in C_j} s_i \|p_{\mathcal{L}^\perp}(v_i)\|$.

If neither norm δ_j dominates the sum of the others, formally, $\delta_{\hat{\jmath}} \leq \sum_{j \in M \setminus \{\hat{\jmath}\}} \delta_j$ for all $\hat{\jmath} \in M$, all operations can be fully executed and the resulting b_j, $j \in M$ can be split up into three linearly dependent directions $d_1, d_2, d_3 \in \mathcal{L}^\perp$. Thus, the dimension of an optimal embedding may be reduced to a value of at most $\dim \mathcal{L} + 2$. This is Theorem 33.

If one component is "heavier" than the others, this means $\delta_{\hat{\jmath}} > \sum_{j \in M \setminus \{\hat{\jmath}\}} \delta_j$ for a $\hat{\jmath} \in M$, then the points of the components C_j, $j \in M \setminus \{\hat{\jmath}\}$ can all be collapsed into the same direction $\bar{b}$. But the transformation for $C_{\hat{\jmath}}$ cannot be fully executed, this means the points remain spread out. This is Theorem 34.

We start with the observation that in the first case appropriate directions d_1, d_2, d_3 exist so as to fulfill the equilibrium constraint.

Observation 32 *Given scalars $\delta_j \geq 0$ for $j \in M = \{1, \ldots, m\}$, $m \geq 2$, so that, for each $\hat{\jmath} \in M$, $\delta_{\hat{\jmath}} \leq \sum_{j \in M \setminus \{\hat{\jmath}\}} \delta_j$, there exist vectors $d_1, d_2, d_3 \in \mathbb{R}^2$ with $\|d_1\| = \|d_2\| = \|d_3\| = 1$ and an assignment $\kappa : M \to \{1, 2, 3\}$ so that $\sum_{j \in M} \delta_j d_{\kappa(j)} = 0$. This also holds if in addition $|\{j \in M : \kappa(j) = 1\}| = 1$ is required.*

Proof. If $|M| = 2$ then $\delta_1 = \delta_2$ and the claim holds for $d_1 = -d_2$ and κ correspondingly. Otherwise let $\hat{\jmath} \in M$ be the smallest number so that $\sum_{j=1}^{\hat{\jmath}-1} \delta_j < \frac{1}{2} \sum_{j \in M} \delta_j \leq \sum_{j=1}^{\hat{\jmath}} \delta_j$, set $\kappa(\hat{\jmath}) = 1$, $\kappa(j) = 2$ for $\hat{\jmath} > j \in M$ and $\kappa(j) = 3$ for $\hat{\jmath} < j \in M$. Set $\bar{\delta}_h := \sum_{j \in M, \kappa(j) = h} \delta_j$, $h \in \{1, 2, 3\}$. Note that $\bar{\delta}_1 \leq \bar{\delta}_2 + \bar{\delta}_3$, $\bar{\delta}_2 \leq \bar{\delta}_1 + \bar{\delta}_3$, $\bar{\delta}_3 \leq \bar{\delta}_1 + \bar{\delta}_2$. Assume, w.l.o.g., that $\bar{\delta}_1 \leq \bar{\delta}_2 \leq \bar{\delta}_3$. Set $d_1(\alpha) := (\cos \alpha, -\sin \alpha)^T$ for $0 \leq \alpha \leq \pi$, $d_2(\alpha) := (\cos \gamma(\alpha), \sin \gamma(\alpha))^T$ where $\gamma(\alpha)$ is defined implicitly by $\bar{\delta}_2 \sin \gamma(\alpha) = \bar{\delta}_1 \sin \alpha$, and $d_3 = (-1, 0)^T$. Then $b(\alpha) := \bar{\delta}_1 d_1(\alpha) + \bar{\delta}_2 d_2(\alpha) + \bar{\delta}_3 d_3$ satisfies $[b(\alpha)]_2 = 0$ for all $0 \leq \alpha \leq \pi$, $[b(0)]_1 \geq 0$ and $[b(\pi)]_1 \leq 0$, so by continuity of $b(\alpha)$ there is an $\hat{\alpha} \in [0, \pi]$ with $b(\hat{\alpha}) = 0$. ∎

Now we can state the result of case one.

Theorem 33 *Given a connected graph $G = (N, E)$ and data $s > 0$, $l > 0$ let $v_i \in \mathbb{R}^n$ for $i \in N$ be an optimal solution of (2.8), and let $S \subseteq N$ with $0 \in \mathcal{S} := \operatorname{conv}\{v_i : i \in S\}$ be a separator in G giving rise to separated sets $C_j \subseteq N$, $j \in M := \{1, \ldots, m\}$. Put $\mathcal{L} := \operatorname{span} \mathcal{S}$ and, for $j \in M$, $\delta_j := \sum_{i \in C_j} s_i \|p_{\mathcal{L}^\perp}(v_i)\|$.*

If $\delta_{\hat{\jmath}} \le \sum_{j\in M\setminus\{\hat{\jmath}\}} \delta_j$ *for all* $\hat{\jmath} \in M$ *then there exist vectors* $d_1, d_2, d_3 \in \mathcal{L}^\perp$, $\|d_1\| = \|d_2\| = \|d_3\| = 1$ *with* $\dim\operatorname{span}\{d_1, d_2, d_3\} \le 2$, $b_j \in \{d_1, d_2, d_3\}$, $j \in M$, *so that the embedding* v_i', $i \in N$, *with*

$$v_i' := \begin{cases} v_i & \text{for } i \in S, \\ p_{\mathcal{L}}(v_i) + \|p_{\mathcal{L}^\perp}(v_i)\| b_j & \text{for } i \in C_j. \end{cases}$$

is also an optimal embedding of (2.8). *Furthermore, such an embedding exists with* $b_j = d_1$ *for at most one* $j \in M$ *and satisfies* $\dim\operatorname{span}\{v_i' : i \in N\} \le \dim\mathcal{L} + 2 \le |S| + 1$.

Proof. Observe that $\dim\mathcal{L} \le |S|-1$ because by $0 \in \mathcal{S}$, the v_i, $i \in S$ are linearly dependent. Choose h and define $\mathcal{H}$ as specified in Observation 21. If $\delta_j = 0$ for all $j \in M$ then the statement holds for $d_1 = d_2 = d_3 = h$ because $v_i' = v_i \in \mathcal{L}$ for $i \in N$. So we may assume $\delta_j > 0$ for at least two $j \in M$. In the case $\dim(\mathcal{H}\cap\mathcal{L}^\perp) = 1$ we must have $|S| = n-2$, $m = 2$, and $|C_1| = |C_2| = 1$, so $b_1 = d_1 = -b_2 = -d_2 = -d_3$ with $d_1 = p_{\mathcal{L}^\perp}(v_i)/\|p_{\mathcal{L}^\perp}(v_i)\|$, $i \in C_1$, satisfies all requirements. It remains to consider the case $\dim(\mathcal{H}\cap\mathcal{L}^\perp) \ge 2$.

By Observation 32 we find three vectors $d_1, d_2, d_3 \in \mathcal{H}\cap\mathcal{L}^\perp$ of norm one and an assignment $\kappa : M \to \{1, 2, 3\}$ satisfying $\sum_{j\in M} \delta_j d_{\kappa(j)} = 0$ and $\{j \in M : \kappa(j) = 1\} = 1$. For $j \in M$ set $b_j = d_{\kappa(j)}$ and let $u_i(t)$, $i \in C_j$, be the transformations of Observation 27 for the respective b_j. Then $v_i' = u_i(1)$ for $i \in C_j$, $j \in M$, by Observation 27(ii). The distance constraints are satisfied for the new embedding because for $\{i, k\} \in E$ either

$i, k \in S$:	$\|v_i' - v_k'\| = \|v_i - v_k\|$ by definition,
$i \in C_j$ for some $j \in M, k \in S$:	$\|v_i' - v_k'\| = \|v_i - v_k\|$ by Observation 27(iv),
$i, k \in C_j$ for some $j \in M$:	$\|v_i' - v_k'\| \le \|v_i - v_k\|$ by Observation 27(v).

The equilibrium constraint is satisfied on $\mathcal{L}$, because $p_{\mathcal{L}}(v_i) = p_{\mathcal{L}}(v_i')$ for all $i \in N$ (by definition for $i \in S$ and by Observation 27(iii) otherwise). It is also satisfied on $\mathcal{L}^\perp$, because

$$\sum_{i\in N} s_i p_{\mathcal{L}^\perp}(v_i') = \sum_{i\in S} s_i \underbrace{p_{\mathcal{L}^\perp}(v_i')}_{=0} + \sum_{j\in M}\sum_{i\in C_j} s_i p_{\mathcal{L}^\perp}(v_i') = \sum_{j\in M}\sum_{i\in C_j} s_i \|p_{\mathcal{L}^\perp}(v_i)\| b_j = \sum_{j\in M} \delta_j d_{\kappa(j)} = 0$$

by construction of the d_j. Finally, the objective value has not changed because $\|v_i\| = \|v_i'\|$ for all $i \in N$ (by definition for $i \in S$ and by Observation 27(iii) otherwise). ■

Now we treat the case of a "heavy" component.

Theorem 34 *Given the setting of Theorem 33 assume that there is a* $\hat{\jmath} \in M$ *with* $\delta_{\hat{\jmath}} > \sum_{j\in M\setminus\{\hat{\jmath}\}} \delta_j$. *There exists an* $h \in \operatorname{span}\{v_i : i \in N\}^\perp$ *and an optimal embedding* v_i', $i \in N$, *of* (2.8) *with*

$$\begin{aligned} & v_i' \in \operatorname{span}\{h, v_i : i \in C_{\hat{\jmath}}\} && \text{for } i \in C_{\hat{\jmath}}, \\ & v_i' = v_i && \text{for } i \in S, \\ & v_i' = p_{\mathcal{L}}(v_i) + \|p_{\mathcal{L}^\perp}(v_i)\|\bar{b} && \text{for } i \in C_j \text{ with } j \in M \setminus \{\hat{\jmath}\}, \end{aligned}$$

where $\bar{b} := -p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}})/\|p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}})\|$ *if* $\bar{v}'_{C_{\hat{\jmath}}} := \sum_{i\in C_{\hat{\jmath}}} s_i v_i' \notin \mathcal{L}$ *and* $\bar{b} := 0$ *otherwise.*

Furthermore, if there is some direction $\hat{b} \in \operatorname{span}\{v_i : i \in C_{\hat{\jmath}}\} \cap \mathcal{L}^\perp \setminus \{0\}$ *with* $\hat{b}^T v_i \ge 0$ *for all* $i \in C_{\hat{\jmath}}$, *then such an embedding exists with* $v_k' \in \operatorname{span}\{v_i : i \in C_{\hat{\jmath}}\}$ *for all* $k \in C_{\hat{\jmath}}$.

Proof. If $\sum_{j\in M\setminus\{\hat{\jmath}\}}\delta_j = 0$ then we may choose $h = \bar{b} = 0$ and not transform the embedding at all to obtain the result. Therefore assume $\sum_{j\in M\setminus\{\hat{\jmath}\}}\delta_j > 0$. Choose h and define $\mathcal{H}$ as specified in Observation 21. Since $\delta_{\hat{\jmath}} > 0$ we can find a $b_{\hat{\jmath}} \in \mathcal{L}^\perp \cap \operatorname{span}\{v_i : i \in C_{\hat{\jmath}}\}$ with $\|b_{\hat{\jmath}}\| = 1$. Let $u_i(t)$, $i \in C_{\hat{\jmath}}$ denote the transformations of Observation 27 for this $b_{\hat{\jmath}}$, set $\bar{u}_{C_{\hat{\jmath}}}(t) := \sum_{i\in C_{\hat{\jmath}}} s_i u_i(t)$. By Observation 27, the function $\|p_{\mathcal{L}^\perp}(\bar{u}_{C_{\hat{\jmath}}}(t))\|$ is continuous and nondecreasing. As the equilibrium constraint is satisfied for the v_i, $i \in N$, we have

$$\begin{aligned}
\|p_{\mathcal{L}^\perp}(\bar{u}_{C_{\hat{\jmath}}}(0))\| &\overset{\text{Obs.27(i)}}{=} \Big\|\sum_{i\in C_{\hat{\jmath}}} s_i p_{\mathcal{L}^\perp}(v_i)\Big\| \overset{\text{equilib.}}{=} \Big\|\sum_{i\in N\setminus C_{\hat{\jmath}}} s_i p_{\mathcal{L}^\perp}(v_i)\Big\| \\
&\overset{p_{\mathcal{L}^\perp}(v_i)=0, i\in S}{=} \Big\|\sum_{j\in M\setminus\{\hat{\jmath}\}}\sum_{i\in C_j} s_i p_{\mathcal{L}^\perp}(v_i)\Big\| \\
&\leq \sum_{j\in M\setminus\{\hat{\jmath}\}}\sum_{i\in C_j} s_i \big\|p_{\mathcal{L}^\perp}(v_i)\big\| \overset{\text{by def.}}{=} \sum_{j\in M\setminus\{\hat{\jmath}\}}\delta_j
\end{aligned}$$

and, by assumption, $\|p_{\mathcal{L}^\perp}(\bar{u}_{C_{\hat{\jmath}}}(1))\| = \delta_{\hat{\jmath}} > \sum_{j\in M\setminus\{\hat{\jmath}\}}\delta_j$. So there is a $\hat{t} \in [0,1]$ with

$$\|p_{\mathcal{L}^\perp}(\bar{u}_{C_{\hat{\jmath}}}(\hat{t}))\| = \sum_{j\in M\setminus\{\hat{\jmath}\}}\delta_j. \tag{4.1}$$

Choose $v'_i = u_i(\hat{t})$ for $i \in C_{\hat{\jmath}}$ and put

$$\bar{v}'_{C_{\hat{\jmath}}} = \sum_{i\in C_{\hat{\jmath}}} s_i v'_i = \bar{u}_{C_{\hat{\jmath}}}(t_{\hat{\jmath}}) \quad \text{and} \quad \bar{b} = -p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}})/\|p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}})\|. \tag{4.2}$$

For $j \in M \setminus \{\hat{\jmath}\}$ choose $b_j = \bar{b}$ and let $u_i(t)$, $i \in C_j$, be the transformations of Observation 27 for the respective b_j. Then, by Observation 27(ii), $v'_i = u_i(1)$ for $i \in C_j$ with $j \in M\setminus\{\hat{\jmath}\}$ satisfies the requirements of the theorem. The equilibrium constraint is satisfied for the embedding v'_i, $i \in N$, because it holds on $\mathcal{L}$ due to $p_{\mathcal{L}}(v_i) = p_{\mathcal{L}}(v'_i)$ for $i \in N$ by Observation 27(iii) and it holds on $\mathcal{L}^\perp$, because

$$\begin{aligned}
\sum_{i\in N} s_i p_{\mathcal{L}^\perp}(v'_i) &= \sum_{i\in S} s_i \underbrace{p_{\mathcal{L}^\perp}(v'_i)}_{=0} + \sum_{i\in C_{\hat{\jmath}}} s_i p_{\mathcal{L}^\perp}(v'_i) + \sum_{j\in M\setminus\{\hat{\jmath}\}}\sum_{i\in C_j} s_i p_{\mathcal{L}^\perp}(v'_i) \\
&\overset{\text{by def.}}{=} p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}}) + \sum_{j\in M\setminus\{\hat{\jmath}\}}\sum_{i\in C_j} s_i \|p_{\mathcal{L}^\perp}(v_i)\|\bar{b} \\
&\overset{(4.2)}{=} \left(\|p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}})\| - \sum_{j\in M\setminus\{\hat{\jmath}\}}\delta_j\right)\frac{p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}})}{\|p_{\mathcal{L}^\perp}(\bar{v}'_{C_{\hat{\jmath}}})\|} \overset{(4.1)}{=} 0.
\end{aligned}$$

Feasibility of v'_i, $i \in N$, with respect to the distance constraints and optimality follows from Observation 27(iv) and (v) as in the proof of Theorem 33.

Finally, suppose $\hat{b}$ exists as described in the statement of the theorem. Then we may choose $b_{\hat{\jmath}} = \frac{\hat{b}}{\|\hat{b}\|}$ and by construction (3.4) of the u_i, $i \in C_{\hat{\jmath}}$, we have $u_i(t) = v_i$ for $t \in [0, \frac{1}{2}]$

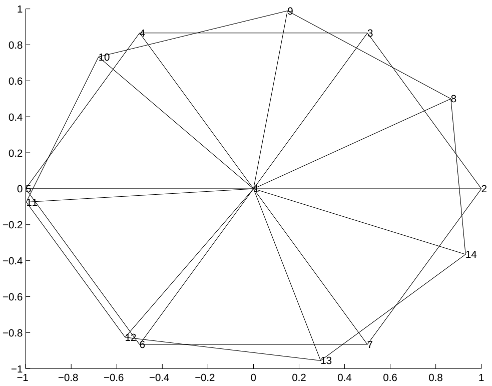

Figure 4.3: Optimal two dimensional embedding of two wheels with identical hub, see Remark 35. The construction of the proof of Theorem 34 would yield a three dimensional embedding.

(see Observation 23 for φ_i) and $u_i(t) \in \mathcal{L} + \operatorname{span}\{\hat{b}, v_i\}$ for $t \in [\frac{1}{2}, 1]$ (see Observation 25 for ψ_i). Thus, there is no need for the vector h of Observation 21. This completes the proof. ■

Remark 35 *A solution corresponding to the modified solution of this theorem is not necessarily an optimal embedding of minimal dimension. Consider, e.g., the graph consisting of two wheels with identical hub and rims of* 6 *and* 7 *nodes,*

$$\begin{aligned} G &= (\{1, \dots, 14\}, \{\{1, k\} : 2 \leq k \leq 14\} \cup E_1 \cup E_2) \text{ with} \\ E_1 &= \{\{2,3\}, \{3,4\}, \{4,5\}, \{5,6\}, \{6,7\}, \{7,2\}\} \text{ and} \\ E_2 &= \{\{8,9\}, \{9,10\}, \{10,11\}, \{11,12\}, \{12,13\}, \{13,14\}, \{14,8\}\}, \end{aligned}$$

together with data $s = e$ and $l = e$. Figure 4.3 shows an optimal two dimensional embedding of this graph. What happens if we execute the transformation given in the proof of Theorem 34? We would stop in the following situation. The node v_1 would stay at the origin. The rim consisting of 6 *nodes would be embedded in* $\operatorname{span}\{\bar{b}\}$ *(with $\bar{b} \neq 0$ as in Theorem 34). The rim consisting of* 7 *nodes would not be fully collapsed. The nodes would lie on a circle in a plane perpendicular to $\bar{b}$. Thus, the transformation would result in a three dimensional embedding.*

A refinement of Theorem 33 will help to obtain the tree-width-bound of section 4.3. As starting point assume that the v_i, $i \in N$ are already embedded in dimension $|S| + 1$ as described in Theorem 33 with each node set C_j lying in some flat halfspace $\mathcal{L} + \{\beta d_{\kappa(j)} : \beta \geq 0\}$. We denote by $D_i := \bigcup_{j \in M : \kappa(j) = i} C_j$ the sets of nodes which are embedded in direction d_i, $i = 1, 2, 3$. Let the embedding be chosen in such a way that $C_j = D_1$ is the only component assigned to direction d_1. In the case that D_1 is not connected to some $\hat{\imath} \in S$ we are able to reduce the bound on the dimension of the embedding to $|S|$ by using the squeezing transformation of Observation 28 separately for each D_i. This can be done simultanuosly so that the equilibrium constraint will not be violated. Figure 4.4 shows this operation projected onto $\mathcal{L}'^{\perp}$ (as defined within Observation 28).

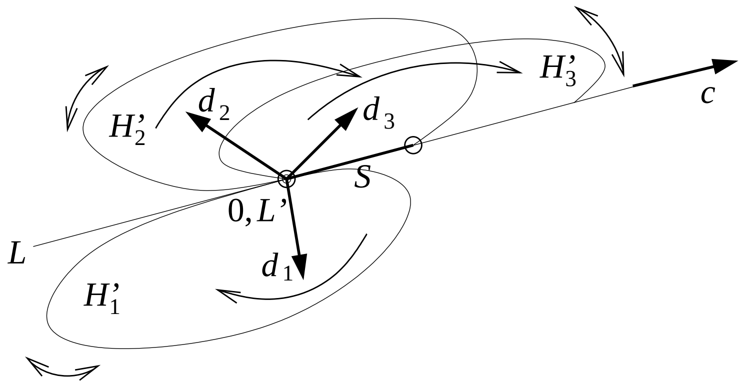

Figure 4.4: Transformation in the proof of Theorem 37.

The next observation will serve to find the correct balancing of the parameters for each D_i in order to guarantee the equilibrium constraint on the subspace spanned by g (as defined within Observation 28) and appropriately chosen d_j.

Observation 36 *Given continuous functions* $\lambda_j : [0,1] \to \mathbb{R}^2$, $j \in \{1,2,3\}$ *and* $\sigma \in \mathbb{R}$ *with*

(i) $[\lambda_1(t)]_1$ *is strictly decreasing,* $[\lambda_2(t)]_1$ *and* $[\lambda_3(t)]_1$ *are strictly increasing,*
(ii) $[\lambda_i(t)]_2 \geq 0$ *for* $t \in [0,1]$ *and* $i = 1,2,3$,
(iii) $[\lambda_1(0)]_1 + [\lambda_2(0)]_1 + [\lambda_3(0)]_1 + \sigma = 0$,
(iv) $[\lambda_i(0)]_2 < [\lambda_j(0)]_2 + [\lambda_k(0)]_2$ *for pairwise distinct* $i,j,k \in \{1,2,3\}$,
(v) $[\lambda_1(1)]_2 = [\lambda_2(1)]_2 = [\lambda_3(1)]_2 = 0$.

There exist $t_1, t_2, t_3 \in [0,1]$ *and pairwise distinct* $\tilde{\imath}, \tilde{\jmath}, \tilde{k} \in \{1,2,3\}$ *satisfying*

(vi) $[\lambda_1(t_1)]_1 + [\lambda_2(t_2)]_1 + [\lambda_3(t_3)]_1 + \sigma = 0$,
(vii) $[\lambda_{\tilde{\imath}}(t_{\tilde{\imath}})]_2 = [\lambda_{\tilde{\jmath}}(t_{\tilde{\jmath}})]_2 + [\lambda_{\tilde{k}}(t_{\tilde{k}})]_2$.

Proof. Due to continuity, the monotonicity property (i), and the initial condition (iii) there exists a continuous nondecreasing function $\tau : [0, \bar{\tau}] \to [0,1]$ defined implicitly via

$$[\lambda_1(t)]_1 + [\lambda_2(\tau(t))]_1 + [\lambda_3(\tau(t))]_1 + \sigma = 0,$$

where

$$\bar{\tau} := \max\{t \in [0,1] : [\lambda_1(t)]_1 + [\lambda_2(t')]_1 + [\lambda_3(t')]_1 + \sigma = 0 \text{ for some } t' \in [0,1]\}.$$

By definition, $(t_1', t_2', t_3') = (\bar{\tau}, \tau(\bar{\tau}), \tau(\bar{\tau}))$ satisfies (vi) and by monotonicity at least one of t_1', t_2', t_3' is equal to one. Then (v) and (ii) imply that there are pairwise distinct $i,j,k \in \{1,2,3\}$ with $[\lambda_i(t_i')]_2 \geq [\lambda_j(t_j')]_2 + [\lambda_k(t_k')]_2$. By the initial condition (iv) and the continuity of the λ_j and τ, there must be a smallest $t_1 \in (0, \bar{\tau}]$ so that $t_2 = t_3 = \tau(t_1)$ satisfy (vi) and (vii). ∎

Now we are ready for proving Theorem 33:

Theorem 37 *Given the setting of Theorem 33 assume that $\delta_{\hat{\jmath}} \le \sum_{j \in M\setminus\{\hat{\jmath}\}} \delta_j$ holds for all $\hat{\jmath} \in M$ and let $\bar{\jmath} \in M$ be the only index with $b_{\bar{\jmath}} = d_1$ within the new embedding of Theorem 33. If at most $|S|-1$ nodes of S are adjacent to nodes in $C_{\bar{\jmath}}$, then there is an optimal embedding of dimension at most $|S|$.*

Proof. Let v_i, $i \in N$ be the optimal embedding resulting from Theorem 33 with normalized vectors $d_1, d_2, d_3 \in \mathcal{L}^\perp$ satisfying $\dim \operatorname{span}\{d_1, d_2, d_3\} \le 2$ and an assignment $\kappa : M \to \{1, 2, 3\}$ with $b_j = d_{\kappa(j)}$ for $j \in M$. Choose $D_k := \bigcup_{j \in M : \kappa(j) = k} C_j$ for $k \in \{1, 2, 3\}$. Then,

$$v_i \in \mathcal{L} + \{\beta d_j : \beta \ge 0\} \quad \text{for } i \in D_j,\ j \in \{1, 2, 3\}. \tag{4.3}$$

Together with $\mathcal{L} = \operatorname{span} \mathcal{S}$ and $0 \in \mathcal{S} = \operatorname{conv}\{v_i : i \in S\}$ the dimension of this embedding is bounded by $\dim \mathcal{L} + \dim \operatorname{span}\{d_1, d_2, d_3\}$ and $\dim \mathcal{L} \le |S| - 1$. If $\dim \mathcal{L} < |S| - 1$ or $\dim \operatorname{span}\{d_1, d_2, d_3\} < 2$ then the statement holds, so we may assume $\dim \mathcal{L} = |S| - 1$ and $\dim \operatorname{span}\{d_1, d_2, d_3\} = 2$. Next suppose there is a $j \in \{1, 2, 3\}$ with $v_i^T d_j = 0$ for all $i \in D_j$, w.l.o.g. assume this to hold for $j = 1$. Then the equilibrium constraint on $\mathcal{L}^\perp$ simplifies to $\sum_{i \in H_2} s_i \|p_{\mathcal{L}^\perp}(v_i)\| d_2 = \sum_{i \in H_3} s_i \|p_{\mathcal{L}^\perp}(v_i)\| d_3$. Thus, the embedding on $\mathcal{L}^\perp$ is restricted to a one dimensional subspace and the dimension of the embedding is again bounded by $|S|$. So it remains to consider the case

$$\text{for each } j \in \{1, 2, 3\}, \quad v_i^T d_j > 0 \text{ for some } i \in D_j. \tag{4.4}$$

By assumption there is a node $\hat{\imath} \in S$ not adjacent to any node in $D_1 = C_{\bar{\jmath}}$. Put $S' := S \setminus \{\hat{\imath}\}$. This set S' separates D_1 from G. We have $0 \in \mathcal{S}' := \operatorname{conv}\{v_i : i \in S'\}$, because otherwise the Separator-Shadow Theorem 30 would imply $v_i \in \mathcal{L}' := \operatorname{span} \mathcal{S}'$ for $i \in D_1$, in contradiction to (4.4). Now $0 \in \mathcal{S}'$ yields $\dim \mathcal{L}' = |S'| - 1$ and as $\dim \mathcal{L} = |S| - 1$ we find a vector $\hat{g}$ with

$$0 \ne \hat{g} = \frac{p_{\mathcal{L}'^\perp}(v_{\hat{\imath}})}{\|p_{\mathcal{L}'^\perp}(v_{\hat{\imath}})\|} \in \mathcal{L} \cap \mathcal{L}'^\perp \quad \text{and} \quad \hat{g}^T v_i = 0 \text{ for all } i \in S'. \tag{4.5}$$

Set $g_1 := -\hat{g}$ and $g_2 := g_3 := \hat{g}$, then by (4.3)

$$\text{for each } j \in \{1, 2, 3\} : \quad v_i \in \{x \in \mathcal{L}' + \operatorname{span}\{d_j, g_j\} : d_j^T x \ge 0\} \text{ for all } i \in D_j.$$

Therefore we may use Observation 28 for $j \in \{1, 2, 3\}$ with $C = D_j$, $d = d_j$, $g = g_j$ to define transformations $\theta_i(t)$ for $i \in D_j$ and $\bar{\theta}_j(t) := \bar{\theta}_{D_j}(t)$. Observe that $\mathcal{S}' \subseteq \mathcal{L}'$ and $\mathcal{S} \subseteq \mathcal{L}' + \{\beta g_j : \beta \ge 0\}$ for $j \in \{2, 3\}$, so Observation 28(iv) and (v) establish that for $j \in \{1, 2, 3\}$ and $t_j \in [0, 1]$ the distance constraints of edges incident to nodes $i \in D_j$ remain satisfied for embedding $\theta_i(t_j)$ and the objective value remains unchanged due to Observation 28(iii) by $0 \in \mathcal{L}'$. Also note, that replacing d_j by some other normalized

$d'_j \in \mathcal{L}^\perp$ will not affect distance constraints but only the equilibrium constraint. So it remains to find appropriate $t_j \in [0,1]$ and normalized $d'_j \in \mathcal{L}^\perp$ so that the equilibrium constraint holds while the dimension of the embedding is reduced by at least one. For this purpose, define for $j \in \{1,2,3\}$ the function $\lambda_j : [0,1] \to \mathbb{R}^2$ by

$$\lambda_j(t) := \begin{pmatrix} \hat{g}^T \bar{\theta}_j(t) \\ d_j^T \bar{\theta}_j(t) \end{pmatrix} \qquad \text{for } t \in [0,1].$$

We show that the λ_j and $\sigma := \hat{g}^T v_{\hat{\imath}}$ satisfy the requirements of Observation 36. Observation 36(i) holds because of Observation 28(vii) and (4.4). Observation 36(ii) follows from Observation 28(vi). Observation 36(iii) is implied by the feasibility of the equilibrium constraint on the linear subspace spanned by $\hat{g}$ for the embedding v_i, $i \in N$; for this, use Observation 28(i), (4.5) and the definition of σ. Suppose Observation 36(iv) does not hold and assume, w.l.o.g., that $\lambda_1(0) \geq \lambda_2(0) + \lambda_3(0)$, then by (4.3) and Observation 28(i) this is equivalent to

$$\sum_{i \in D_1} s_i \|p_{\mathcal{L}^\perp}(v_i)\| \geq \sum_{i \in D_2 \cup D_3} s_i \|p_{\mathcal{L}^\perp}(v_i)\|$$

and together with the equilibrium constraint

$$\sum_{i \in D_1} s_i \|p_{\mathcal{L}^\perp}(v_i)\| d_1 + \sum_{i \in D_2} s_i \|p_{\mathcal{L}^\perp}(v_i)\| d_2 + \sum_{i \in D_3} s_i \|p_{\mathcal{L}^\perp}(v_i)\| d_3 = 0$$

this implies $d_1 = -d_2 = -d_3$ in contradiction to $\dim \operatorname{span}\{d_1, d_2, d_3\} = 2$. Thus, Observation 36(iv) holds. Finally, Observation 36(v) follows from Observation 28(viii). Hence, there exist $t_1, t_2, t_3 \in [0,1]$ and pairwise distinct $\tilde{\imath}, \tilde{\jmath}, \tilde{k} \in \{1,2,3\}$ so that Observation 36(vi) and (vii) hold. Now,

$$\text{choose } \hat{d} \in \mathcal{L}^\perp, \|\hat{d}\| = 1, \quad \text{set } d'_{\tilde{\imath}} := -d'_{\tilde{\jmath}} := -d'_{\tilde{k}} := \hat{d} \tag{4.6}$$

and (use γ_i of Observation 28)

$$v'_i := \begin{cases} v_i & i \in S, \\ p_{\mathcal{L}'}(v_i) + \delta_i[g_j \cos(\gamma_i - t_j\gamma_i) + d'_j \sin(\gamma_i - t_j\gamma_i)] & i \in D_j, j \in \{1,2,3\}. \end{cases}$$

Since only the d_j have been replaced by d'_j, $j \in \{1,2,3\}$, the distance constraints are still valid for the new embedding v'_i, $i \in N$, and the objective value is unchanged. Furthermore, setting

$$\bar{\theta}'_j(t) := \sum_{i \in H_j} s_i (p_{\mathcal{L}'}(v_i) + \delta_i[g_j \cos(\gamma_i - t\gamma_i) + d'_j \sin(\gamma_i - t\gamma_i)]) \quad \text{for } j \in \{1,2,3\},$$

we see that the functions λ_j, $j \in \{1,2,3\}$, also satisfy

$$\lambda_j(t) = \begin{pmatrix} \hat{g}^T \bar{\theta}'_j(t) \\ d_j'^T \bar{\theta}'_j(t) \end{pmatrix} \qquad \text{for } t \in [0,1].$$

Therefore Observation 36(vi) and (vii) still hold for t_1, t_2, t_3 and $\tilde{\imath}, \tilde{\jmath}, \tilde{k}$ yielding

$$\begin{aligned} 0 &= \sigma + \hat{g}^T(\bar{\theta}_1'(t_1) + \bar{\theta}_2'(t_2) + \bar{\theta}_2'(t_2)) = \hat{g}^T(s_{\tilde{\imath}} v_{\tilde{\imath}} + \sum_{j\in\{1,2,3\}} \sum_{i\in D_j} s_i v_i') \overset{(4.5)}{=} \hat{g}^T \sum_{i\in N} s_i v_i' \\ 0 &= d_{\tilde{\imath}}'^T \bar{\theta}_{\tilde{\imath}}'(t_{\tilde{\imath}}) - d_{\tilde{\jmath}}'^T \bar{\theta}_{\tilde{\jmath}}'(t_{\tilde{\jmath}}) - d_{\tilde{k}}'^T \bar{\theta}_{\tilde{k}}'(t_{\tilde{k}}) \overset{(4.6)}{=} \hat{d}^T \sum_{j\in\{1,2,3\}} \sum_{i\in D_j} s_i v_i' \overset{\hat{d}\in\mathcal{L}^\perp}{=} \hat{d}^T \sum_{i\in N} s_i v_i' \end{aligned}$$

So the equilibrium constraint holds on the linear subspaces spanned by $\hat{g}$ and $\hat{d}$. It also holds on $\mathcal{L}'$ because $p_{\mathcal{L}'}(v_i) = p_{\mathcal{L}'}(v_i')$ for $i \in N$ and the embedding v_i was feasible. Since $v_i' \in \mathcal{L}' + \operatorname{span}\{\hat{g}, \hat{d}\} = \mathcal{L} + \operatorname{span}\{\hat{d}\}$ for $i \in N$, the new embedding satisfies the equilibrium constraint on the entire space. Therefore it is an optimal embedding of dimension at most $\dim \mathcal{L} + 1 = |S|$. ■

4.3 The tree-width bound

The two previous sections suggest that there exists a low dimensional optimal embedding if all separators are small in size. Indeed we will prove that there always exists an embedding of dimension tree-width of the graph plus one (see Corollary 46). In order to state this property we first recall the definitions of tree-decomposition and tree-width as given in [11].

Definition 38 *For a graph $G = (N, E)$ a* tree-decomposition *of G is a tree $T := (\mathcal{N}, \mathcal{E})$ with $\mathcal{N} \subseteq 2^N$ and $\mathcal{E} \subseteq \binom{\mathcal{N}}{2}$ satisfying the following requirements:*
(i) $N = \bigcup_{U\in\mathcal{N}} U$.
(ii) For every $e \in E$ there is a $U \in \mathcal{N}$ with $e \subseteq U$.
(iii) If $U_1, U_2, U_3 \in \mathcal{N}$ with U_2 on the $T-$path from U_1 to U_3, then $U_1 \cap U_3 \subseteq U_2$.
The width of T is the number $\max\{|U| - 1 : U \in \mathcal{N}\}$. *The* tree-width $tw(G)$ *is the least width of any tree-decomposition of G.*

For example, trees have tree-width one (each edge forms one set U, so choose $\mathcal{N} = E$ and for $\mathcal{E}$ use the edge set of any spanning tree of the original tree's line graph). It is beneficial to keep this example in mind throughout this section, because it is very convenient to illustrate the proofs in an easy way.

We will show that for any tree-decomposition $T = (\mathcal{N}, \mathcal{E})$ of G there is always an optimal embedding of dimension at most $\max\{|U| : U \in \mathcal{N}\}$. As this also holds for a tree-decomposition giving the tree-width of G, this will prove the bound. Note that in a tree-decomposition any $U \in \mathcal{N}$ and any $U \cap U'$ with $\{U, U'\} \in \mathcal{E}$ is a separator of G (see, *e. g.*, Lemma 12.3.1 in [11]). Hence, we may apply the theorems of Section 4.2 (which implicitly use the results of Section 4.1) to these sets. By successively transforming the optimal embedding v_i, $i \in N$, we will find a separator of the form $U \in \mathcal{N}$ or $U \cap U'$ for some $\{U, U'\} \in \mathcal{E}$ containing 0 in the convex hull of its points so that either Theorem 33 or Theorem 37 yield an optimal embedding of appropriate dimension.

We start by showing that there always exists a node $U \in \mathcal{N}$ that contains the origin in its convex hull:

Observation 39 *Consider a tree-decomposition $T = (\mathcal{N}, \mathcal{E})$ of a connected graph $G = (N, E)$ and an optimal embedding $v_i \in \mathbb{R}^n$, $i \in N$ of* (2.8). *There is a $U \in \mathcal{N}$ with $0 \in \text{conv}\{v_u : u \in U\}$.*

Proof. Consider a subtree $(\mathcal{N}', \mathcal{E}') =: T'$ of T with $|\mathcal{N}'|$ minimal so that $0 \in \text{conv}\{v_i : i \in \bigcup_{U \in \mathcal{N}'} U\}$. Such a tree exists since the condition holds for $T' = T$ by the equilibrium constraint. Let the convex combination giving the origin be described by $C := \bigcup_{U \in \mathcal{N}'} U$ and $\alpha \in \mathbb{R}^C_+$ with $\alpha^T e = 1$ so that $\sum_{i \in C} \alpha_i v_i = 0$. If $|\mathcal{N}'| = 1$, we are done.

Assume, for contradiction, that $|\mathcal{N}'| > 1$. Then there is an edge $\{U, U'\} \in \mathcal{E}'$ and $S' := U \cap U'$ is a separator of G. Deleting edge $\{U, U'\}$ from T' splits T' into two nonempty subtrees $(\mathcal{N}'_j, \mathcal{E}'_j) =: T'_j$ for $j \in \{1, 2\}$ with $0 \notin \text{conv}\{v_i : i \in \bigcup_{U \in \mathcal{N}'_j} U\}$ by assumption. Set $N'_j := \bigcup_{U \in \mathcal{N}'_j} U$. Because $S' \subseteq N'_j$ for $j \in \{1, 2\}$ we obtain $0 \notin \mathcal{S}' := \text{conv}\{v_i : i \in S'\}$. Applying the Separator-Shadow-Theorem 30 with respect to $S = S'$ and $C_j = N'_j \setminus S'$, $j \in \{1, 2\}$ yields, w.l.o.g., $\text{conv}\{v_i, 0\} \cap \mathcal{S}' \neq \emptyset$ for all $i \in C_1 = N'_1 \setminus S'$. But then the origin must be contained in the convex hull of subtree T'_2 as we show next. Put $C'_1 := N'_1 \setminus S'$, $C'_2 := N'_2$ and set, for $j \in \{1, 2\}$, $\bar{\alpha}_j := \sum_{i \in C'_j} \alpha_i$ and $\bar{v}_j := \frac{1}{\bar{\alpha}_j} \sum_{i \in C'_j} \alpha_i v_i \in \text{conv}\{v_i : i \in N'_j\}$. Then $0 = \bar{\alpha}_1 \bar{v}_1 + \bar{\alpha}_2 \bar{v}_2 \in \text{conv}\{\bar{v}_1, \bar{v}_2\}$ (by definition of the α_i) and $\emptyset \neq \mathcal{S}' \cap \text{conv}\{\bar{v}_1, 0\} \subset \text{conv}\{\bar{v}_1, \bar{v}_2\}$ (as the separator-shadow property holds for C'_1), so there is a $p \in \mathcal{S}' \subseteq \text{conv}\{v_i : i \in N'_2\}$ with $0 \in \text{conv}\{p, \bar{v}_2\} \subseteq \text{conv}\{v_i : i \in N'_2\}$, a contradiction to the minimality of $|\mathcal{N}'|$. Hence, T' consists of only one node. ■

We will call a node $U \in \mathcal{N}$ a *zero-node* (with respect to the embedding v_i, $i \in N$) if $0 \in \text{conv}\{v_i : i \in U\}$ and an edge $\{U, U'\} \in \mathcal{E}$ a *zero-edge* (with respect to the embedding v_i, $i \in N$) if $0 \in \text{conv}\{v_i : i \in U \cap U'\}$. Note that for a zero-edge both endpoints are zero-nodes.

Observation 40 *The subgraph $T' := (\mathcal{N}', \mathcal{E}')$ of $T = (\mathcal{N}, \mathcal{E})$ induced by the zero-nodes of an optimal embedding v_i, $i \in N$ of* (2.8) *is a tree and $\mathcal{E}'$ is the set of zero-edges.*

Proof. Suppose that there are two zero-nodes U_1 and U_2 that are not connected in T' or that they are connected in T' by an edge that is not a zero-edge. In both cases there is an edge $\{\bar{U}, \bar{U}'\} \in \mathcal{E}$ inducing a separator $S := \bar{U} \cap \bar{U}'$ in G with $0 \notin \mathcal{S} := \text{conv}\{v_i : i \in S\}$ on the path connecting U_1 and U_2 in T. Deleting edge $\{\bar{U}, \bar{U}'\}$ from T splits T into two nonempty subtrees $T_j := (\mathcal{N}_j, \mathcal{E}_j)$ with $U_j \in \mathcal{N}_j$ for $j \in \{1, 2\}$ so that the node sets $C_j := \bigcup_{U \in \mathcal{N}_j} U \setminus S$ have no common incident edge in G. For S, C_1 and C_2 the Separator-Shadow Theorem 30 implies, w.l.o.g., that $\text{conv}\{v_i, 0\} \cap \mathcal{S} \neq \emptyset$ for all $i \in C_1$. Because $U_1 \subseteq C_1 \cup S$ we obtain $0 \notin \text{conv}\{v_i : i \in U_1\}$, which contradicts the assumption that U_1 is a zero-node. ■

Hence, for a given tree-decomposition $T = (\mathcal{N}, \mathcal{E})$ any optimal embedding induces a *zero-tree* (with respect to the embedding v_i, $i \in N$) consisting of the zero-nodes and zero-edges.

In particular, all zero-nodes and zero-edges are connected in T. This helps to carry out the following algorithmic approach:

We start with a zero-node U and transform the given optimal embedding for $S = U$ as suggested in Theorems 33, 34, 37. In the case that the δ_j, $j \in M$ are balanced, as required in Theorem 33, we will show that the resulting dimension is at most $|U|$, and we are done (this case is treated in Observation 41). Otherwise, we obtain the setting of Theorem 34 where one component $C_{\hat{\jmath}}$ cannot be flattened out fully. It will turn out, that in the zero-tree of the new optimal embedding, U has a unique incident zero-edge $\{U, \widehat{U}\}$ leading to that part of the graph containing $C_{\hat{\jmath}}$ (of course, U remains a zero-node since its embedding does not change in this transformation). This is the content of Observation 42. Now the algorithm will transform the new optimal embedding with respect to the separator $S = U \cap \widehat{U}$. This may again lead to a sufficiently flat optimal embedding (balanced case). If not (unbalanced case), $\widehat{U}$ will be the part that is not yet flat enough. Thus, the algorithm steps from zero-node to zero-node (though the zero-tree may change within the algorithm) getting the situation more and more balanced. This procedure will continue until the algorithm has found a zero-edge which is balanced in some sense. This will finally help to produce a sufficently flat optimal embedding. This is treated by Observation 43.

We start with the case of having found a zero-node which forms a separator yielding the assumptions of Theorem 33. Now, we are able to construct an optimal embedding of the required dimension with the help of this theorem (via the geometrical transformations used within its proof).

Observation 41 *Consider a tree-decomposition $T = (\mathcal{N}, \mathcal{E})$ of a connected graph $G = (N, E)$, an optimal embedding $v_i \in \mathbb{R}^n$, $i \in N$ of (2.8), and a zero-node $S \in \mathcal{N}$ whose deletion splits T into m subtrees $(\mathcal{N}_j, \mathcal{E}_j) =: T_j$ ($j \in M := \{1, \ldots, m\}$). Put*

$$\begin{aligned}
\mathcal{L} &:= \operatorname{span}\{v_i : i \in S\}, \\
C_j &:= \bigcup_{U \in \mathcal{N}_j} U \setminus S, \quad j \in M, \\
\delta_j &:= \sum_{i \in C_j} s_i \|p_{\mathcal{L}^\perp}(v_i)\|, \quad j \in M.
\end{aligned}$$

If $\delta_{\hat{\jmath}} \le \sum_{j \in M \setminus \{\hat{\jmath}\}} \delta_j$ for all $\hat{\jmath} \in M$ then there is an optimal embedding v_i', $i \in N$ of dimension at most $|U'|$ for some $U' \in \{S, U : \{S, U\} \in \mathcal{E}\}$.

Proof. We distinguish two cases. In the first case assume that S has a neighbor U' in T with $|U'| > |S|$ and apply Theorem 33 with respect to S and the C_j, $j \in M$. The resulting optimal embedding v_i' has dimension at most $\dim \mathcal{L} + 2$ and since $\dim \mathcal{L} \le |S| - 1$ ($0 \in \operatorname{conv}\{v_i : i \in S\}$) the dimension is at most $|U'|$.

In the second case all neighbors U of S in T satisfy $|U| \le |S|$. By definition, no two nodes in $\mathcal{N}$ are identical, so each set C_j is separated from S by a subset $S_j := S \cap U_j$ induced by an edge $\{S, U_j\} \in \mathcal{E}$ with $|S_j| < |S|$. Applying Theorem 33 with respect to S and the C_j, $j \in M$ we obtain the corresponding embedding v_i', $i \in N$ with a unique index

$\bar{\jmath} \in M$ satisfying $b_{\bar{\jmath}} = d_1$. Because $S_{\bar{\jmath}} \subset S$ separates S and $C_{\bar{\jmath}}$, at most $|S| - 1$ nodes of S are incident to nodes in $C_{\bar{\jmath}}$. Therefore we may apply Theorem 37 with respect to S, the C_j, $j \in M$ and the embedding v'_i, $i \in N$ and obtain an optimal embedding v''_i, $i \in N$ of dimension at most $|S|$. ∎

If, however, one of the sets is too "big" to be flattened out, we can find a unique edge that leads us towards a more balanced center in the "big" set.

Observation 42 *Given the setting of Observation 41, assume that* $\delta_{\hat{\jmath}} > \sum_{j \in M \setminus \{\hat{\jmath}\}} \delta_j$ *for a* $\hat{\jmath} \in M$. *Let* v'_i, $i \in N$ *be an optimal embedding arising from Theorem 34 for this* S *and the* C_j, $j \in M$. *The (unique) edge* $\{S, \widehat{U}\} \in \mathcal{E}$ *with* $\widehat{U} \in \mathcal{N}_{\hat{\jmath}}$ *is a zero-edge with respect to this new optimal embedding.*

Proof. Since $\delta_{\hat{\jmath}} > 0$, neither the subtree $T_{\hat{\jmath}}$ nor $C_{\hat{\jmath}}$ are empty, so there is an edge $\{S, \widehat{U}\} \in \mathcal{E}$ with $\widehat{U} \in \mathcal{N}_{\hat{\jmath}}$. Suppose, for contradiction, that it is not a zero edge with respect to the embedding v'_i, $i \in N$. Then $S' := S \cap \widehat{U}$ separates G into $C_{\hat{\jmath}}$ and $N \setminus (S' \cup C_{\hat{\jmath}})$. By assumption, $0 \notin \operatorname{conv}\{v_i : i \in S'\}$ and $0 \in \operatorname{conv}\{v_i : i \in S\}$, so the Separator-Shadow Theorem 30 applied with respect to the separator S' implies that $v_i \in \operatorname{cone}\{v_k : k \in S'\} \subseteq \mathcal{L}$ for $i \in C_{\hat{\jmath}}$. But then $\delta_{\hat{\jmath}} = 0$. ∎

$\widehat{U}$ is a zero-node of the embedding v'_i and we could continue with transforming v'_i with respect to $\widehat{U}$ ending up in Observations 41 or 42. But maybe, now the situation with respect to the separator $S' = S \cap \widehat{U}$ gives S as the "big" component in comparison to $\widehat{U}$. Then the algorithm would like to switch back to zero-node S again. If this is the case, however, we can immediately construct an optimal embedding of the required dimension:

Observation 43 *Consider the setting of Observation 42 with* $\{S, \widehat{U}\} \in \mathcal{E}$ *being the zero-edge with respect to embedding* v'_i, $i \in N$ *satisfying* $\widehat{U} \in \mathcal{N}_{\hat{\jmath}}$. *Deleting this edge in* T *splits* T *into two subtrees* $(\mathcal{N}'_j, \mathcal{E}'_j) =: T'_j$ *with* $j \in \{S, \widehat{U}\}$ *so that* $S \in \mathcal{N}'_S$ *and* $\widehat{U} \in \mathcal{N}'_{\widehat{U}}$. *Put*

$$\begin{aligned} S' &:= S \cap \widehat{U}, \\ \mathcal{L}' &:= \operatorname{span}\{v_i : i \in S'\}, \\ C'_j &:= \bigcup_{U \in \mathcal{N}'_j} U \setminus S', \quad j \in \{S, \widehat{U}\}, \\ \delta'_j &:= \sum_{i \in C_j} s_i \|p_{\mathcal{L}'^\perp}(v'_i)\|, \quad j \in \{S, \widehat{U}\}. \end{aligned}$$

If $\delta'_S \geq \delta'_{\widehat{U}}$ *then there is an optimal embedding* v''_i, $i \in N$ *of dimension at most* $|S|$.

Proof. If $\delta'_S = \delta'_{\widehat{U}}$ then Theorem 33 applied to embedding v'_i with respect to S' and C'_j for $j \in \{S, \widehat{U}\}$ yields an optimal embedding

$$v''_i := \begin{cases} v'_i & \text{for } i \in S', \\ p_{\mathcal{L}'}(v_i) + \|p_{\mathcal{L}'^\perp}(v_i)\| b & \text{for } i \in C'_S \\ p_{\mathcal{L}'}(v_i) - \|p_{\mathcal{L}'^\perp}(v_i)\| b & \text{for } i \in C'_{\widehat{U}}. \end{cases}$$

for some normalized $b \in \mathcal{L}'^{\perp}$ and the dimension is bounded by $\dim \mathcal{L}' + 1 \leq |S'| \leq |S|$.

For $\delta'_S > \delta'_{\widehat{U}}$ remember that the v'_i were constructed via Theorem 34. So with the definitions of $\bar{b}$ and the v'_i given there, we have

$$v'_i = p_{\mathcal{L}}(v_i) + \|p_{\mathcal{L}^{\perp}}(v_i)\|\bar{b} \quad \text{for } i \in C'_S = \bigcup_{j \in M \setminus \{\hat{\jmath}\}} C_j \cup S \setminus S'.$$

If $\bar{b} = 0$ then all these v'_i lie in $\mathcal{L}$ and by applying Theorem 34 to v'_i with respect to S' and C'_j for $j \in \{S, \widehat{U}\}$, the space of the new optimal embedding v''_i, $i \in N$, will be $\mathcal{L}$ enlarged by some direction h at most, so its dimension is bounded by $\dim \mathcal{L} + 1 \leq |S|$.

If $\bar{b} \neq 0$, then $p_{\mathcal{L}^{\perp}}(v_i) \neq 0$ for some $i \in C'_S$ and using $\bar{b} \in \mathcal{L}^{\perp}$, $\|\bar{b}\| = 1$, we get

$$\bar{b}^T v'_i = \bar{b}^T p_{\mathcal{L}}(v_i) + \|p_{\mathcal{L}^{\perp}}(v_i)\|\bar{b}^T\bar{b} = \|p_{\mathcal{L}^{\perp}}(v_i)\| \geq 0 \quad \text{for all } i \in C'_S.$$

Since $\mathcal{L}' \subseteq \mathcal{L}$ we obtain $\bar{b} \in \text{span}\,\{v'_i : i \in C'_S\} \cap \mathcal{L}'^{\perp} \setminus \{0\}$ and $\bar{b}^T v'_i \geq 0$ for all $i \in C'_S$. So, with $\hat{b} := \bar{b}$ we are in the special case of Theorem 34. Thus, applying Theorem 34 to v'_i with respect to S' and C'_j for $j \in \{S, \widehat{U}\}$ yields a new optimal embedding v''_i, $i \in N$, with $v''_i \in \text{span}\,\{v'_i : i \in C'_S\} \subseteq \mathcal{L} + \text{span}\,\{\bar{b}\}$ for $i \in C'_S$ and therefore $v''_i \in \mathcal{L} + \text{span}\,\{\bar{b}\}$ for all $i \in N$. The dimension of this new embedding is again bounded by $|S|$. ■

All possible situations with corresponding transformations have now been described. We fit all pieces together:

Algorithm 44
Input: *a connected graph $G = (N, E)$, a tree-decomposition $T = (\mathcal{N}, \mathcal{E})$ of G, an optimal embedding v_i, $i \in N$, of* (2.8).
Step 0: *Set S to a zero-vertex of T with respect to the embedding.*
Step 1: *Using the notation of Observation 41 with respect to S, determine δ_j for $j \in M$.*
Step 2: *If $\delta_{\hat{\jmath}} \leq \sum_{j \in M \setminus \{\hat{\jmath}\}} \delta_j$ for all $\hat{\jmath} \in M$, apply the proof of Observation 41 to find an optimal embedding of dimension at most the width of T plus one and stop.*
Step 3: *Transform, as described in Observation 42, the optimal embedding to v'_i, $i \in N$ and compute the corresponding zero-edge $\{S, \widehat{U}\}$. Determine δ'_S and $\delta'_{\widehat{U}}$ in the notation of Observation 43.*
Step 4: *If $\delta'_S \geq \delta'_{\widehat{U}}$ apply the proof of Observation 43 to find an optimal embedding of dimension at most the width of T plus one and stop.*
Step 5: *Set $S \leftarrow \widehat{U}$, $v_i \leftarrow v'_i$ for $i \in N$ and goto Step 1.*

What remains to be proven is the correctness and finiteness of the algorithm. We will see in the proof of the next theorem that the values δ'_j of Observation 43 do not change if the algorithm turns back in $\widehat{U}$ to cross the same edge again. Hence, the condition $\delta'_S \geq \delta'_{\widehat{U}}$ will be met the second time at the latest. This ensures termination of the algorithm.

Theorem 45 *Let $G = (N, E)$ be a connected graph and $T = (\mathcal{N}, \mathcal{E})$ a tree decomposition of G. Algorithm 44 is correct and stops with an optimal embedding for* (2.8) *of dimension at most width of T plus one in at most $|\mathcal{N}|$ iterations.*

Proof. Step 0 can be carried through by Observation 39.

If in Step 1 the set M is empty ($\mathcal{N} = \{S\}$), then the condition in Step 2 is vacuously satisfied and the transformation of Observation 41 is the identity. But in this case $S = |N|$ and any optimal embedding has dimension at most $|N| - 1$ by Observation 21, so the algorithm stops correctly.

We will prove that the algorithm steps over any edge at most once without stopping and this will yield the iteration bound. Suppose $\{S, \widehat{U}\}$ is the first edge of T to be considered a second time and that the algorithm just stepped from S to $\widehat{U}$ and now considers stepping back to S. Then $\widehat{U}$ transforms, by means of Observation 42 the embedding v_i' that was generated by S via Observation 42. By construction (see Theorem 34), both transformations have $\mathcal{L}' := \operatorname{span}\{v_i' : i \in S \cap \widehat{U}\}$ as an invariant subspace. Therefore the numbers δ_S' and $\delta_{\widehat{U}}'$ of Observation 43 computed in Step 3 have identical values in both cases (but with names interchanged), so the condition of Step 4 is certainly satisfied the second time and the algorithm stops.

The correctness of the statement regarding the dimension of the optimal embedding at termination is a consequence of the respective Observations 41 and 43. ■

Corollary 46 *For each connected graph G there exists an optimal embedding of* (2.8) *of dimension at most $tw(G) + 1$.*

We conclude this section with two examples. First we look at complete graphs. These have unique optimal embeddings, not fulfilling the tree-width bound. Second we will construct graphs with tight tree-width bound. We choose for both examples the data $s = e$ and $l = e$ (with appropriate dimension).

Complete graphs - Unique high dimensional embedding

For $K_n := (\{1, \ldots, n\}, \{\{i,j\} : 1 \le i < j \le n\})$ we show that the unique optimal embedding is the regular $(n-1)$-dimensional simplex with all points lying on the ball of radius $r_n := \sqrt{\frac{n-1}{2n}}$.

The optimal X for (2.4) is given by $X_{ii} = r_n^2 = \frac{n-1}{2n}$ for $1 \le i \le n$, $X_{ij} = X_{ji} = -\frac{r_n^2}{n-1} = -\frac{1}{2n}$ for $1 \le i < j \le n$, and the optimal weights are $w_{ij} = \frac{1}{n}$ for $1 \le i < j \le n$. Choosing $\mu = \frac{1}{n}$ we compute $L_w + \mu ee^T - I = 0$, so (w, μ) is feasible for (2.2) with objective $\frac{n-1}{2}$. Likewise, X is feasible for (2.4) and $\langle I, X \rangle = \frac{n-1}{2}$, so optimality is shown. Furthermore, since $w_{ij} > 0$ for all ij, the constraints $\langle E_{ij}, X \rangle = 1$ hold for all optimal X, i.e., the embedding must have all points pairwise at distance one.

So the regular $n-1$ dimensional simplex is the only optimal embedding. Note that the tree-width of K_n is $n-1$, thus the complete graphs are not tight with respect to the bound of Corollary 46.

Graphs with tight tree-width bound

We append to K_n three independent vertices that are completely linked to K_n resulting in a graph $G(n) := (\{1, \dots, n+3\}, E(n) := \{\{i,j\} : 1 \le i \le n, i < j \le n+3\})$. The tree-width of $G(n)$ is n and for $n \ge 4$ the minimal dimension of an optimal embedding of $G(n)$ is $n+1$.

In fact, we show that, for $n \ge 4$, the vertices of K_n are again arranged as a centrally symmetric $(n-1)$-dimensional simplex with all points lying on a ball of radius $r_n := \sqrt{\frac{n-1}{2n}}$ and the three new points are arranged centrally symmetric on a circle orthogonal to this simplex with radius $\bar{r} := \sqrt{\frac{n+1}{2n}}$.

The optimum of (2.4) is obtained by extending the optimum of the previous example with $X_{ii} = \bar{r}^2 = \frac{n+1}{2n}$ for $n < i \le n+3$, $X_{ij} = X_{ji} = -\frac{\bar{r}^2}{2} = -\frac{n+1}{4n}$ for $n < i < j \le n+3$, and $X_{ij} = X_{ji} = 0$ for $1 \le i \le n$, $n < j \le n+3$. The optimal weights are $w_{ij} = \frac{1}{n}$ for $1 \le i \le n$, $n < j \le n+3$ and $w_{ij} = \frac{1}{n} - \frac{3}{n^2}$ for $1 \le i < j \le n$ (use (2.7) and symmetry). Setting $\mu = \frac{1}{n}$ the slack matrix of (2.2) computes to

$$Z := L(G, w) + \frac{1}{n} ee^T - I = \begin{bmatrix} \frac{3}{n^2} J_n & 0 \\ 0 & \frac{1}{n} J_3 \end{bmatrix} \succeq 0, \qquad (4.7)$$

where J_k denotes the square matrix of all ones of order k. Therefore (w, μ) is feasible for (2.2), the objective value is

$$\sum_{ij \in E(n)} w_{ij} = 3n\frac{1}{n} + \frac{n(n-1)}{2}\left(\frac{1}{n} - \frac{3}{n^2}\right) = 1 + \frac{n}{2} + \frac{3}{2n}.$$

Likewise, X is positive semidefinite because it is a Gram matrix. Furthermore, X satisfies all distance constraints and has the same objective value

$$\langle I, X \rangle = n \cdot \frac{n-1}{2n} + 3 \cdot \frac{n+1}{2n} = 1 + \frac{n}{2} + \frac{3}{2n}.$$

Hence the primal and the dual solution are optimal.

Now take any optimal embedding v_i, $i = 1, \dots, n$, so $V = [v_1, \dots, v_n]$. Since $w > 0$, all optimal embeddings must have all edge lengths equal to one, $\|v_i - v_j\| = 1$ for all $ij \in E(n)$. By (4.7) and semidefinite complementarity it holds that $\langle V^T V, Z \rangle = 0$, thus $\sum_{i=1}^n v_i = 0$ and $\sum_{i=n+1}^{n+3} v_i = 0$. So the embedding of K_n must be centrally symmetric like in the previous example, and by the distance constraints each of the three additional vertices must be embedded orthogonal to the embedding of K_n with distance $\bar{r}$ to the origin. As the three vectors have to sum up to zero, this can only be done in two additional dimensions. This completes the proof.

For $n = 1$ the construction yields a star with one central and three exterior nodes and the bound is also tight. For $n = 2$ the embedding described above is not optimal (it would collapse to the image of the star), for $n = 3$ the embedding is optimal but not of minimal dimension. Without going into details, the cases $n = 2, 3$ can be extended to tight examples by appending to each node of K_n yet another node by a single edge, see Figure 4.5 for an illustration of the resulting embedding for $n = 2$.

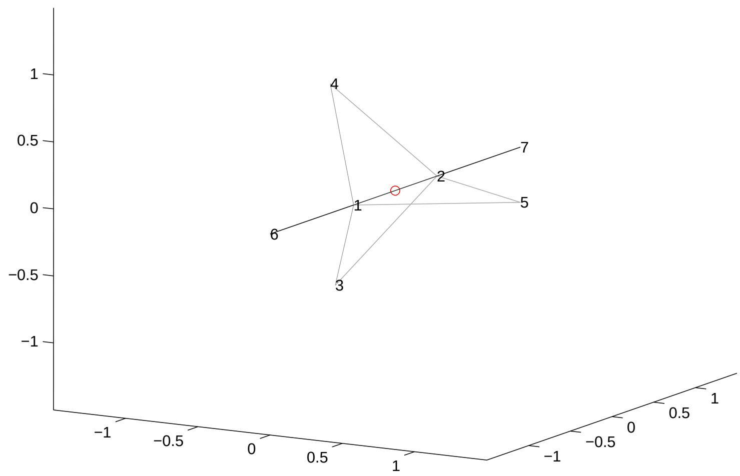

Figure 4.5: A graph with tree-width 2 and optimal embedding of dimension at least three (the central circle indicates the origin).

4.4 Application to trees

The results of this chapter prove especially powerful if we consider trees. The reason is that each node (except leaves) is a separator. The Separator-Shadow Theorem 30 applied to a tree $T = (N, E)$ yields that for each node $i \in N$ with $v_i \neq 0$ all but one of the components of $T - \{i\}$ are embedded in the ray $\{\beta v_i : \beta \geq 0\}$.

So we will succeed in proving major parts of the main theorem of [15] in another way with the tools of the previous sections. We will restrict ourselves to the case $s = e$ and $l = e$, as M. Fiedler did. But the reasoning could be carried out verbatim for arbitrary data $s > 0$, $l > 0$.

We start by recalling some definitions from [15]. Given a tree $T = (N, E)$ a metric space $(\mathcal{X}_T, d)$ can be assigned to it as follows. $\mathcal{X}_T$ consists of all nodes of T as well as of all metric points on the edges understood as copies of the intervall $[0, 1]$. Each point x on the edge ij is uniquely determined by its distances $d(i, x) \geq 0$ and $d(j, x) \geq 0$ from the incident nodes, they satisfy $d(i, x) + d(j, x) = 1$. The distance between any two points $x, y \in \mathcal{X}_T$ is the canonical length of the unique path along the edges of the tree that connects x and y.

Every point $x^* \in \mathcal{X}_T$ for which the function

$$g(x) = \sum_{i \in N} d(x, i)^2$$

attains its minimum is called an *absolute center of gravity* of $\mathcal{X}_T$ with respect to $T = (N, E)$. The number

$$\text{var}(T) := \frac{1}{|E|} \min_{x \in \mathcal{X}_T} g(x)$$

is called *variance* of T. The definitions may be extended to general graphs as well. M. Fiedler points out that for the corresponing definitions for general graphs there may be several absolute centers of gravity, e. g., for a triangle, but that trees induce a unique center of gravity (see Theorem 3.3 of [15]). This can also be observed directly by interpreting $\mathcal{X}_T$ as a convex space. In this sense $g(\cdot)$ is a strictly convex function and has a unique minimizer x^*.

This point can be characterized by a kind of directional derivative. Compare this to sufficient and necessary optimality conditions in convex optimization. We distinguish between two cases.

First, let $x \in \mathcal{X}_T$ coincide with a node $i \in T$. Let $C_1, \ldots, C_m$ be the components of $T - \{i\}$, and denote by $\mathcal{X}_{ij}$ for $j \in M := \{1, \ldots, m\}$ those points of $\mathcal{X}_T$ that belong to the edge $ik \in E$, $k \in C_j$ incident to i and C_j. For each "direction" $j \in M$ denote by $x_j(t) \in \mathcal{X}_{ij}$ for $t \in [0, 1]$ the point with $d(x, x_j(t)) = t$, and by $g_j(t) := g(x_j(t))$ the value of $g(\cdot)$ occuring by stepping from x into direction of j with step length $t \geq 0$. We have for $\hat{\jmath} \in M$:

$$g_{\hat{\jmath}}(t) = \sum_{j \in M \setminus \{\hat{\jmath}\}} \sum_{k \in C_j} (d(x, k) + t)^2 + \sum_{k \in C_{\hat{\jmath}}} (d(x, k) - t)^2.$$

We consider the directional derivative for $t = 0$:

$$\begin{aligned} g'_{\hat{\jmath}}(0, 1) &:= \lim_{t \downarrow 0} \frac{g_{\hat{\jmath}}(t) - g_{\hat{\jmath}}(0)}{t} \\ &= 2 \left(\sum_{j \in M \setminus \{\hat{\jmath}\}} \sum_{k \in C_j} d(x, k) - \sum_{k \in C_{\hat{\jmath}}} d(x, k) \right). \end{aligned}$$

Now, x is a minimizer of $g(\cdot)$ if and only if for all $\hat{\jmath} \in M$ the directional derivative for $t = 0$ satisfies $g'_{\hat{\jmath}}(0, 1) \geq 0$. Thus,

$$\sum_{k \in C_{\hat{\jmath}}} d(x, k) \leq \sum_{j \in M \setminus \{\hat{\jmath}\}} \sum_{k \in C_j} d(x, k), \quad \text{for all } \hat{\jmath} \in M, \tag{4.8}$$

is a sufficient and necessary optimality condition for the unique point solving $\min_{x \in \mathcal{X}_T} g(x)$ in case that it is a node of T.

Second, let x be an inner point of an edge $ij \in E$, thus $d(x, i) > 0$ and $d(x, j) > 0$. Again we define a function $\tilde{g}_x(\cdot)$ which describes the value of $g(\cdot)$ if we move a small step of t away from x. Let $C_i \ni i$ and $C_j \ni j$ be the components of $T - \{ij\}$. For $t \in [-d(x, i), d(x, j)]$ let

$$\tilde{g}_x(t) := \sum_{k \in C_i} (d(x, k) + t)^2 + \sum_{k \in C_j} (d(x, k) - t)^2.$$

This time optimality of x is equivalent to $\tilde{g}'_x(0) = 0$. This leads to

$$\sum_{k \in C_i} d(x, k) = \sum_{k \in C_j} d(x, k) \tag{4.9}$$

as a sufficient and necessary condition for the unique point solving $\min_{x\in\mathcal{X}_T} g(x)$ in case that it is no node of T.

Now, let us turn back to optimal embeddings of $T = (N, E)$ with respect to data $s = e$, $l = e$. Let v_i, $i \in N$ be an optimal embedding of (2.8). Let T_V be the active subgraph of T with respect to v_i, $i \in N$. We know from Observation 19 that it is connected, which implies that $T_V = T$. Hence, each edge of T has a length of 1 in the embedding.

Consider the sets $\mathcal{N} := \{\{i,j\} \subseteq N : ij \in E\}$ and $\mathcal{E} := \{\{U_1, U_2\} \in \binom{\mathcal{N}}{2} : |U_1 \cap U_2| = 1\}$ and choose $\tilde{\mathcal{E}} \subseteq \mathcal{E}$ so that $(\mathcal{N}, \tilde{\mathcal{E}})$ forms a spanning tree of the graph $(\mathcal{N}, \mathcal{E})$. Then $(\mathcal{N}, \tilde{\mathcal{E}})$ gives a tree-decomposition yielding the tree-width $tw(T) = 1$. According to Observation 39 there exists a zero-node $U = \{i, k\} \in \mathcal{N}$ corresponding to an edge $ik \in E$ with $0 \in \operatorname{conv}\{v_i, v_k\}$. Again, we distinguish two cases (which will fit to the cases considered above).

First suppose $v_i = 0$ for some $i \in N$. Let $M \subseteq N$ be the set of all neighbors of i and denote by C_j, $j \in M$ the components of $T - \{i\}$ respectively. Since each edge has a length of 1 we have $v_j \neq 0$ for all $j \in M$ and we may apply the Separator-Shadow Theorem 30 with $S = \{v_j\}$ for all $j \in M$. Proceeding inductively for increasing $d(i, \cdot)$, the embedding of each component C_j is fully determined by v_j, $j \in M$. We obtain for each $r \in C_j$ that $v_r = d(i, r)v_j$. Now fix some $\hat{\jmath} \in M$ and define $\mathcal{L}_{\hat{\jmath}} := \operatorname{span}\{v_{\hat{\jmath}}\}$. The equilibrium constraint yields:

$$\sum_{r\in C_{\hat{\jmath}}} d(i,r) = \left\| \sum_{r\in C_{\hat{\jmath}}} p_{\mathcal{L}_{\hat{\jmath}}}(v_r) \right\| = \left\| \sum_{j\in M\setminus\{\hat{\jmath}\}} \sum_{r\in C_j} (-p_{\mathcal{L}_{\hat{\jmath}}}(v_r)) \right\| \leq \sum_{j\in M\setminus\{\hat{\jmath}\}} \sum_{r\in C_j} d(i,r).$$

This holds for each $\hat{\jmath} \in M$. Hence, condition (4.8) holds for i which therefore is the (unique) absolute center of gravity of $\mathcal{X}_T$.

If there is no i with $v_i = 0$ then there is an edge $ik \in E$ with $0 = v_i + \lambda(v_k - v_i)$ for a $0 < \lambda < 1$. Let $x^0 \in \mathcal{X}_T$ be the point with $d(x^0, i) = \lambda$ and $d(x^0, k) = 1 - \lambda$. Let $C_i \ni i$ and $C_k \ni k$ be the components of $T - \{ik\}$. The Separator-Shadow Theorem 30 inductively, fully determines the embedding: $v_r = d(x^0, r)\frac{v_i}{\|v_i\|}$ for $r \in C_i$ and $v_r = d(x^0, r)\frac{v_k}{\|v_k\|} = -d(x^0, r)\frac{v_i}{\|v_i\|}$ for $r \in C_k$ (we made use of the generalized distance of $\mathcal{X}_T$ since the origin lies on the metric edge ik). The equilibrium constraint with the straight line $\mathcal{L} := \operatorname{span}\{v_i\}$ yields

$$\sum_{r\in C_i} d(x^0,r) = \left\| \sum_{r\in C_i} p_{\mathcal{L}}(v_r) \right\| = \left\| \sum_{r\in C_k} (-p_{\mathcal{L}}(v_r)) \right\| = \sum_{r\in C_k} d(x^0,r).$$

This is (4.9) with $x = x^0$. Thus, x^0 is the (unique) absolute center of gravity of $\mathcal{X}_T$. We summarize:

Observation 47 *Let $T = (N, E)$ be a tree, $\mathcal{X}_T$ the corresponding metric space and v_i, $i \in N$ an optimal embedding of* (2.8) *with data $s = e$ and $l = e$. Then the origin with respect to the embedded nodes and edges marks the position of the unique absolute center of gravity of $\mathcal{X}_T$.*

This implies that we are able to construct an optimal embedding once we know the absolute center of gravity. It determines the position of the origin and allows to make use of the Separator-Shadow Theorem 30 within the branches of the tree as already described. This leads to a major part of the main theorem of [15]. We give a new independent proof.

Theorem 48 (cf. [15], Theorem 4.3) *Let $T = (N, E)$, $|N| \geq 2$ be a tree, let x^* be the absolute center of gravity of $\mathcal{X}_T$. Then, the absolute algebraic connectivity of T is the reciprocal of the variance of T:*

$$\hat{a}(T) = \frac{1}{\mathrm{var}(T)}. \tag{4.10}$$

For each $ij \in E$ let C_{ij} be a component of $T - \{ij\}$ that does not contain x^*. The edge weights $w^* \in \mathbb{R}^E_+$ which solve (1.3) are uniquely determined as follows:

$$w^*_{ij} = \frac{1}{\mathrm{var}(T)} \sum_{k \in C_{ij}} d(x^*, k). \tag{4.11}$$

We consider the two cases concerning whether x^* is a node of T:

1. *x^* is not a node: An eigenvector $y \in \mathbb{R}^N$ of $L(T, w^*)$ corresponding to $\hat{a}(T)$ is obtained as follows: Let $ij \in E$ be the edge containing x^* and C_1, C_2 the components of $T - \{ij\}$. Then $y_k = d(x^*, k)$ for $k \in C_1$ and $y_k = -d(x^*, k)$ for $k \in C_2$.*

2. *x^* is a node $i \in N$: Let m be the degree of i in T. Eigenvectors of $L(T, w^*)$ corresponding to $\hat{a}(T)$ are obtained as follows:*

   Let $C_1, \ldots, C_m$ be the components of $T - \{i\}$. For each $j \in \{1, \ldots, m\}$ let $y^{(j)} = (y^{(j)}_k)_{k \in N}$ be the valuation on N for which $y^{(j)}_k = d(x^*, k)$ if $k \in C_j$ and $y^{(j)}_k = 0$ otherwise. Then every vector $y = (y_k)_{k \in N}$ of the form

   $$y = \sum_{j=1}^{m} \alpha_j y^{(j)}, \tag{4.12}$$

   where $\alpha_1, \ldots, \alpha_m$ are numbers not all equal to zero and so that

   $$\sum_{j=1}^{m} \alpha_j \sum_{k \in N} y^{(j)}_k = 0, \tag{4.13}$$

   is an eigenvector of $L(T, w)$ corresponding to $\hat{a}(T)$.

Proof. Let v_i, $i \in N$ be an optimal embedding of (2.8) with data $s = e$ and $l = e$. As already described above, we know the stucture of the embedding from the Separator-Shadow Theorem 30 and Observation 19 together with Observation 47:

In case of x^* not being a node, the embedding is one dimensional and obtained by identifying span $\{v_i,\, i \in N\}$ with $\mathbb{R}^1$ (up to the sign),

$$v_i = d(x^*, i), \text{ for } i \in C_1 \text{ and } v_i = -d(x^*, i), \text{ for } i \in C_2.$$

In the case that x^* is a node i we see that each component C_j of $T - \{i\}$ is embedded in a halfray and stretched as much as possible:

$$v_k = d(x^*, k)b_j, \text{ for } k \in C_j \text{ and all } j = 1, \ldots, m, \tag{4.14}$$

where $b_j \in \mathbb{R}^n$, $j \in \{1, \ldots, m\}$, are vectors with $\|b_j\| = 1$ so that the equilibrium constraint is fulfilled.

In both cases it is easy to compute the optimal value of the embedding (2.8) which by Theorem 17 equals the optimal value of (2.1):

$$\frac{|E|}{\hat{a}(T)} = \sum_{i \in N} (d(x^*, i))^2 = |E| \cdot \text{var}(T).$$

We have shown (4.10).

To confirm (4.11) we prove the equivalent fact that

$$w_{ij} = \sum_{k \in C_{ij}} d(x^*, k),\ ij \in E, \tag{4.15}$$

is the unique optimizer of (2.1).

This will be done inductively with the help of the force equilibrium conditions (2.11). For an edge $e = ij \in E$ let us define its distance to the absolute center of gravity by

$$d(x^*, e) := \max\{d(x^*, i)\, ,\, d(x^*, j)\}.$$

Note, that in the case that e does not contain x^*, the node of e which belongs to C_{ij} (unique in this case) yields this maximum.

We number the edges of T so that the distance to the absolute center of gravity is nonincreasing, i. e. $E = \{e_1, \ldots, e_{|E|}\}$ and $d(x^*, e_r) \geq d(x^*, e_t)$ for $1 \leq r < t \leq |E|$. We proceed the induction on increasing $1 \leq r \leq |E|$. Note, that the following reasoning for an edge $ij = e_r$, $1 \leq r \leq |E|$ holds for the case that x^* lies on ij as well as for the case that x^* does not lie on ij. We will not distinguish both cases, as the formulas remain the same.

Consider $ij = e_1$ with node i satisfying $d(x^*, i) = d(x^*, e_1) \geq d(x^*, j)$. Then i is a leaf and (2.11) evaluated at i reads:

$$v_i = w_{ij}(v_i - v_j) = w_{ij} \frac{v_i}{\|v_i\|}. \tag{4.16}$$

This yields

$$w_{ij} = \|v_i\| = d(x^*, i),$$

which is (4.15) in this case.

Now, consider an edge $e_t \in E$ with $1 < t \leq |E|$ and let (4.15) be already proven for all edges $e_r \in E$ with $r < t$.

For $ij = e_t$ let, w.l.o.g., the node $i \in N$ belong to C_{ij}. In the case that i is a leaf we may again use (4.16) to obtain (4.15). Otherwise let $k_1, \dots, k_m$ be all neighbors of i within C_{ij}. Then every edge $e_q \in \{ik_1, \dots, ik_m\}$ fulfills (4.15) due to $q < t$ as well as

$$v_i - v_{k_q} = -\frac{v_i}{\|v_i\|}.$$

Then we have (using the force equilibrium (2.11) at i):

$$v_i = w_{ij}(v_i - v_j) + \sum_{q=1}^{m} w_{ik_q}(v_i - v_{k_q}) = \left(w_{ij} - \sum_{q=1}^{m} w_{ik_q} \right) \frac{v_i}{\|v_i\|}.$$

This yields

$$w_{ij} = \|v_i\| + \sum_{q=1}^{m} w_{ik_q} = d(x^*, i) + \sum_{q=1}^{m} \sum_{t \in C_{ik_q}} d(x^*, t) = \sum_{k \in C_{ij}} d(x^*, k).$$

Finally we will validate the given eigenvectors. We know from Theorem 17 that for arbitrary $z \in \mathbb{R}^n \setminus \{0\}$ the vector $y := [z^T v_1, \dots, z^T v_n]^T$ forms an eigenvector to the second smallest eigenvalue of the optimal Laplacian. In case that x^* is not a node, we will choose an appropriate vector z to obtain that the so constructed y has the desired structure. In case that x^* is a node, we will again choose an appropriate vector z to obtain an eigenvector y that has the given structure. With the help of y, we will show that all vectors of the given structure are eigenvectors, indeed.

Let x^* not be a node. We choose $z = \frac{v_k}{\|v_k\|}$ for a $k \in C_1$. Then y has the desired form.

Now let x^* be a node, say w.l.o.g. $x^* = 1$. We can choose $z \in \mathbb{R}^n \setminus \{0\}$ such that $\alpha_j := z^T b_j \neq 0$ for all $j = 1, \dots, m$. Taking equation (4.14) into account we obtain that y has the form given in (4.12). Since y is an eigenvector to the second smallest eigenvalue of the optimal Laplacian it is perpendicular to its null space, in particular $e^T y = 0$. But this is equivalent to (4.13). Hence we have constructed an eigenvector of the given structure. To show that all vectors of this structure are eigenvectors we use the block structure of $L(T, w^*)$: Let $k_1, \dots, k_m \in N$ be the neighbours of 1. By L_i, $i \in \{1, \dots, m\}$ we denote the optimal Laplacian block of all nodes belonging to the branch C_{1k_i}. Then we may order the nodes such that

$$
L(T, w^*) = \left[\begin{array}{c|c|c|c|c}
\sum_{i=1}^m w^*_{1k_i} & -w^*_{1k_1} 0 \dots 0 & -w^*_{1k_2} 0 \dots 0 & \cdots & -w^*_{1k_m} 0 \dots 0 \\ \hline
\begin{matrix} -w^*_{1k_1} \\ 0 \\ \vdots \\ 0 \end{matrix} & L_1 & 0 & \cdots & 0 \\ \hline
\begin{matrix} -w^*_{2k_1} \\ 0 \\ \vdots \\ 0 \end{matrix} & 0 & L_2 & \cdots & 0 \\ \hline
\vdots & \vdots & \vdots & \ddots & \\ \hline
\begin{matrix} -w^*_{2k_m} \\ 0 \\ \vdots \\ 0 \end{matrix} & 0 & 0 & & L_m
\end{array}\right]
$$

gives the block structure of the optimal Laplacian. Let $\hat{y} = \sum_{j=1}^m \beta_j y^{(j)}$ be a vector of the form given by (4.12) and (4.13). Note that $\hat{y}_1 = 0$ and therefore the first column of $L(T, w^*)$ does not play any role in the following. Since $L(T, w^*)y = \hat{a}(T)y$ we have $L_i y^{(i)} = \hat{a}(T)y^{(i)}$, for all $i = 1, \dots, m$, due to the block structure. With $\hat{y}^{(i)} = \frac{\beta_i}{\alpha_i} y_i$ we obtain that $\hat{y}$ also fulfills these eigenvalue equations. Thus, we have verified $L(T, w^*)\hat{y} = \hat{a}(T)\hat{y}$ up to the first row. The first row of $L(T, w^*)\hat{y}$ reads:

$$
-\sum_{j=1}^m w^*_{1k_j} \beta_j \underbrace{y^{(j)}_{k_j}}_{=d(x^*, k_j)=1} \overset{(4.11)}{=} -\frac{1}{\text{var}(T)} \sum_{j=1}^m \beta_j \sum_{k \in C_{1k_j}} \underbrace{d(x^*, k)}_{=y^{(j)}_k} \overset{(4.13)}{=} 0 = \hat{a}(T)\hat{y}_1.
$$

Hence, $\hat{y}$ is an eigenvector of the optimal Laplacian $L(T, w^*)$. ■

In [15] M. Fiedler has not only shown that the vectors given in the two cases of Theorem 48 are eigenvectors of the optimal Laplacian, but that all eigenvectors of the optimal Laplacian have these structures respectively. We conjecture, that this may also be proven with help of the tools used in this section.

Theorem 49 (cf. [15], Theorem 4.3) *Given the setting of Theorem 48, there holds:*

1. *x^* is not a node: Then $\hat{a}(T)$ is a simple eigenvalue of $L(T, w)$. The eigenvector $y \in \mathbb{R}^N$ of $L(T, w)$ corresponding to $\hat{a}(T)$ is obtained as follows (up to a scalar multiple): Let $ij \in E$ be the edge containing x^* and C_1, C_2 the components of $T - \{ij\}$. Then $y_k = d(x^*, k)$ for $k \in C_1$ and $y_k = -d(x^*, k)$ for $k \in C_2$.*

2. *x^* is a node $i \in N$: Let m be the degree of i in T. Unless $|N| = 1$ we have always $m \geq 2$. The multiplicity of $\hat{a}(T)$ as eigenvalue of $L(T, w)$ is then $m - 1$ and the linear*

space containing all the eigenvectors of $L(T, w)$ *corresponding to* $\hat{a}(T)$ *is obtained as follows:*

Let $C_1, \ldots, C_m$ *be the components of* $T - \{i\}$*. For each* $j \in \{1, \ldots, m\}$ *let* $y^{(j)} = (y_k^{(j)})_{k \in N}$ *be the valuation on* N *for which* $y_k^{(j)} = d(x^*, k)$ *if* $k \in C_j$ *and* $y_k^{(j)} = 0$ *otherwise. Then every vector* $y = (y_k)_{k \in N}$ *of the form* (4.12) *where* $\alpha_1, \ldots, \alpha_m$ *are numbers not all equal to zero and so that* (4.13) *is fulfilled is an eigenvector of* $L(T, w)$ *corresponding to* $\hat{a}(T)$*.*

Chapter 5

The Rotational Dimension of a graph

In the previous chapter we have seen that the structure of optimal embeddings of (2.8) is closely linked to the separator structure of the underlying graph. If one looks for a low dimensional embedding, the dimension will depend on the size of the separator which contains the origin in the convex hull.

Arbitrary choices of the data s and l allow to get different separators to contain the origin. This motivates the introduction of the rotational dimension as graph invariant measuring the complexity in the respective convex hull.

The contents of Sections 5.1 and 5.2 follow [20] almost verbatim. Section 5.3 compares the rotational dimension of a graph with the Colin de Verdière number of that graph, another interesting graph property.

5.1 Definition and basic properties

Definition 50 *For a connected graph $G = (N, E)$, the* rotational dimension *of G with respect to node weights $s \in \mathbb{R}^N_+$ and edge lengths $l \in \mathbb{R}^E_+$ is*

$$\operatorname{rotdim}_G(s, l) := \min\{\dim \operatorname{span}\{v_i,\ i \in N\} : v_i,\ i \in N,\ \textit{is an optimal solution of}\ (2.8)\}.$$

(by convention, $\dim \emptyset := -1$*) and the* rotational dimension of a connected graph G *is*

$$\operatorname{rotdim}(G) := \max\{\operatorname{rotdim}_G(s, l) : s \in \mathbb{Z}^N_+,\ l \in \mathbb{Z}^E_+\}.$$

For a graph consisting of several connected components the rotational dimension of G *is*

$$\operatorname{rotdim}(G) := \max\{\operatorname{rotdim}(C) : C\ \textit{is a connected component of}\ G\}.$$

*A graph G is called d-*embeddable*, if* $\operatorname{rotdim}(G) \le d$*, i.e., for any data $s \in \mathbb{Z}^N_+$, $l \in \mathbb{Z}^E_+$ all components of G have an optimal d-dimensional embedding.*

Note that we allow entries of the data s respectively l to be zero. The embedding problem (2.8) is properly defined, even though the primal optimization problem (2.1) might not be meaningful. The zeros will help to get rid of nodes ($s_i = 0$) or to contract edges ($l_{ij} = 0$) in order to reflect minor operations (see Observation 51).

Furthermore, the data is reduced to integral values in the definition of the rotational dimension. We will see (Observation 53) that there is no difference to a definition with continuous data.

Now, let us work out the important fact, that the rotational dimension of a graph is closed under minor operations:

Observation 51 *d-embeddability is a minor monotone graph property.*

Proof. By definition every minor of a graph can be obtained by consecutive application of the following three operations: contraction of an edge, deletion of an edge, deletion of an isolated node. At this we delete loops or multiple edges whenever they appear. It suffices to show that these operations preserve d-embeddability. This is clear for the deletion of an isolated node, because we just loose one component.

So, let us consider the edge operations. Let $G = (N, E)$ and $\hat{G} = (\hat{N}, \hat{E})$ be graphs, where G arises from $\hat{G}$ by execution of an edge operation. We show $\text{rotdim}(G) \leq \text{rotdim}(\hat{G})$. Let $s \in \mathbb{Z}_+^N$, $l \in \mathbb{Z}_+^E$ be data for the embedding problem (2.8) for G. Our strategy is to express this as an embedding problem (2.8) for $\hat{G}$ by appropriate choice of the data $\hat{s} \in \mathbb{Z}_+^{\hat{N}}$, $\hat{l} \in \mathbb{Z}_+^{\hat{E}}$. It suffices to do this for the component of $\hat{G}$ where the operation takes place. So, w.l.o.g. let $\hat{G}$ be connected.

- Deletion of an edge. We number the nodes of G and $\hat{G}$ in the same way, and such that the considered edge of $\hat{G}$ is $\{1, 2\}$. We set $\hat{l}_e := l_e$ for all $e \in E$, and $\hat{l}_{12} := \sum_{e \in E} l_e + 1$.

  If G is also connected we set $\hat{s} := s$. The edge $\{1, 2\}$ can adopt every possible length with respect to the other edges, and therefore its length restriction is not relevant. With these data every optimal solution of (2.8) for $\hat{G}$ is also an optimal solution of (2.8) for G and vice versa. We have $\text{rotdim}_G(s, l) = \text{rotdim}_{\hat{G}}(\hat{s}, \hat{l})$.

  If G is split into two components C_1, C_2 with $\text{rotdim}(G) = \text{rotdim}(C_1) \geq \text{rotdim}(C_2)$, then we set $\hat{s}_i := s_i$, $i \in C_1$, and $\hat{s}_i := 0$, $i \in C_2$. Now, every optimal solution of (2.8) for $\hat{G}$ is also an optimal solution of (2.8) for C_1 and vice versa. We have $\text{rotdim}_{C_1}(s, l) = \text{rotdim}_{\hat{G}}(\hat{s}, \hat{l})$.

- Contraction of an edge. We number the nodes of G and $\hat{G}$ in the same way, and such that the considered edge of $\hat{G}$ is $\{1, 2\}$. We denote the arising node of G by 0. We set the node weights to $\hat{s}_1 := s_0$, $\hat{s}_2 := 0$, $\hat{s}_i := s_i$, $i \in N \setminus \{0\}$ and the edge lengths to $\hat{l}_{12} := 0$, $\hat{l}_{1i} := l_{0i}$, $1i \in \hat{E}$, $\hat{l}_{2i} := l_{0i}$, $2i \in \hat{E}$. Thus, the edge $\{1, 2\} \in \hat{G}$ behaves like the node $0 \in G$. Again, every optimal solution of (2.8) for $\hat{G}$ is also an optimal solution of (2.8) for G and vice versa and we have $\text{rotdim}_G(s, l) = \text{rotdim}_{\hat{G}}(\hat{s}, \hat{l})$.

Doing this for all possible data $s \in \mathbb{Z}_+^N$, $l \in \mathbb{Z}_+^E$ we get $\text{rotdim}(G) \leq \text{rotdim}(\hat{G})$. ■

It is possible to define $\text{rotdim}_G(s, l)$ and $\text{rotdim}(G)$ in the same way for data $s \geq 0$, $l \geq 0$. The then occuring graph property of d-dimensional embeddability is also minor monotone since the proof of Observation 51 does not make use of the fact that the entries of s and l are integral. One could ask whether there is a connection between the two graph properties. There is, they are the same. Before we will prove this, we state that the embedding problem (2.8) is invariant under orthogonal transformations, which is geometrically evident.

Lemma 52 *Given a connected graph $G = (N, E)$ with data $s \in \mathbb{Z}_+^N$, $l \in \mathbb{Z}_+^E$ for the embedding problem* (2.8)*, let $Q \in \mathbb{R}^{N\times N}$ be an orthogonal matrix. The embedding problem* (2.8) *is equivalent to the problem*

$$\begin{array}{ll} \text{maximize} & \sum_{i\in N} s_i \|Qv_i\|^2, \\ \text{subject to} & \sum_{i\in N} s_i Q v_i = 0, \\ & \|Qv_i - Qv_j\| \le l_{ij} \qquad \textit{for } ij \in E, \\ & v_i \in \mathbb{R}^n \textit{ for } i \in N. \end{array}$$

Proof. Let $v_i \in \mathbb{R}^N, i \in N$ be a feasible solution of the embedding problem (2.8). Then v_i, $i \in N$ is also feasible for the orthogonally transformed problem and has the same objective value:

$$\sum_{i\in N} s_i Q v_i = Q \sum_{i\in N} s_i v_i = 0,$$

$$\begin{aligned} \|Qv_i - Qv_j\|^2 &= (v_i - v_j)^T Q^T Q (v_i - v_j) \\ &= (v_i - v_j)^T (v_i - v_j) \\ &\le l_{ij}^2, \end{aligned}$$

$$\sum_{i\in N} s_i \|Qv_i\|^2 = \sum_{i\in N} s_i v_i^T Q^T Q v_i = \sum_{i\in N} s_i \|v_i\|^2.$$

Since we can swap the roles of both problems using the transformation matrix Q^T, the proof is complete. ■

Observation 53 *Let $G = (N, E)$ be a connected graph. Then*

$$\operatorname{rotdim}(G) = \max\{\operatorname{rotdim}_G(s, l) : s \ge 0,\ l \ge 0\}.$$

Proof. Let $s \in \mathbb{Q}_+^N$, $l \in \mathbb{Q}_+^E$. Let $\alpha \in \mathbb{Z}$ be a common denominator of the entries of s and $\beta \in \mathbb{Z}$ be a common denominator of the entries of l. Then the embedding problem (2.8) with data $s \in \mathbb{Q}_+^N$, $l \in \mathbb{Q}_+^E$ is equivalent to the embedding problem (2.8) with data $\hat{s} := \alpha s \in \mathbb{Z}_+^N$, $\hat{l} := \beta l \in \mathbb{Z}_+^E$. Hence, the assertion holds for fractional s and l.

Let $(s^k)_{k\ge1}$ and $(l^k)_{k\ge1}$ be sequences of data with $s^k > 0$, $l^k > 0$, $k \ge 1$, and $s^k \to s$, $l^k \to l$, $k \to \infty$. Let $\operatorname{rotdim}_G(s^k, l^k) \le d$ for all $k \ge 1$. We will show that also $\operatorname{rotdim}_G(s, l) \le d$, which eventually will complete the proof. We denote by (P^k) the embedding problems (2.8) for G with data s^k, l^k and by (P) the embedding problem (2.8) for G with data s, l. For $k \ge 1$ let v_i^k, $i \in N$ be an optimal solution of dimension at most d. According to Lemma 52 we can consider all v_i^k, $i \in N$, $k \ge 1$ to lie in the same affine subspace $\mathcal{L} \subset \mathbb{R}^N$ with $\dim \mathcal{L} = d$. Since the sequence $(l^k)_{k\ge1}$ converges, it is certainly bounded. That yields that the sequences $(v_i^k)_{k\geq 1}$ are bounded for all $i \in N$. Hence, we can find for all $i \in N$ compact balls $B_i \subseteq \mathcal{L}$ with $v_i^k \in B_i$ for all $k \geq 1$. Therefore, every sequence $(v_i^k)_{k\geq 1}$ has a cluster point $v_i \in \mathcal{L}$. W.l.o.g. let $v_i^k \to v_i$, $k \to \infty$ for all $i \in N$. (Go to a subsequence k_l of k such that $v_1^{k_l} \to v_1$, $k \to \infty$ and use the same argumentation to get $v_2^{k_l}$ converging and so on.) We will show that v_i, $i \in N$ is an optimal solution of (P). Let $\hat{v}_i$, $i \in N$ be an arbitrary optimal solution of (P). Let $k \geq 1$ be fixed. For $i \in N$ we set $\alpha_i^k := s_i/s_i^k$ and for $ij \in E$ we set

$$\beta_{ij}^k := \begin{cases} l_{ij}^k/(l_{ij} + |1-\alpha_i^k|\|\hat{v}_i\| + |1-\alpha_j^k|\|\hat{v}_j\|),\ l_{ij} > 0, \\ 1,\ l_{ij} = 0. \end{cases}$$

With $\beta^k := \min_{ij\in E} \beta_{ij}^k$ we define $\hat{v}_i^k := \alpha_i^k \beta^k \hat{v}_i$, $i \in N$. This is a feasible solution of (P^k):

$$\sum_{i\in N} s_i^k \hat{v}_i^k = \beta^k(\sum_{i\in N} s_i \hat{v}_i) = 0,$$

$$\begin{aligned} \|\hat{v}_i^k - \hat{v}_j^k\| &\leq \beta^k(\|\hat{v}_i - \hat{v}_j\| + \|\alpha_i^k \hat{v}_i - \hat{v}_i\| + \|\hat{v}_j - \alpha_j^k \hat{v}_j\|) \\ &\leq l_{ij}^k \beta^k (l_{ij} + |1-\alpha_i^k|\|\hat{v}_i\| + |1-\alpha_j^k|\|\hat{v}_j\|)/l_{ij}^k \\ &\leq l_{ij}^k. \end{aligned}$$

Because of the optimality of v_i^k, $i \in N$ for (P^k) we obtain

$$\sum_{i\in N} s_i^k \|v_i^k\|^2 \geq \sum_{i\in N} s_i^k \|\hat{v}_i^k\|^2 = \sum_{i\in N} \alpha_i^k (\beta^k)^2 s_i \|\hat{v}_i\|^2.$$

Using the continuity of the objective function and $\alpha_i^k \to 1$, $k \to \infty$ for all $i \in N$, $\beta^k \to 1$, $k \to \infty$ we get for $k \to \infty$:

$$\sum_{i\in N} s_i \|v_i\|^2 \geq \sum_{i\in N} s_i \|\hat{v}_i\|^2.$$

Hence, v_i, $i \in N$ is an optimal solution of (P). ■

Directly from the limit consideration of the previous proof follows:

Corollary 54 *Let $G = (N, E)$ be a connected graph, let S be a dense subset of $\mathbb{R}_+^N$, and let L be a dense subset of $\mathbb{R}_+^E$. Then*

$$\text{rotdim}(G) = \max\{\text{rotdim}_G(s, l) : s \in S,\ l \in L\}.$$

Consequently, it does not matter whether we consider rotdim(G) for data $s \in \mathbb{Z}_+^N$, $l \in \mathbb{Z}_+^E$, or for data $s \geq 0$, $l \geq 0$, or for data $s > 0$, $l > 0$.

5.2 Characterization of graphs with small rotational dimension

In this section we will verify the following:

Theorem 55 *For a graph $G = (N, E)$ holds:*

- $\text{rotdim}(G) = 0 \Leftrightarrow$ *G has no edges.*
- $\text{rotdim}(G) \leq 1 \Leftrightarrow$ *G is a disjoint union of paths.*
- $\text{rotdim}(G) \leq 2 \Leftrightarrow$ *G is outerplanar.*

As shown, the d-embeddability is a minor monotone graph property. Thus, we can use Theorem 2 to characterize all graphs, that are d-embeddable. The proof of Theorem 55 splits into two parts and will be given by the next observations. First we want to show that 0-embeddable graphs have no edges, 1-embeddable graphs consist of paths, and 2-embeddable graphs are outerplanar. This can be done by showing, that the forbidden minors of these classes of graphs do not fit into the corresponding rotational dimension.

Observation 56

(i) $\text{rotdim}(K_n) = n - 1$ *for* $n \geq 1$*,*

(ii) $\text{rotdim}(K_{1,3}) = 2$*,*

(iii) $\text{rotdim}(K_{2,3}) = 3$.

Proof. W.l.o.g. we suppose a d-embedding given by $v_i \in \mathbb{R}^d$, $i \in N$.

(i) In Section 4.3 it was shown that $\text{rotdim}_{K_n}(e, e) = n-1$. Furthermore $\text{rotdim}_{K_n}(s, l) \leq n-1$ for arbitrary data $s > 0$, $l > 0$ because of the equilibrium constraint $\sum_{i \in N} s_i v_i = 0$.

(ii) Let node 1 be the central node of $K_{1,3}$ and consider the data $s = e$, $l = e$. A best 1-embedding is $v_1 = \frac{1}{4}$, $v_2 = \frac{5}{4}$, $v_3 = v_4 = -\frac{3}{4}$. Its objective value is $\frac{11}{4}$. But this is smaller than 3, which is the objective value of the following feasible 2-embedding: $v_1 = (0, 0)$, $v_2 = (\cos 0, \sin 0)$, $v_3 = (\cos \frac{2\pi}{3}, \sin \frac{2\pi}{3})$, $v_4 = (\cos \frac{4\pi}{3}, \sin \frac{4\pi}{3})$ (this is optimal). We have shown that $\dim(K_{1,3}) \geq 2$.

Let $s > 0$, $l > 0$ be arbitrary data. We will show that we can find an optimal 2-embedding. Let v_i, $i \in N$ be an optimal embedding. If $v_1 \neq 0$, the embedding is even 1-dimensional - apply the Separator-Shadow Theorem 30 with $S = \{1\}$. If $v_1 = 0$, we can construct a 2-embedding using Theorem 33 with $S = \{1\}$.

(iii) Let G be the complete bipartite graph on the node partition $\{1,2\} \cup \{3,4,5\}$. Let $s := e$, $l_{1i} := 1$, $l_{2i} := 2$, $i = 3,4,5$. We will show, that an arbitrary optimal solution of the embedding problem (2.8) with these data requires at least three dimensions. Assume, for contradiction, $v_i \in \mathbb{R}^2$, $i \in N$ is an optimal 2-embedding. Let $w \geq 0$ be an optimal solution of (2.1) with the defined data s and l.

According to Observation 19 the graph G_w is connected. Therefore at least one edge $e = 1k$, $k \in \{3,4,5\}$ and one edge $\tilde{e} = 2\tilde{k}$, $\tilde{k} \in \{3,4,5\}$ have positive weight $w_e > 0$ and $w_{\tilde{e}} > 0$. Because of symmetry every edge has a positive weight in at least one optimal solution. According to Observation 15 the primal program (2.1) is convex. Hence, a convex combination with positive coefficients of the optimal solution yields an optimal solution $\tilde{w} > 0$ of (2.1).

The Complementary Slackness Conditions (2.9) force all edges of the embedding to be tight. Thus, the distances of v_3, v_4, v_5 to v_1 and v_2 are fixed, coincide resp. and yield $v_1 \neq v_2$. There are only two places in the plane, that realize these distances depending on v_1, v_2. Hence, w.l.o.g. $v_3 = v_4$. Furthermore $0 \in \operatorname{conv}\{v_1, v_2\}$, otherwise the Separator-Shadow Theorem 30 with $S = \{1,2\}$ would yield a contradiction to the equilibrium constraint $\sum_{i \in N} s_i v_i = 0$. But, this is only possible for $v_3 = v_4 = v_5 \in \operatorname{span}\{v_1, v_2\}$.

We get as unique, up to congruences, solution: $v_1 = \frac{6}{5}b$, $v_2 = -\frac{9}{5}b$, $v_3 = v_4 = v_5 = \frac{1}{5}b$ for a vector $b \in \mathbb{R}^2$, $\|b\| = 1$. The optimal value would be $\frac{24}{5}$. This is a contradiction, since the value of the following feasible 3-dimensional embedding is greater: $v_1 = (\frac{\sqrt{3}}{5}, 0, 0)$, $v_2 = (-\frac{4\sqrt{3}}{5}, 0, 0)$, $v_3 = (\frac{\sqrt{3}}{5}, \cos 0, \sin 0)$, $v_4 = (\frac{\sqrt{3}}{5}, \cos\frac{2\pi}{3}, \sin\frac{2\pi}{3})$, $v_5 = (\frac{\sqrt{3}}{5}, \cos\frac{4\pi}{3}, \sin\frac{4\pi}{3})$. Its objective value is $\frac{27}{5}$.

It remains to prove $\dim(K_{2,3}) \leq 3$. Let $s > 0$, $l > 0$ be arbitrary data, and v_i, $i \in N$ an optimal embedding. If $0 \notin \operatorname{conv}\{v_1, v_2\}$ the embedding is 2-dimensional due to the Separator-Shadow Theorem 30 with $S = \{1,2\}$. If $0 \in \operatorname{conv}\{v_1, v_2\}$ we apply Theorem 33 with $S = \{1,2\}$ which yields an optimal 3-embedding.

■

Now, we show that an arbitrary graph of the given classes is embeddable in the respective rotational dimension. For graphs without edges as well as for graphs, that are a disjoint union of paths we even show that every optimal embedding for positive weights is 0-dimensional or 1-dimensional, resp. For outerplanar graphs we prove for positive weights that every optimal embedding is at most 2-dimensional, if the graph has a maximum degree of 3. Since every outerplanar graph is a minor of an outerplanar graph of maximum degree 3, we will then have shown 2-embeddability for outerplanar graphs.

Observation 57 *Let $G = (\{1\}, \emptyset)$ be the graph that consists of one isolated node. Every optimal solution of the embedding problem* (2.8) *with data $s_1 > 0$ has dimension* 0.

Proof. The equilibrium condition for the isolated node 1 reads $s_1 v_1 = 0$. Hence, $v_1 = 0$. ■

Observation 58 *Let $G = (N, E)$ be a nontrivial path. Every optimal solution of the embedding problem* (2.8) *with data $s > 0$, $l > 0$ has dimension* 1.

Proof. Let $w \geq 0$ be an optimal solution of (2.1), and $v_i \in \mathbb{R}^N$, $i \in N$ be an optimal embedding of (2.8). We have $w > 0$ since the strictly active subgraph of G has to be connected. From (2.9) follows that all edges of the embedding are tight. We consider the following tree-width decomposition $\mathcal{T} = (\mathcal{N}, \mathcal{E})$ of G:

$$\mathcal{N} = \{\{i, j\} \subseteq N : ij \in E\}, \mathcal{E} = \{N_1 N_2 \in \binom{\mathcal{N}}{2} : |N_1 \cap N_2| = 1\}.$$

We know from Observation 39 that in every optimal embedding of G one edge contains 0 in its convex hull. If 0 is contained in the interior of the convex hull, then we apply the Separator-Shadow Theorem 30 to the nodes incident to this edge as separators. Otherwise there is one node, that is embedded in 0. Its neighbors cannot be embedded in zero too, since all edges are tight. We apply the Separator-Shadow Theorem 30 to its neighbors as separators. The equilibrium condition $\sum_{i \in N} s_i v_i = 0$ yields the assertion. ■

The case of outerplanar graphs requires more work. First we will show that any outerplanar graph is a minor of an outerplanar graph of maximum degree three. Together with minor monotonicity this yields that we have only to show 2-embedabbility of outerplanar graphs of maximum degree three.

Lemma 59 *A minor monotone graph property holds for all outerplanar graphs if and only if it holds for outerplanar graphs of maximum degree three.*

Proof. Necessity is immediate. The following construction shows sufficiency. Each outerplanar graph G is a minor of an outerplanar graph G' obtained as follows: Since G is outerplanar, it has a plane embedding such that each vertex is situated on the boundary of the outer (infinite) face of this embedding.

Let r be a positive real number small enough, so that for each node the circle of radius r around the node intersects each edge incident to this node (an only those) exactly once and all circles are disjont. The edges subdivide the circles into arcs. Because the embedding is outerplanar, each of the circles contains an arc belonging to the outer face. For each of the circles delete it's whole interior together with exactly one such arc from the drawing. Interpret the intersection points of the circles with the edges of G as vertices of G' and the remaining arcs and parts of the edges of G as edges of G'.

Clearly, the maximum degree of G' is three, the outer face of G' contains the interior of all circles and hence we constructed an outerplanar embedding of G'. Finally, contracting all arcs of the drawing results in G. ■

By Corollary 54 we only need to consider algebraically independent edge lengths and for these, optimal embeddings have favorable properties.

Lemma 60 *Given an outerplanar graph $G = (N, E)$ with maximum degree* 3 *and data $s > 0$, $l > 0$, suppose the entries of l are algebraically independent and let $v_i \in \mathbb{R}^n$, $i \in N$ be an optimal solution of* (2.8). *Suppose C is the set of nodes of a chordless cycle in the active subgraph G_V, then* $\dim \operatorname{span} \{v_i : i \in C\} = 2$.

Proof. Let $C \subseteq N$ be a set of nodes so that $G_V[C]$ is a cycle. Note that $\dim \operatorname{span}\{v_i : i \in C\}$ cannot be 0 or 1, because all edge lengths are tight in the embedding and by algebraic independence of the entries in l any sum of signed lengths of cycle edges cannot cancel out.

It remains to show that $\dim \operatorname{span}\{v_i : i \in C\} \leq 2$. Assume, for contradiction, that there are three nodes in C, say 1, 2, and 3 with $\dim \operatorname{span}\{v_1, v_2, v_3\} = 3$. Then $0 \notin \operatorname{conv}\{v_1, v_2, v_3\}$ and in G_V any node $i \in N \setminus \{1, 2, 3\}$ is separated from one of the three nodes by the other two, because otherwise G_V would contain a forbidden minor or $G_V[C]$ would have a chord.

So, if i is separated, say, from 1 in G_V by 2 and 3 then Theorem 30 (Separator-Shadow) implies $\operatorname{conv}\{v_i, 0\} \cap \operatorname{conv}\{v_2, v_3\} \neq \emptyset$, because $\operatorname{conv}\{v_1, 0\} \cap \operatorname{conv}\{v_2, v_3\} = \emptyset$. Thus, for $i \in N$ we have $\operatorname{conv}\{v_i, 0\} \cap \operatorname{conv}\{v_1, v_2, v_3\} \neq \emptyset$. Therefore zero is strictly separated from the v_i, $i \in N$ by the affine plane containing the points v_1, v_2 and v_3. This contradicts the equilibrium constraint. ∎

We are now ready for the decisive step.

Observation 61 *Given an outerplanar graph $G = (N, E)$ with maximum degree 3 and data $s > 0$, $l > 0$, suppose the entries of l are algebraically independent and let $v_i \in \mathbb{R}^n$, $i \in N$ be an optimal solution of* (2.8)*. The dimension of the embedding is at most two,* $\dim \operatorname{span}\{v_i : i \in N\} \leq 2$.

Proof. Because the active subgraph $G_V = (N, E_V)$ is outerplanar, the sets of nodes spanning chordless cycles in G_V together with the sets of endnodes of bridges of G_V form the set $\mathcal{N}$ of a tree decomposition $T = (\mathcal{N}, \mathcal{E})$ of G_V. By Observation 39 there is at least one set $U \in \mathcal{N}$ with $0 \in \operatorname{conv}\{v_i, i \in U\}$.

Suppose first that each such $U \in \mathcal{N}$ with $0 \in \operatorname{conv}\{v_i : i \in U\}$ is the node set of a bridge in G_V. If there is such a $U = \{i, j\} \in \mathcal{N}$ with $0 \in \operatorname{conv}\{v_i, v_j\} \setminus \{v_i, v_j\}$ then Theorem 30 (Separator-Shadow) implies that the embedding is in fact one dimensional. Otherwise there is a node $\hat{\imath} \in N$ with $v_{\hat{\imath}} = 0$. By the current assumption on the zero-nodes of $\mathcal{N}$, each edge $\{\hat{\imath}, j\} \in E_V$ is a bridge in G_V with $v_j \neq 0$ because $l_{\hat{\imath}j} > 0$.

Furthermore, there are at most three edges incident to $\hat{\imath}$. Thus each $i \in N$ is separated from $\hat{\imath}$ in G_V by some neighbor j of $\hat{\imath}$, and Theorem 30 (Separator-Shadow) implies $v_j \in \operatorname{conv}\{v_i, 0\}$. In consequence, all points are embedded in at most three halfrays emanating from the origin. By the equilibrium constraint, these have to lie in a common two dimensional subspace.

So we may assume in the following that there is a $C \in \mathcal{N}$ with $G_V[C]$ a cycle and $0 \in \operatorname{conv}\{v_i : i \in C\}$. Put $E_C := \{\{i, j\} \in E_V : i, j \in C\}$ and call $e \in E_C$ an *inner edge* if it is contained in another chordless cycle of G_V and an *outer edge* otherwise. Because G_V is outerplanar, for each node $k \in N \setminus C$ there is an edge $ij \in E_C$ such that k and $C \setminus \{i, j\}$ are in different components of $G_V - \{i, j\}$. If $0 \notin \operatorname{conv}\{v_i, v_j\}$ for all $ij \in E_C$, then by Theorem 30 (Separator-Shadow) all nodes of G_V are embedded in the subspace $\operatorname{span}\{v_c : c \in C\}$ which is 2-dimensional by Lemma 60.

The same argument still works if $v_h \neq 0$ for all $h \in C$ and $0 \notin \operatorname{conv}\{v_{i'}, v_{j'}\}$ for all inner edges $i'j' \in E_C$. It remains to consider the case of $0 \in \operatorname{conv}\{v_i, v_j\}$ for some edge

$ij \in E_C$ where ij is either an inner edge or $v_i = 0$ for some $i \in C$ and both edges incident to i in $G_V[C]$ are outer edges. By $l_{ij} > 0$ we may assume $v_j \neq 0$. Let $N' \subset N$ be the set of nodes in the connected component of $G_V - \{i, j\}$ that contains $C - \{i, j\}$ and put $G_1 := G_V[N' \cup \{i, j\}]$ and $G_2 := G_V[N \setminus N']$.

We claim that G_1 is embedded in a halfplane bounded by span $\{v_j\}$. Indeed, let $k \in C$ with $k \neq j$ be the other neighbour of i in $G_V[C]$. By the properties of ij and because the degree of i is at most 3, the edge ki is an outer edge. Hence, if v_k and v_j are linearly independent, all vertices h of $G - \{i, j\}$ in the component of k are separated from i by the set $\{j, k\}$ and so Theorem 30 (Separator-Shadow) asserts $\text{conv}\{v_h, 0\} \cap \text{conv}\{v_j, v_k\} \neq \emptyset$ proving the claim in this case.

If v_k and v_j are linearly dependent, Lemma 60 ensures the existence of a vertex $k' \in C$ such that $v_{k'}$ is linearly independent to v_j. Because $l_{ik} > 0$, there is an $i' \in \{i, k\}$ such that $0 \neq v_{i'}$. Now Theorem 30 (Separator-Shadow) applied to the separators $\{i', k'\}$ and $\{j, k'\}$ of G_V completes the proof of the claim.

It remains to show that the embedding of G_2 aligns nicely with that of G_1. If the edge ij is an inner edge, the same argument shows that G_2 is embedded in a halfplane bounded by span $\{v_j\}$. The equilibrium constraint then ensures that the halfplanes of G_1 and G_2 lie in a common two dimensional subspace.

If the edge ij is an outer edge we have $v_i = 0$, ij is a bridge in G_2 and i has at most one other neighbor $k \neq j$ in G_2. Consider some node $h \in N \setminus (N' \cup \{i, j\})$. In G_2 node h is separated from i by either j or k. If h is separated from i by j then Theorem 30 (Separator-Shadow) implies $v_j \in \text{conv}\{0, v_h\}$, otherwise we get in the same way $v_k \in \text{conv}\{0, v_h\}$. So nodes of G_2 lie in span $\{v_j\}$ or are embedded in a halfray emanating from the origin through v_k. Again the equilibrium constraint forces the halfplane of G_1 and the halfray of G_2 to lie in a common two dimensional subspace. ■

We have shown, that graphs without edges are 0-embeddable, disjoint unions of paths are 1-embeddable, and outerplanar graphs are 2-embeddable. Together with Observation 56 this verifies Theorem 55.

5.3 The Colin de Verdière graph parameter

After having studied graphs with small rotational dimension, we can obtain similarities with another minor monotone graph property, namely the Colin de Verdière graph parameter. We will see that for small numbers the lists of forbidden minors match. Similarities are founded in the more general setting of Discrete Schrödinger Operators. The Laplacian is one example of a Discrete Schrödinger Operator, the Colin de Verdière number is based on Discrete Schrödinger Operators as well, joined with a somewhat weird condition, the Strong Arnold Hypothesis. The Colin de Verdière graph parameter was introduced in [7], resp. [8]. A survey and main source of the following definitions and results is [23].

Definition 62 *Let $G = (N, E)$ be a (simple) graph. We call a matrix $M = (m_{ij})_{ij \in N \times N}$ with*

1. $m_{ij} < 0$ *for* $ij \in E$*,*

2. $m_{ij} = 0$ *for* $i \neq j$ *and* $ij \notin E$*,*

Discrete Schrödinger Operator. *We denote the set of all Discrete Schrödinger Operators associated with a graph* G *by* $\mathcal{O}_G$*.*

Each weighted Laplacian $L_d(G, w)$ with $w > 0$ fulfills the criteria of this definition. Moreover, each Discrete Schrödinger Operator M may be obtained by $M = L(G, w) + \text{Diag}(d_1, \dots, d_n)$ for some $w \in \mathbb{R}^E_{++}$ and $(d_1, \dots, d_n)^T \in \mathbb{R}^N$. This is similar to the relation between (continuous) Laplacian and (continuous) Schrödinger Operator.

Since no assumptions are made regarding the main diagonal elements, we may shift the spectrum of a Discrete Schrödinger Operator by a multiple of the identity. By doing so we may investigate the eigenspace to the second smallest eigenvalue of the matrix by shifting λ_2 to zero and considering the kernel of the matrix.

Thus, let M be a Discrete Schrödinger Operator with exactly one negative eigenvalue. In order to examine changes of the underlying graph such as minor operations one may perturbate M. These perturbations shall in first order preserve the corank and the property to be a Discrete Schrödinger Operator. This leads to the Strong Arnold Hypothesis:

Definition 63 *Let* $\mathcal{O}^n_k$ *be the submanifold of all symmetric* $n \times n$*-matrices with corank* k*. For a matrix* $M \in \mathcal{O}_G$ *let* $\mathcal{T}_M\mathcal{O}^n_k$ *denote the tangent space of* $\mathcal{O}^n_k$ *at* M*, and let* $\mathcal{T}_M\mathcal{O}_G$ *denote the tangent space of* $\mathcal{O}_G$ *at* M*.*

We say that $M \in \mathcal{O}_G$ *fulfills the* Strong Arnold Hypothesis *if* $\mathcal{T}_M\mathcal{O}^n_k + \mathcal{T}_M\mathcal{O}_G$ *is the whole space of all real-valued symmetric* $n \times n$*-matrices.*

An algebraic equivalent is given by:

Theorem 64 (cf. [23]) *A matrix* $M \in \mathcal{O}_G$ *fulfills the Strong Aronld Hypothesis if and only if there is no nonzero symmetric matrix* $X = (x_{ij})^n_{i,j=1}$ *with* $x_{ij} = 0$ *if* $i = j$ *or* i *and* j *are adjacent, such that* $MX = 0$*.*

Now, join Discrete Schrödinger Operators and the Strong Aronld Hypothesis together to define the Colin de Verdière number of a graph.

Definition 65 *Let* G *be a simple, not necessarily connected graph. The* Colin de Verdière graph parameter $\mu(G)$ *is defined as the largest corank of any matrix* $M \in \mathcal{O}_G$ *with exactly one negative eigenvalue and such that* M *fulfills the Strong Arnold Hypothesis. It is also called the* Colin de Verdière number *of* G*.*

It turns out, that the Colin de Verdière graph parameter is also a minor monoton graph property, and small values can be characterized by the following result:

Theorem 66 (cf. [23]) *The Colin de Verdière number* $\mu(\cdot)$ *is a minor monotone graph property, i.e. if* G' *is a minor of* G *then we have* $\mu(G') \leq \mu(G)$*. Furthermore we have for a graph* G*:*

- $\mu(G) = 0$ *if and only if* G *has no edges.*
- $\mu(G) \leq 1$ *if and only if* G *is a disjoint union of paths.*
- $\mu(G) \leq 2$ *if and only if* G *is outerplanar.*
- $\mu(G) \leq 3$ *if and only if* G *is planar.*

We may compare this to Theorem 55. As we can see, the graph classes yielding the values $0, 1,$ and 2 for the rotational dimension and the Colin de Verdière number coincide. But whether there is a deeper relation and how both parameters behave to each other is still an open problem.

We conjecture that $\mathrm{rotdim}(G) \leq \mu(G)$. Moreover, we conjecture that the classes of graphs characterized by both parameters already differ for the case of three dimensions. The supposed example is the $K_{3,3}$. So we conclude this work with these open problems:

Conjecture 67 *Let* $G = (N, E)$ *be a (simple) connected graph. Then* $\mathrm{rotdim}(G) \leq \mu(G)$.

Conjecture 68 $\mathrm{rotdim}(K_{3,3}) \leq 3$.

List of Figures

Bibliography

[1] M. Armbruster. Branch-and-Cut for a Semidefinite Relaxation of Large-scale Minimum Bisection Problems. *Dissertation*, Chemnitz University of Technology, Department of Mathematics, 2007.

[2] D. Bertsimas and Y. Ye. Semidefinite relaxations, multivariate normal distributions, and order statistics. In D.-Z. Du and P. Pardalos, editors, *Handbook of Combinatorial Optimization*, pages 1–19. Kluwer Academic Publishers, 1998.

[3] S. Boyd, P. Diaconis, and L. Xiao. Fastest mixing Markov chain on a graph. *SIAM Rev. 46*, No. 4, pages 667–689, 2004.

[4] K. L. Boyer and K. Sengupta. Modelbase partitioning using property matrix spectra. *Computer Vision and Image Understanding*, 70(2):177–196, May 1998.

[5] T. F. Chan, P. Ciarlet, and W. K. Szeto. On the optimality of the median cut spectral bisection graph partitioning method. *SIAM J. Sci. Comput.*, 18(3):943–948, May 1997.

[6] Y. Colin de Verdière. Sur la multiplicité de la première valeur propre non nulle du laplacien. *Comment. Math. Helv.*, 61:254-270, 1986.

[7] Y. Colin de Verdière. Sur un nouvel invariant des graphes et un critère de planarité. *Journal of Combinatorial Theory, Series B 50*, 11-21, 1990.

[8] Y. Colin de Verdière. On a new graph invariant and a criterion for planarity. *Graph Structure Theory, Contemporary Mathematics*, American Mathematical Society, Rhode Island, 137-147, 1993.

[9] Y. Colin de Verdière. Multiplicités des valeurs propres Laplaciens discrets et Laplaciens continus *Rend. Mat.*, VII. Ser. **13**:433-460, 1993.

[10] D. Cvetković, M. Doob, and H. Sachs. *Spectra of Graphs. Theory and application.* J. A. Barth Verlag, Leipzig, 3rd edition, 1995.

[11] R. Diestel. *Graph Theory.* Springer, Berlin, 2nd edition, 2000.

[12] M. Fiedler. Algebraic connectivity of graphs. *Czechoslovak Mathematical Journal*, 23:298–305, 1973.

[13] M. Fiedler. A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory. *Czechoslovak Mathematical Journal*, 25:619–633, 1975.

[14] M. Fiedler. Laplacian of graphs and algebraic connectivity. *Combinatorics and Graph Theory*, 25:57–70, 1989.

[15] M. Fiedler. Absolute algebraic connectivity of trees. *Linear and Multilinear Algebra*, 26:85–106, 1990.

[16] M. Fiedler. A geometric approach to the Laplacian matrix of a graph. *IMA Vol. Math. Appl.*, 50:73–98, 1993.

[17] M. Fiedler. Some minimax problems for graphs. *Discrete Mathematics*, 121:65–74, 1993.

[18] M. X. Goemans and D. P. Williamson. Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming. *J. ACM*, 42:1115–1145, 1995.

[19] F. Göring, C. Helmberg, M. Wappler. Embedded in the Shadow of the Separator. *SIAM J. Optim.*, 19(1):472-501, 2008.

[20] F. Göring, C. Helmberg, M. Wappler. The Rotational Dimension of a Graph. *Journal of Graph Theory*, 66(4):283-302, April 2011.

[21] C. Helmberg. Semidefinite Programming for Combinatorial Optimization. *ZIB-Report* ZR-00-34, Konrad-Zuse-Zentrum Berlin, Oct 2000.

[22] C. Helmberg, B. Mohar, S. Poljak, and F. Rendl. A spectral approach to bandwidth and separator problems in graphs. *Linear and Multilinear Algebra*, 39:73–90, 1995.

[23] H. van der Holst, L. Lovász, and A. Schrijver. The Colin de Verdière graph parameter. *Graph Theory and Combinatorial Biology, Bolyai Soc. Math. Stud.*, 7:29–85. János Bolyai Mathematical Society, Budapest, 1999.

[24] R. A. Horn and C. R. Johnson. *Matrix Analysis.* Cambridge University Press, 1985.

[25] X. Ji and H. Zha. Extracting shared topics of multiple documents. *Lect. Notes Comput. Sci.*, 2637:100–110, 2003.

[26] M. Juvan and B. Mohar. Laplace eigenvalues and bandwidth-type invariants of graphs. *J. Graph Theory*, 17(3):393–407, 1993.

[27] A. Kaveh and H. A. Rahimi Bondarabady. Spectral trisection of finite element models. *International Journal of Numerical Methods for Heat & Fluid Flow*, 11(4):358-370, 2001.

[28] A. Kaveh and H. A. Rahimi Bondarabady. Bisection for parallel computing using Ritz and Fiedler vectors. *Acta Mechanica*, 167:131–144, Feb. 2004.

[29] J. Keuchel, C. Schnörr, C. Schellewald, and D. Cremers. Unsupervised Image Partitioning with Semidefinite Programming. *CVGPR-Group, Dept. Math. and Comp. Science*, University of Mannheim, 2002.

[30] J. Keuchel, C. Schnörr, C. Schellewald, and D. Cremers. Binary partitioning, perceptual grouping, and restoration with semidefinite programming. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 25(11):1364–1379, Nov. 2003.

[31] E. de Klerk. Exploiting special structure in semidefinite programming: A survey of theory and applications. *European Journal of Operational Research*, 201(1):1-10, 2010.

[32] M. Laurent and S. Poljak. On a positive semidefinite relaxation of the cut polytope. *Linear Algebra and its Applications*, 223/224:439-461, 1995.

[33] L. Lovász. On the Shannon capacity of a graph. *IEEE Transactions on Information Theory*, IT-25(1):1–7, Jan. 1979.

[34] B. Mohar. The Laplacian spectrum of graphs. In *Graph Theory, Combinatorics, and Applications*, pages 871–898. John Wiley and Sons, 1991.

[35] B. Mohar. Graph Laplacians. In B. et al., editor, *Topics in algebraic graph theory*, volume 102 of *Encyclopedia of Mathematics and Its Applications*, pages 113–136. Cambridge University Press, 2004.

[36] B. Mohar and S. Poljak. Eigenvalues in combinatorial optimization. In Brualdi, Friedland, and Klee, editors, *Combinatorial and Graph Theoretic Problems in Linear Algebra*. IMA Volume in Mathematics and Applications, Vol. 50, 1993.

[37] A. Pothen, H. D. Simon, and K. Liou. Partitioning sparse matrices with eigenvectors of graphs. *SIAM J. Matrix Anal. Appl.*, 11:430–452, 1990.

[38] S. Reiß. Optimizing Extremal Eigenvalues of Weighted Graph Laplacians and Associated Graph Realizations. *Dissertation*, Chemnitz University of Technology, Department of Mathematics, 2012.

[39] N. Robertson, P. D. Seymour. Graph minors. XX. Wagner's conjecture. *J. Comb. Theory, Ser. B*, 92(2):325-357, 2004.

[40] H. D. Simon, A. Sohn, and R. Biswas. Harp: A dynamic sprectral partitioner. *Journal of Parallel and Distributed Computing*, 50:83–103, 1998.

[41] J. F. Sturm. Using SeDuMi 1.02, a MATLAB toolbox for optimization over symmetric cones (updated for version 1.05). Manual, Department of Econometrics, Tilburg University, P.O. Box 90153, 5000 LE Tilburg, The Netherlands, Oct. 2001.

[42] J. Sun, S. Boyd, L. Xiao, and P. Diaconis. The Fastest Mixing Markov Process on a Graph and a Connection to a Maximum Variance Unfolding Problem. *SIAM Rev.*, accepted 9/2005.

[43] H. Wolkowicz, R. Saigal, and L. Vandenberghe, editors. *Handbook of Semidefinite Programming*, volume 27 of *International Series in Operations Research and Management Science*. Kluwer Academic Publishers, Boston/Dordrecht/London, 2000.

[44] C. W. Wu. On Rayleigh-Ritz ratios of a generalized Laplacian matrix of directed graphs. *Linear Algebra Appl.*, 402:207–227, 2005.

Theses

1. We consider the problem of maximizing the second smallest eigenvalue of the weighted Laplacian of a (simple) graph over all nonnegative edge weightings with bounded total weight.

2. We generalize this problem by introducing node significances and edge lengths.

3. We give a formulation of this generalized problem as a semidefinite program.

4. The dual program can be equivalently written as embedding problem. This is finding an embedding of the n nodes of the graph in n-space so that their barycenter is at the origin, the distance between adjacent nodes is bounded by the respective edge length, and the embedded nodes are spread as much as possible. (The sum of the squared norms is maximized.)

5. We proof the following necessary condition for optimal embeddings. For any separator of the graph at least one of the components fulfills the following property: Each straight-line segment between the origin and an embedded node of the component intersects the convex hull of the embedded nodes of the separator.

6. There exists always an optimal embedding of the graph whose dimension is bounded by the tree-width of the graph plus one.

7. We define the rotational dimension of a graph. This is the minimal dimension k such that for all choices of the node significances and edge lengths an optimal embedding of the graph can be found in $\mathbb{R}^k$.

8. The rotational dimension of a graph is a minor monotone graph parameter.

9. We characterize the graphs with rotational dimension up to two.

Erklärung

Ich erkläre an Eides Statt, dass ich die von mir eingereichte Dissertation
“On Graph Embeddings and a new Minor Monotone Graph Parameter associated with the Algebraic Connectivity of a Graph”
selbständig und nur unter Verwendung der angegebenen Quellen und Hilfsmittel angefertigt habe.

Ich erkläre an Eides Statt, dass ich diese Dissertation in dieser oder ähnlicher Form an keiner anderen Stelle zum Zwecke eines Promotionsverfahrens vorgelegt habe.

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Chemnitz, den 5. Februar 2013 Markus Wappler