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Graph Realizations Associated with Minimizing the Maximum Eigenvalue of the Laplacian

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Abstract

In analogy to the absolute algebraic connectivity of Fiedler, we study the problem of minimizing the maximum eigenvalue of the Laplacian of a graph by redistributing the edge weights. Via semidefinite duality this leads to a graph realization problem in which nodes should be placed as close as possible to the origin while adjacent nodes must keep a distance of at least one. We prove three main results for a slightly generalized form of this embedding problem. First, given a set of vertices partitioning the graph into several or just one part, the barycenter of each part is embedded on the same side of the affine hull of the set as the origin. Second, there is an optimal realization of dimension at most the tree-width of the graph plus one and this bound is best possible in general. Finally, bipartite graphs possess a one dimensional optimal embedding.

Keywords: spectral graph theory, semidefinite programming, eigenvalue optimization, embedding, graph partitioning, tree-width
MSC 2000: 05C50; 90C22, 90C35, 05C10, 05C78

1 Introduction

Let $G = (N, E)$ be an undirected simple graph with node set $N = \{1, \dots, n\}$ and edge set $E \subseteq \{\{i, j\} : i, j \in N, i \neq j\}$. For an edge $\{i, j\}$ we also write ij if there is no danger of confusion. Given edge weights $c \in \mathbb{R}^E$ the weighted Laplacian of G is the matrix $L_c(G) := \sum_{ij \in E} c_{ij} E_{ij}$ where E_{ij} is an $N \times N$ matrix with value 1 on diagonal elements (i, i) and (j, j), value -1 on offdiagonal elements (i, j) and (j, i) and value zero otherwise. If G is clear from the context or if $c = \mathbf{1}$ (throughout, $\mathbf{1}$ will denote the vector of all ones of appropriate size) we simply write L_c or $L(G)$.

Spectral properties of the Laplacian are a central topic in spectral graph theory [2, 3, 6, 19, 20, 22, 24, 29, 32] but also appear in theoretical chemistry [12, 15, 16] and in

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communication networks [25]. While the minimal eigenvalue of L_c is trivial, $\lambda_1(L_c) = 0$ with eigenvector $\mathbf{1}$, the second smallest eigenvalue $\lambda_2(L_c)$ and the maximal eigenvalue $\lambda_{\max}(L_c)$ appear in several bounds on combinatorial graph parameters [21]. The associated eigenspaces are of interest, as well. Indeed, the eigenvector of λ_2, often referred to as Fiedler vector, is the basis of spectral graph partitioning, see [28] and the references therein. In [9, 10] Fiedler introduced the absolute algebraic connectivity

$$\hat{a}(G) := \max\{\lambda_2(L_c) : c \in \mathbb{R}^E_+, \sum_{e \in E} c_e = |E|\}, \tag{1}$$

and exhibited several relations to the connectivity of the graph. This number reappeared recently in several different contexts [11, 13, 26]. The main interest in [13] was to obtain insight into structural connections between the eigenspace of (1) and connected G by studying the (scaled) semidefinite dual to (1),

$$\begin{array}{rll} \frac{|E|}{\hat{a}(G)} = & \text{maximize} & \sum_{i \in N} \|v_i\|^2 \\ & \text{subject to} & \sum_{i \in N} v_i = 0, \\ & & \|v_i - v_j\| \leq 1 \qquad \text{for } ij \in E, \\ & & v_i \in \mathbb{R}^n \text{ for } i \in N. \end{array} \tag{2}$$

Interpreting optimal solutions of (2) as embeddings or, using the terminology of [1], as realizations of the graph in Euclidean space, several close relations to the separator structure of G can be proven, *e.g.*, a separator shadow theorem and the existence of optimal solutions of dimension at most the tree-width of G plus one. In [14] a generalized form of (2) gave rise to the definition of the rotational dimension of a graph, which is a minor monotone graph parameter closely in spirit to the graph parameter of Colin de Verdière [23, 27].

Motivated by these results, this paper is devoted to the study of

$$\min\{\lambda_{\max}(L_c) : c \in \mathbb{R}^E_+, \sum_{e \in E} c_e = |E|\}, \tag{3}$$

or rather its slightly generalized dual with node weights $s \in \mathbb{R}^N$, $s > 0$, and edge lengths $l \in \mathbb{R}^E$, $l > 0$,

$$\begin{array}{rll} \text{minimize} & \sum_{i \in N} s_i \|v_i\|^2 \\ \text{subject to} & \|v_i - v_j\|^2 \geq l_{ij}^2 & \text{for } ij \in E, \\ & v_i \in \mathbb{R}^n & \text{for } i \in N. \end{array} \tag{4}$$

Interpreted as a graph realization problem, the nodes should be embedded as close to the origin as possible, but, like in tensegrities [4, 5], adjacent nodes are separated by struts of length equal to the edge length. Our three main results for optimal realizations of (4) are as follows. Given any set S of vertices of G, the barycenter of each component of $G - S$ is embedded on the same side of the affine hull of the separator as the origin (for a precise statement see Theorem 9). There exists an optimal realization of dimension at most the tree-width of G plus one (Theorem 12) and this bound cannot be improved in general. Finally, bipartite graphs have a one dimensional optimal embedding (Theorem 13).

The paper is organized as follows. In Section 2 we clarify why (4) is a generalization of the dual to (3). Some basic properties of (4) are studied in Section 3. Section 4 states the main results and presents a family of graphs for which the tree-width bound is tight. The technical parts of the proofs of theorems 9 and 12 are presented in sections 5 and 6. In Section 7 we conclude the paper with some thoughts on deriving a graph parameter from (4) in the style of the rotational dimension of a graph.

Our notation is quite standard. We recall that $\mathbf{1}$ denotes the vector of all ones of appropriate size, $\mathbf{e}_i$ denotes the ith unit vector of the canonical basis of $\mathbb{R}^n$, and we use $\|\cdot\|$ for the Euclidean norm. The inner product of matrices $A,\ B \in \mathbb{R}^{m\times n}$ is $\langle A, B\rangle := \sum_{ij} A_{ij}B_{ij}$. For vectors $a, b \in \mathbb{R}^n$ we prefer the notation $a^\top b := \langle a, b\rangle$. If $A - B$ is positive semidefinite for symmetric matrices A and B, this is denoted by $A \succeq B$. For $I \subseteq \{1, \ldots, m\}$ and a matrix $A = [a_1, \ldots, a_m] \in \mathbb{R}^{m\times n}$ we denote by A_I the set $\{a_i : i \in I\}$ and by $\operatorname{lin}(A_I)$ the linear hull, by $\operatorname{aff}(A_I)$ the affine hull, and by $\operatorname{cone}(A_I)$ the convex conic hull of A_I. For a closed convex set C the projection onto C is denoted by $p_C(\cdot)$.

2 The primal and dual problem

Throughout, we assume that $G = (N, E)$ has at least one edge. Our starting point is (3),

$$\lambda^* := \min\left\{\lambda_{\max}(L_c) : c \in \mathbb{R}^E_+, \sum_{ij\in E} c_{ij} = |E|\right\}.$$

As in [13] we first transform the problem so that its dual may be viewed as an embedding or realization of G in $\mathbb{R}^n$. The main steps are as follows.

The standard semidefinite programming representation of the eigenvalue problem reads,

$$\begin{aligned} \lambda^* = \text{minimize} \quad & \lambda \\ \text{subject to} \quad & \sum_{ij\in E} c_{ij}E_{ij} \preceq \lambda I, \\ & \sum_{ij\in E} c_{ij} = |E|, \\ & c \geq 0, \lambda \text{ free.} \end{aligned} \tag{5}$$

Because $E \neq \emptyset$ we have $L_c \neq 0$ and so $L_c \succeq 0$ implies $\lambda > 0$. Dividing (5) by λ and maximizing the sum over the scaled weights $w_{ij} := \frac{c_{ij}}{\lambda}$ yields the equivalent problem

$$\begin{aligned} \frac{|E|}{\lambda^*} = \quad \text{maximize} \quad & \sum_{ij\in E} w_{ij} \\ \text{subject to} \quad & \sum_{ij\in E} w_{ij}E_{ij} \preceq I, \\ & w \geq 0. \end{aligned} \tag{6}$$

The dual program of (6) is

$$\begin{array}{rll} \text{minimize} & \langle I, X\rangle & \\ \text{subject to} & \langle E_{ij}, X\rangle \geq 1 \quad \text{for } ij \in E, \\ & X \succeq 0. \end{array} \tag{7}$$

Note, as $w_{ij} = 0$ ($ij \in E$) is a strictly feasible solution of (6) with respect to the semidefinite constraint, the dual problem (7) attains its optimal solution (by semidefinite duality theory and strict feasibility, see, *e.g.*, [31]).

The positive semidefiniteness of X admits a Gram representation $X = V^\top V$ with $V \in \mathbb{R}^{n\times n}$. We denote the i-th column of V by v_i, *i.e.*, $V = [v_1, \ldots, v_n]$. Then $X_{ij} = v_i^\top v_j$ and $\langle E_{ij}, X\rangle = \|v_i\|^2 - 2v_i^\top v_j + \|v_j\|^2 = \|v_i - v_j\|^2$. With this, (7) transforms to

$$\begin{array}{rl} \text{minimize} & \sum\limits_{i\in N} \|v_i\|^2 \\ \text{subject to} & \|v_i - v_j\|^2 \geq 1 \quad \text{for } ij \in E, \\ & v_i \in \mathbb{R}^n \quad \text{for } i \in N. \end{array} \tag{8}$$

So the dual problem of (3) is equivalent to finding a realization of the graph's nodes in n-space so that the distances of adjacent nodes are at least one (the *distance constraints*) and the sum of the squared norms is minimized. Note that by semidefinite complementarity, any optimal X and thus V is restricted to the eigenspace of the optimum eigenvalue of (3), compare Remark 2 of [13].

Motivated by [14], we prefer to study the generalized form (4) of this problem from the onset. Indeed, setting $s = \mathbf{1}$ and $l = \mathbf{1}$ we regain problem (8) from (4). In principle, the requirements $s > 0$ and $l > 0$ could be replaced by $s \geq 0$ and $l \geq 0$ without altering the basic arguments but as this would entail some cumbersome special cases, we exclude zeros for ease of presentation.

Like in [14] it can be worked out that for (4) there is a corresponding eigenvalue optimization problem. Tracing back the steps above, use $D := \text{Diag}([s_1^{-1}, \ldots, s_n^{-1}])$ with $V^T V = DXD$ for an analogue of (7), dualize to obtain

$$\begin{array}{rl} \text{maximize} & \sum\limits_{ij\in E} l_{ij}^2 w_{ij} \\ \text{subject to} & \sum\limits_{ij\in E} w_{ij} D E_{ij} D \preceq I, \\ & w_{ij} \geq 0 \quad \text{for } ij \in E. \end{array} \tag{9}$$

Finally the same scaling argument yields the eigenvalue formulation

$$\begin{array}{rl} \text{minimize} & \lambda_{\max}(DL_cD) \\ \text{subject to} & \sum\limits_{ij\in E} l_{ij}^2 c_{ij} = |E|, \\ & c_{ij} \geq 0 \quad \text{for } ij \in E. \end{array}$$

Remark 1 *As in [13], the KKT conditions of* (4) *with the Lagrange multipliers* w_{ij} *of* (9) *provide an intuitive physical interpretation. Without feasibility conditions these read*

$$\begin{aligned} s_i v_i - \sum_{ij\in E} w_{ij}(v_i - v_j) &= 0 \qquad \text{for } i \in N, \\ (\|v_i - v_j\|^2 - l_{ij}^2) w_{ij} &= 0 \qquad \text{for } ij \in E. \end{aligned} \tag{10}$$

Consider each node $i \in N$ *as having a point mass of size* s_i*, and imagine each edge* ij *being a mass-free strut of length* ij *between adjacent points. Now the optimum solution of* (4) *corresponds to an equilibrium configuration within a force field that acts with force* $-\sigma v$ *on a point of mass* σ *at position* v*. The* w_{ij} *of* (9) *are the forces acting along strut* ij*. In particular, the forces are in equilibrium in each point.*

3 Basic properties of the embedding

We first consider the barycenter of the embedding. Throughout this text a vector $s \in \mathbb{R}^n_+$ is fixed and we frequently need to sum up several weights s_i over nodes $i \in A \subseteq N$ or calculate weighted barycenters (with weights s_i) of the embeddings of the nodes in A. For this we introduce the notations

$$\bar{s}(A) = \sum_{i\in A} s_i \qquad \text{for } A \subseteq N$$

for the weight of the barycenter and

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

for the barycenter of the embedding of the nodes in A.

Observation 2 *For an optimal realization* $[v_1, \ldots, v_n]$ *of* (4) *the barycenter is in the origin,* i.e., $\bar{v}(N) = 0$*. Hence, any optimal realization is at most* $(n-1)$ *dimensional.*

Proof. This follows by taking the sum over $i \in N$ of the first line in (10) because all w_{ij} cancel out. ■

Edges, whose distance constraints are inactive or whose weights are zero in optimal solutions are mostly of no importance in the considerations to follow and may be dropped. This motivates the following definition.

Definition 3 *For* $G = (N, E)$ *with given data* s *and* l *let* $V = [v_1, \ldots, v_n]$ *be an optimal solution of* (4) *and* w_{ij} $(ij \in E)$ *a corresponding optimal solution of* (9)*. The edge set* $E_{V,l} := \{ij \in E : \|v_i - v_j\| = l_{ij}\}$ *gives rise to the* active subgraph $G_{V,l} = (N, E_{V,l})$ of G with respect to V*. The* strictly active subgraph $G_w = (N, E_w)$ of G with respect to w *has edge set* $E_w := \{ij \in E : w_{ij} > 0\}$*.*

Note that by complementarity, $E_w \subseteq E_{V,l}$. Recall that a component of a graph is a maximal connected subgraph, and so a component of G may split into several components in $G_{V,l}$ which may again split into several components in G_w. The following result is proved by the same argument used for Observation 2.

Observation 4 *Given optimal solutions to* (4) *and* (9) *the barycenter of each component of the strictly active subgraph as well as of the active subgraph as well as of the graph itself is in the origin.*

The next result states that any optimal embedding of (8) is contained within the unit ball.

Observation 5 *All optimal solutions* $[v_1, \ldots, v_n]$ *of* (4) *satisfy* $\|v_i\| < \hat{l} := \max\{l_{ij} : ij \in E\}$ *for* $i \in N$.

Proof. Given an optimal solution $[v_1, \ldots, v_n]$, assume, for contradiction, there exists a vector v_k for some $k \in N$ with $\|v_k\| \geq \hat{l}$. By Observation 2 we may choose a vector $h \in \mathbb{R}^n$, $\|h\| = 1$, with h perpendicular to all v_i ($i \in N$). Define a new embedding $[v'_1, \ldots, v'_n]$ via $v'_i := v_i$ for $i \in N \setminus \{k\}$ and $v'_k := \hat{l}h$. Because $\|v'_i - v'_k\| \geq \|\hat{l}h\| = \hat{l}$ for $i \in N \setminus \{k\}$, the new embedding is feasible. In addition, $s_k\|v'_k\| \leq s_k\|v_k\|$, so the objective value is at least as good. The barycenter of the new embedding, however, is not in the origin. Indeed, $h^\top \bar{v}'(N) = s_k\hat{l}/\bar{s}(N) \neq 0$, so by Observation 2 the new embedding is not optimal. This contradicts optimality of the original embedding. ∎

If $l = \mathbf{1}$ this allows to characterize those nodes that are embedded in the origin.

Observation 6 *In an optimal solution* $[v_1, \ldots, v_n]$ *of* (4) *for* $G = (N, E)$ *with* $l = \mathbf{1}$*, a node is embedded in the origin if and only if it is an isolated node in* G.

Proof. For an isolated node $j \in N$, $v_j = 0$ is feasible and best possible. Conversely, if $j \in N$ has a neighbor i in G then any feasible solution with $v_j = 0$ satisfies $\|v_i\| \geq 1$. By Observation 5 this cannot be optimal. ∎

At the end of this section we consider alternative formulations of the objective function of problem (4). The objective function may be bounded by (see Lemma 8 below)

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

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

$$\begin{array}{rl} \text{minimize} & \sum_{i,j\in N} s_i s_j \|v_i - v_j\|^2 \\ \text{subject to} & \|v_i - v_j\|^2 \geq l_{ij}^2 \quad \text{for } ij \in E, \\ & v_i \in \mathbb{R}^n \quad \text{for } i \in N, \end{array} \tag{11}$$

we obtain the following result.

Observation 7 *Each optimal solution of* (4) *is an optimal solution of* (11) *with the same active subgraph.*

For $s = \mathbf{1}$ the objective function of (11) is also known as the variance of the data v_i (see, *e.g.*, [30]), it appears in statistics (see, *e.g.*, [18]) and as the moment of inertia of rotating rigid bodies in physics (see, *e.g.*, [8]). In the following sections we will frequently group nodes into clusters and consider the relative positions between these clusters while keeping the relative positions within each cluster fixed. It is well known from physics that it then suffices to study the relative positions of the weighted barycenters of the clusters. We collect these properties in the next lemma and include a proof for the convenience of the reader.

Lemma 8 *Given* $v_i \in \mathbb{R}^d$ *and weights* $s_i > 0$ *for* $i \in N$ *with finite* N *partitioned into* $N = \dot{\bigcup}_{I \in \mathcal{P}} I$ *for some finite family* $\mathcal{P}$*, there holds*

$$\bar{v}(N) = \frac{1}{\bar{s}(N)} \sum_{I \in \mathcal{P}} \bar{s}(I)\bar{v}(I) \tag{12}$$

and

$$\begin{aligned}
&\sum_{i \in N} s_i \|v_i - \bar{v}(N)\|^2 = \\
&= -\bar{s}(N)\|\bar{v}(N)\|^2 + \sum_{i \in N} s_i \|v_i\|^2 && (13)\\
&= \frac{1}{2\bar{s}(N)} \sum_{i,j \in N} s_i s_j \|v_i - v_j\|^2 && (14)\\
&= \sum_{I \in \mathcal{P}} \sum_{i \in I} s_i \|v_i - \bar{v}(I)\|^2 + \sum_{I \in \mathcal{P}} \bar{s}(I)\|\bar{v}(I) - \bar{v}(N)\|^2 && (15)\\
&= \sum_{I \in \mathcal{P}} \left(\sum_{i \in I} s_i \|v_i - \bar{v}(I)\|^2 + \frac{1}{2\bar{s}(N)} \sum_{J \in \mathcal{P}} \bar{s}(I)\bar{s}(J)\|\bar{v}(I) - \bar{v}(J)\|^2 \right). && (16)
\end{aligned}$$

Proof. Equation (12) is verified by direct computation. Equation (13) follows by

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

For (14),

$$
\begin{aligned}
\sum_{i\in N} s_i\|v_i-\bar v(N)\|^2 &= \sum_{i\in N} s_i\|v_i\|^2 - \frac{2}{\bar s(N)}\sum_{i,j\in N} s_i s_j v_i^\top v_j + \frac{1}{\bar s(N)}\sum_{i,j\in N} s_i s_j v_i^\top v_j\\
&= \sum_{i\in N} s_i\|v_i\|^2 - \frac{1}{\bar s(N)}\sum_{i,j\in N} s_i s_j v_i^\top v_j\\
&= \frac{1}{2\bar s(N)}\sum_{i,j\in N}\left(s_i s_j\|v_i\|^2 - 2 s_i s_j v_i^\top v_j + s_i s_j\|v_j\|^2\right)\\
&= \frac{1}{2\bar s(N)}\sum_{i,j\in N} s_i s_j\|v_i-v_j\|^2.
\end{aligned}
$$

Next, (15) is proved by

$$
\begin{aligned}
\sum_{i\in N} s_i\|v_i-\bar v(N)\|^2 =& \sum_{I\in\mathcal P}\sum_{i\in I} s_i\|v_i-\bar v(I)+\bar v(I)-\bar v(N)\|^2\\
=& \sum_{I\in\mathcal P}\sum_{i\in I} s_i\|v_i-\bar v(I)\|^2 + 2\sum_{I\in\mathcal P}\sum_{i\in I} s_i(v_i-\bar v(I))^\top(\bar v(I)-\bar v(N)) +\\
&+\sum_{I\in\mathcal P}\bar s(I)\|\bar v(I)-\bar v(N)\|^2\\
=& \sum_{I\in\mathcal P}\sum_{i\in I} s_i\|v_i-\bar v(I)\|^2 + 2\sum_{I\in\mathcal P}(\bar v(I)-\bar v(N))^\top \underbrace{\sum_{i\in I} s_i(v_i-\bar v(I))}_{=0} +\\
&+\sum_{I\in\mathcal P}\bar s(I)\|\bar v(I)-\bar v(N)\|^2.
\end{aligned}
$$

Finally, (16) follows from using (12) and (14) for the second summand in (15). ■

4 Main results

The structural properties of optimal embeddings $[v_1,\dots,v_n]$ of (4) are tightly linked to the separator structure of the underlying graph. A (node-)*separator* of a connected graph G is a subset $S\subset N$ of nodes, whose removal disconnects the graph into at least two connected components. Often we will not discern every single component arising this way but simply speak of two or more separated sets of nodes. The first result corresponds to the Separator-Shadow Theorem in [13].

Theorem 9 (Sunny Side) *Given a graph $G=(N,E)$, data $s>0$, $l>0$, an optimal solution $V=[v_1,\dots,v_n]$ of (4), and two disjoint nonempty subsets A and S of N such that each edge of the corresponding active subgraph $G_{V,l}$ leaving A ends in S. Then the barycenter $\bar v(A)$ is contained in $\mathcal S := \operatorname{aff}(V_S)-\operatorname{cone}(V_S)$.*

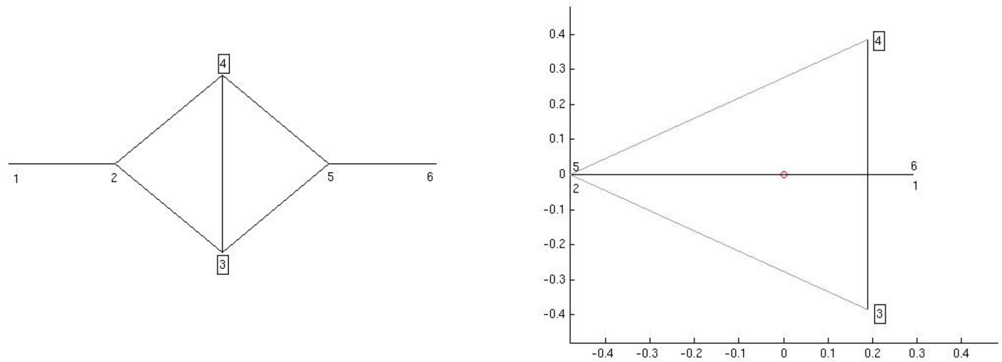

Figure 1: In an optimal embedding, not all nodes need to lie on the sunny side of the separator, see Remark 10.

The proof requires some preparation and is therefore deferred to Section 5.

Remark 10 *In order to motivate the name "sunny side" denote the projection of the origin onto* $\text{aff}(V_S)$ *by* p_0*, then* $\text{aff}(V_S) - \text{cone}(V_S) = \{v - \alpha p_0 : v \in \text{aff}(V_S), \alpha \in \mathbb{R}_+\}$*. If* $0 \notin \text{aff}(V_S)$ *then this is the half space in* $\text{lin}(V_S)$ *containing the origin. If the origin is viewed as the sun, then the barycenter of* V_A *lies in the sunny half space of the affine hull of* V_S*, which separates* V_A *from the - eventually empty - rest of the graph. While the Separator Shadow Theorem of [13] ensures that every single node of at least one of the separated node sets lies in the shadow of the convex hull of the separator, the current theorem is limited to the barycenter of the node sets but holds for all separated node sets at the same time. It is not possible to extend the result to all nodes. This is illustrated in Figure 1, where the node set* $S = \{3, 4\}$ *forms a separator leading to the components* $A = \{1, 2\}$ *and* $B = \{5, 6\}$*. In this optimal embedding for* $s = \mathbf{1}$ *and* $l = \mathbf{1}$ *the nodes* 1 *and* 6 *are not in* $\text{aff}(V_S) - \text{cone}(V_S)$*.*

Depending on the separator structure of the graph, there always exist optimal embeddings of rather small dimension. In order to state this result, we need the notions tree-decomposition and tree-width which we recall here in the form given in [7].

Definition 11 *Let* $G = (N, E)$ *be a graph,* T *a tree, and let* $\mathcal{N} := (N_t)_{t \in T}$ *be a family of node sets* $N_t \subseteq N$ *indexed by the nodes* t *of* T*. The pair* $(T, \mathcal{N})$ *is called a tree-decomposition of* G *if it satisfies the following three conditions:*

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

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

For example, trees have tree-width one (each edge forms one set N_t, so choose $\mathcal{N}=E$, and for the tree's edge set use the edge set of any spanning tree of the original tree's line graph). In general, it is NP-complete to determine the tree-width, but any valid tree-decomposition provides an upper bound.

Theorem 12 *For each graph* G *there exists an optimal embedding of* (4) *of dimension at most* 1 *if* $\mathrm{tw}(G)=1$ *and* $\mathrm{tw}(G)+1$ *otherwise.*

The proof of Theorem 12 is given in Section 6.

Next, we consider some special graph classes. For bipartite graphs the structure of optimal solutions is particularly simple.

Theorem 13 *Let* G *be bipartite. There exists a one-dimensional optimal solution of* (4). *Moreover, if* $l=\mathbf{1}$ *then for any optimal solution of* (4) *and any optimal* w *of* (9), *each non-trivial component of the strictly active subgraph* G_w *is embedded in the endpoints of a straight line segment of length one that contains the origin in its relative interior.*

Proof. Given an optimal d-dimensional embedding $[v_1,\dots,v_n]$ of (4) for $G=(A\dot{\cup}B, E\subseteq\{ij : i\in A, j\in B\})$, consider the one-dimensional embedding

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

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

$$l_{ij}^2 \le \|v_i-v_j\|^2 \le (\|v_i\|+\|v_j\|)^2 = \|v_i'-v_j'\|^2.$$

So all distance constraints are fulfilled and the new embedding is optimal. Now consider the case $l=\mathbf{1}$. For $ij\in E_w$ complementarity ensures $1=\|v_i'-v_j'\|^2=\|v_i-v_j\|^2=(\|v_i\|+\|v_j\|)^2$. This together with observations 5 and 6 shows that the origin is a strict convex combination of v_i and v_j. Continuing this argument along the edges of a spanning tree of each component of G_w completes the proof. ■

For complete graphs and $l=\mathbf{1}$ the structure of optimal embeddings is identical to the λ_2-case.

Example 14 (complete graphs) *For* $K_n := (\{1,\dots,n\},\{\{i,j\} : 1\le i<j\le n\})$ *with data* $l=\mathbf{1}$ *and arbitrary* s *we show that the unique optimal embedding of* (4) *is the regular* $(n-1)$*-dimensional simplex whose weighted barycenter coincides with the origin: We can handle the objective function of* (4) *by Lemma 8 and bound it as follows,*

$$\begin{aligned}\sum_{i\in N} s_i\|v_i\|^2 &= \bar{s}(N)\|\bar{v}(N)\|^2 + \frac{1}{2\bar{s}(N)}\sum_{i,j\in N} s_is_j\|v_i-v_j\|^2\\ &\ge 0+\frac{1}{2\bar{s}(N)}\sum_{i\in N}\sum_{j\in N\setminus\{i\}} s_is_j = \frac{\bar{s}(N)^2-\|s\|^2}{2\bar{s}(N)}.\end{aligned} \tag{17}$$

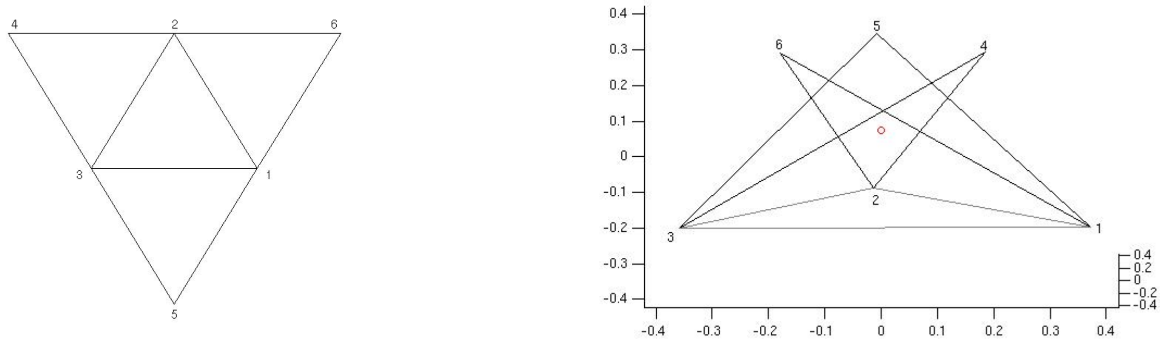

Figure 2: Graph with tight dimension bound, for $d = 3$. The optimal solution is not $d - 1$ but d-dimensional. See Example 15.

Equality holds if and only if $\bar{v}(N) = 0$ *and* $\|v_i - v_j\| = 1$ *for* $i, j \in N$ *with* $i \neq j$. *Note, for use in Example 15, that* $\|v_i\| = \|v_j\|$ *whenever the weights* s_i *and* s_j *are equal, because the exchange of two vertices of a regular simplex is a congruence transformation.*

We conclude this section by giving a family of graphs for which the tree-width bound of Theorem 12 is tight.

Example 15 (graphs with tight dimension bound) *To each node of* K_d *append an additional node and consider the complement of this graph,* i.e., *set* $D := \{1, \dots, d\}$, $N := \{1, \dots, 2d\}$, *and*

$$G(d) := \big(N, \{ij : \ i, j \in D, \ i \neq j\} \cup \{ij : \ i \in D, \ j \in N \setminus (D \cup \{d+i\})\}\big). \tag{18}$$

By construction $G(d)$ *has tree-width* $\mathrm{tw}(G(d)) = d - 1$. *For* $d > 2$ *there is a unique optimal solution* $[v_1, \dots, v_n]$ *of* (8) *(up to congruence) and its dimension is* d. *In order to prove this, set* $N_i := \{d + i\} \cup D \setminus \{i\}$ *for* $i \in D$ *and introduce weights* $s'_j := \frac{1}{d-1}$ *for* $j \in D$ *and* $s'_j := 1$ *for* $j \in N \setminus D$.

We first bound the objective function using (17) *on each weighted sub sum for* $i \in D$,

$$\sum_{k \in N} \|v_k\|^2 = \sum_{i \in D} \sum_{j \in N_i} s'_j \|v_j\|^2 \geq \sum_{i \in D} \frac{1}{2\bar{s}'(N_i)} \left(\bar{s}'(N_i)^2 - \sum_{j \in N_i} {s'_j}^2 \right) = d \frac{3d - 4}{4(d-1)}. \tag{19}$$

By Example 14, equality holds if and only if

$$\forall i \in D : \sum_{j \in N_i} s'_j v_j = 0 \ \wedge \ \forall j, k \in N_i, j \neq k : \|v_j - v_k\| = 1.$$

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

1. $\|v_i\| = \|v_j\|$ *for* $i, j \in D$ *by the concluding remark of Example 14,*

2. $\|v_i - v_j\| = 1$ *for* $i, j \in D$ *with* $i \neq j$, *so* $\operatorname{conv}(V_D)$ *forms a regular simplex with all vertices having the same distance to the origin (thus for* $D' \subseteq D$, *the barycenter* $\bar{v}(D')$ *is the projection of* 0 *onto the simplex corresponding to* D'*),*

3. $v_{d+i} = -\bar{v}(D \setminus \{i\})$ *for* $i \in D$ *by the choice of* s'. *Because* $\operatorname{conv}(V_{N_i})$ *forms a regular simplex with all edge lengths equal to 1, this relation allows to compute* $\|v_{d+i}\|$ *and* $\|v_i\|$ *explicitly, fixing all relative positions uniquely up to congruence. Note, by* $\bar{v}(N_i) = \frac{1}{d} v_{d+i} + \frac{d-1}{d}\bar{v}(D \setminus \{i\})$ *we obtain* $\|v_{d+i}\| < \|v_j\|$ $(j \in D)$ *and* $\|\bar{v}(D)\| > 0$.

The last fact implies $0 \notin \operatorname{conv}(V_D)$, *so the dimension of this realization is* d.

5 Proof of Theorem 9

Proof. If $\bar{v}(A) \in \operatorname{aff}(V_S)$ the assertion is trivial and if $B := N \setminus (A \cup S) = \emptyset$ then Observation 4 implies $\bar{v}(A) = -\bar{v}(S)$ and therefore $\bar{v}(A) \in \operatorname{aff}(V_s) - \operatorname{cone}(V_s)$. Thus we assume $B \neq \emptyset$ and $\bar{v}(A) \notin \operatorname{aff}(V_S)$. In consequence, $|S| \leq n - 2$.

By Observation 7 an optimal solution of (4) is also an optimal solution of (11). Congruence transformations on optimal solutions of (11) influence neither their optimality, their feasibility nor their tight subgraph. Hence we may assume that there is an optimal solution $V' = [v'_1, \ldots, v'_n]$ of (11) congruent to a given optimal solution $V = [v_1, \ldots, v_n]$ of (4) satisfying the following properties:

$0 \in \operatorname{aff}(V'_S) = \operatorname{lin}(V'_S)$,	by invariance of (11) under translations,
$\forall i \in S : [v'_i]_1 = [v'_i]_2 = 0$,	because $\dim \operatorname{aff}(V_S) \leq n - 3$,
$\bar{v}'(A) \in (\operatorname{lin}(V'_S) + \operatorname{cone}\{\mathbf{e}_1\}) \setminus \operatorname{lin}(V'_S)$,	$\mathbf{e}_1$ is the direction $\bar{v}(A) - p_{\operatorname{aff}(V_S)}(\bar{v}(A))$,
$\bar{v}'(B) \in \operatorname{lin}(V'_S \cup \{\mathbf{e}_1\}) + \operatorname{cone}\{\mathbf{e}_2\}$	by choosing $\mathbf{e}_2$ by a similar argument.

Rephrased in this setting we have to prove that $\bar{v}'(A) \in \operatorname{lin}(V'_S) + \operatorname{cone}\{\bar{v}'(N)\}$. For this it suffices to prove $[\bar{v}'(B)]_2 = 0$ and $[\bar{v}'(B)]_1 \geq 0$, *i.e.*, $\bar{v}'(B) \in \operatorname{lin}(V'_S) + \operatorname{cone}\{\mathbf{e}_1\}$, because then $\bar{v}'(N) = \frac{1}{\bar{s}(N)}(\bar{s}(S)\bar{v}'(S) + \bar{s}(A)\bar{v}'(A) + \bar{s}(B)\bar{v}'(B)) \in (\operatorname{lin}(V'_S) + \operatorname{cone}\{\mathbf{e}_1\}) \setminus \operatorname{lin}(V'_S)$ and so $\operatorname{lin}(V'_S) + \operatorname{cone}\{\mathbf{e}_1\} = \operatorname{lin}(V'_S) + \operatorname{cone}\{\bar{v}'(N)\}$. The relations $[\bar{v}'(B)]_2 = 0$ and $[\bar{v}'(B)]_1 \geq 0$ will follow from necessary optimality conditions of the realization V' in comparison to modified realizations obtained by feasible rotations of nodes in A.

From the given properties of V' we obtain

$$[\bar{v}'(A)]_1 > [\bar{v}'(A)]_2 = 0 \quad \text{and} \quad [\bar{v}'(B)]_2 \geq 0. \tag{20}$$

We are interested in the behavior of the objective function, when the v'_i $(i \in A)$ are rotated by an orthogonal matrix

$$R(t) = \begin{bmatrix} 1-t & -\sqrt{2t-t^2} & 0 & 0 & \cdots \\ \sqrt{2t-t^2} & 1-t & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \\ \vdots & \vdots & \vdots & & \ddots \end{bmatrix} \tag{21}$$

near the value $t = 0$, because for small enough t the obtained solutions of (11) remain feasible:

- The distances $v_i - v_j$ of vectors with $i, j \in A \cup S$ do not change, because the rotation is a congruence transformation having all v_i with $i \in S$ as fixed points.
- The distances $v_i - v_j$ of vectors with $i, j \in B \cup S$ do not change because such vectors aren't moved at all.
- The distances $v_i - v_j$ of vectors with $i \in A$, $j \in B$ do not belong to active distance constraints of (11), because the active subgraph does not contain such edges ij, $R(0)$ is the identity, and $R(t)$ is continuous in t.

Let $f(t) := \sum_{i,j \in N} s_i s_j \|v_i^t - v_j^t\|^2$ with $v_k^t = \begin{cases} R(t)v_k' & \text{if } k \in A \text{ and} \\ v_k' & \text{otherwise.} \end{cases}$

Using Lemma 8 with $\mathcal{P} = \{A, B, S\}$ we rewrite the objective function of (11) to fit the partitioning of the nodes,

$$\sum_{i,j \in N} s_i s_j \|v_i - v_j\|^2 = \sum_{I \in \mathcal{P}} \left(\sum_{J \in \mathcal{P}} \bar{s}(I)\bar{s}(J)\|\bar{v}(I) - \bar{v}(J)\|^2 + 2\bar{s}(N) \sum_{i \in I} s_i \|v_i - \bar{v}(I)\|^2 \right).$$

Consequently, using $[\bar{v}'(A)]_2 = 0$, optimality of V' and feasibility of $V^t = [v_1^t, \ldots, v_n^t]$ for all $0 \le t \le \varepsilon$ with $\varepsilon > 0$ small enough, we obtain

$$\begin{aligned} 0 &\le f(t) - f(0) \\ &= \left(\|\bar{v}^t(A) - \bar{v}^t(B)\|^2 - \|\bar{v}'(A) - \bar{v}'(B)\|^2\right) \bar{s}(A)\bar{s}(B) \\ &= \Big(\left([\bar{v}^t(A)]_1 - [\bar{v}^t(B)]_1\right)^2 - \left([\bar{v}'(A)]_1 - [\bar{v}'(B)]_1\right)^2 + \\ &\quad + \left([\bar{v}^t(A)]_2 - [\bar{v}^t(B)]_2\right)^2 - \left([\bar{v}'(A)]_2 - [\bar{v}'(B)]_2\right)^2 \Big) \bar{s}(A)\bar{s}(B) \\ &= \Big(t^2 [\bar{v}'(A)]_1^{\,2} - 2t[\bar{v}'(A)]_1 \left([\bar{v}'(A)]_1 - [\bar{v}'(B)]_1\right) + \\ &\quad + (2t - t^2)[\bar{v}'(A)]_1^{\,2} - 2\sqrt{2t - t^2}[\bar{v}'(A)]_1 [\bar{v}'(B)]_2 \Big) \bar{s}(A)\bar{s}(B) \\ &= 2[\bar{v}'(A)]_1 \bar{s}(A)\bar{s}(B) \left(t[\bar{v}'(B)]_1 - \sqrt{2t - t^2}[\bar{v}'(B)]_2 \right). \end{aligned}$$

With $2[\bar{v}'(A)]_1 \bar{s}(A)\bar{s}(B) > 0$, see (20), we conclude

$$[\bar{v}'(B)]_1 - \sqrt{\tfrac{2}{t} - 1}[\bar{v}'(B)]_2 \ge 0 \qquad \text{for all } 0 < t < \varepsilon.$$

Together with (20) this implies $[\bar{v}'(B)]_2 = 0$ and $[\bar{v}'(B)]_1 \ge 0$. ■

6 Proof of Theorem 12

We will prove the tree-width theorem algorithmically by implicitly exploiting the property of any tree-decomposition $(T, \mathcal{N} = (N_t)_{t\in T})$ that for adjacent nodes t and t' in T the node set $N_t \cap N_{t'}$ is a separator of G (see [7]).

Proof of Theorem 12. Graphs with $\operatorname{tw}(G) = 1$ are trees. For these the theorem follows from Theorem 13. So we may assume $\operatorname{tw}(G) > 1$.

Given any tree-decomposition $(T, \mathcal{N} = (N_t)_{t\in T})$ of G and an optimal embedding $V = [v_1, \ldots, v_n]$ of (4), put $\mathcal{L}_t := \operatorname{lin}(V_{N_t})$ and let

$$d^* := \max\{\dim \mathcal{L}_t : t \in T\}$$

denote the maximum dimension spanned by any bag N_t. Let $t^* \in T$ be a node, for which d^* is attained. Starting from V we show how to construct an optimal embedding $V' = [v'_1, \ldots, v'_n]$ with $v'_i \in \mathcal{L}_{t^*}$ for $i \in N$. Because $\dim \mathcal{L}_{t^*} \le |N_{t^*}|$, the dimension of the new embedding is bounded by the width of the tree-decomposition plus one. As there is a tree-decomposition of width $\operatorname{tw}(G)$ this proves the theorem.

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

Next let $p \in T$ be the (*predecessor*) node adjacent to $\hat{t}$ on the tree-path from $\hat{t}$ to t^*. By assumption, $\mathcal{L}_p \subseteq \mathcal{L}_{t^*}$ and $\hat{d} := \dim \mathcal{L}_{\hat{t}} \le d^*$. The points of $S := N_{\hat{t}} \cap N_p$ span a (possibly empty) common subspace $\mathcal{S} := \operatorname{lin}(V_S) \subseteq \mathcal{L}_{t^*} \cap \mathcal{L}_{\hat{t}}$ whose dimension we denote by $d_{\mathcal{S}}$. Choose an orthonormal basis $\{e_1, \ldots, e_{d_{\mathcal{S}}}\}$ of $\mathcal{S}$, extend it to an orthonormal basis of $\mathcal{L}_{t^*}$ by $\{e_1, \ldots, e_{d_{\mathcal{S}}}, \ldots, e_{d^*}\}$ and then to an orthonormal basis of $\mathbb{R}^n$ by $\{e_1, \ldots, e_{d_{\mathcal{S}}}, \ldots, e_{d^*}, \ldots, e_n\}$. Likewise, extend $\{e_1, \ldots, e_{d_{\mathcal{S}}}\}$ to an orthonormal basis of $\mathcal{L}_{\hat{t}}$ by $\{e_1, \ldots, e_{d_{\mathcal{S}}}, f_{d_{\mathcal{S}}+1}, \ldots, f_{\hat{d}}\}$ and this again to an orthonormal basis of $\mathbb{R}^n$ by $\{e_1, \ldots, e_{d_{\mathcal{S}}}, f_{d_{\mathcal{S}}+1}, \ldots, f_{\hat{d}}, \ldots, f_n\}$. Using the orthogonal matrices $P := [e_1, \ldots, e_n]$ and $\hat{P} := [e_1, \ldots, e_{d_{\mathcal{S}}}, f_{d_{\mathcal{S}}+1}, \ldots, f_n]$, the new embedding is defined by

$$v'_i := \begin{cases} v_i & \text{for } i \in N \setminus \hat{N}, \\ P\hat{P}^\top v_i & \text{for } i \in \hat{N}. \end{cases}$$

Note that by construction, $v'_i = v_i$ for $i \in S$ and $v'_i \in \mathcal{L}_{t^*}$ for $i \in N_{\hat{t}}$. Due to property 3 of Definition 11 we have $S = \hat{N} \cap \bar{N}$. Therefore $v'_i = v_i$ for $i \in \bar{N}$. If $t \in T \setminus \hat{T}$ then $N_t \subseteq \bar{N}$ and so $\|v'_i - v'_j\| = \|v_i - v_j\|$ for all $\{i, j\} \subseteq N_t$. For $t \in \hat{T}$ there holds $N_t \subseteq \hat{N}$, so $\|v'_i - v'_j\| = \|P\hat{P}^\top(v_i - v_j)\| = \|v_i - v_j\|$ for all $\{i, j\} \subseteq N_t$. By property 2 of Definition 11, for each $ij \in E$ there is a $t \in T$ with $ij \in N_t$, thus V' is feasible. Furthermore, $\|v'_i\| = \|v_i\|$ for $i \in N$, so the new realization is again optimal. Letting $\mathcal{L}'_t := \operatorname{lin}(V'_{N_t})$ for $t \in T$ we see that $\mathcal{L}'_t = \mathcal{L}_t$ for $t \in T \setminus \hat{T}$ and (in slight abuse of notation) $\mathcal{L}'_t = P\hat{P}^\top \mathcal{L}_t$ for $t \in \hat{T}$, so $\dim \mathcal{L}'_t = \dim \mathcal{L}_t$ for $t \in T$, completing the proof. ■

7 Dimension bounds as graph parameters

Recently, several graph parameters have been introduced that are based on the rank of certain matrix representations of the graph, [23, 27] or on the existence of certain graph realizations in low dimensions. For example, Belk and Connelly [1] call a graph $G = (N, E)$ d-realizable if, given any realization $V = [v_1, \dots, v_n]$ of the graph in some finite dimensional Euclidean space, there exists a d-dimensional realization $[v'_1, \dots, v'_n]$ with $v'_i \in \mathbb{R}^d$ $(i \in N)$ and $\|v_i - v_j\| = \|v'_i - v'_j\|$ for all $ij \in E$. They show that this is a minor monotone property and give excluded minor characterizations for $d \in \{1, 2, 3\}$. Our proof of the tree-width theorem also works for this case, so $d \leq \mathrm{tw}(G) + 1$. This result should be well known, *e.g.*, it is implicitly contained in the work of Hendrickson [17] on the molecule problem.

Based on a generalization of maximizing the second smallest eigenvalue of the Laplacian, Göring *et al.* [14] introduced the so called rotational dimension of a graph, proved its minor monotonicity and gave excluded minor characterizations for $d \in \{0, 1, 2\}$.

Let us proceed in a similar way for the maximum eigenvalue and define for a graph G and data $s \in \mathbb{R}^N$ with $s > 0$ and $l \in \mathbb{R}^E$ with $l > 0$

$$\mathrm{d}_G^{\lambda_{\max}}(s, l) := \min \{\dim \mathrm{lin}(V_N) : V \text{ is optimal for (4)}\} \tag{22}$$

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

$$\mathrm{d}^{\lambda_{\max}}(G) := \max \left\{ \mathrm{d}_G^{\lambda_{\max}}(s, l) : s \in \mathbb{R}^N,\ s > 0,\ l \in \mathbb{R}^E,\ l > 0 \right\}. \tag{23}$$

In contrast to the rotational dimension of a graph G, $\mathrm{d}^{\lambda_{\max}}(G)$ is not minor monotone: For a complete graph K_n we have $\mathrm{d}^{\lambda_{\max}}(K_n) \geq n - 1$ because of Example 14. But each K_n is a minor of a bipartite graph (subdivide each edge of K_n exactly once), and by Theorem 13, bipartite graphs G have $\mathrm{d}^{\lambda_{\max}}(G) = 1$. So, at this time, this parameter seems less promising than the rotational dimension.

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