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of Graph Laplacians and Associated

Graph Realizations

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Abstract

Extremal eigenvalues and eigenvectors of the Laplace matrix of a graph form the core of many bounds on graph parameters and graph optimization problems. In order to advance the understanding of connections between structural properties of the graph and these eigenvectors and eigenvalues we study the problem minimizing the difference between maximum and second smallest eigenvalue over edge weighted Laplacians of a graph. Building on previous work where these eigenvalues were investigated separately, we show that a corresponding dual problem allows to view eigenvectors to optimized eigenvalues as graph realizations in Euclidean space, whose structure is tightly linked to the separator structure of the graph. In particular, optimal realizations corresponding to the maximum eigenvalue fold towards the barycenter along separators while for the second smallest eigenvalue they fold outwards along separators. Furthermore optimal realizations exist in dimension at most the tree-width of the graph plus one.

Keywords: spectral graph theory, semidefinite programming, eigenvalue optimization, embedding, tree width

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1 Introduction

Let $G = (N, E)$ be a finite, simple, undirected, not necessarily connected graph with node set $N = \{1, \ldots, n\}$, $n \geq 3$, and nonempty edge set $E \subseteq \{\{i, j\} : i \neq j, \ i, j \in N\}$. For given edge weights w_{ij} $(ij \in E)$ the *weighted Laplacian* $L_w = \sum_{ij \in E} w_{ij} E_{ij}$ of G is the weighted sum of matrices $E_{ij} \in \mathbb{R}^{n \times n}$ $(ij \in E)$ having value 1 at entries (i, i) and (j, j), value -1 at (i, j) and (j, i) and value zero otherwise. Each E_{ij} is positive semidefinite $(E_{ij} \succeq 0)$ with smallest eigenvalue zero and a corresponding eigenvector $\mathbf{1}$ of all ones. Thus, if the edge weights w_{ij} are nonnegative, also L_w is positive semidefinite having eigenvector $\mathbf{1}$ in the eigenspace of eigenvalue zero.

The eigenvalues of the (weighted) Laplacian are a classical topic in spectral graph theory [5, 11, 12, 13, 32, 33, 45] and have been studied with revived interest in the last years [2, 16, 37, 39, 41, 43]. They found application in various fields, such as in combinatorial optimization [7, 35], spectral graph partitioning [42], communication networks [1, 38], theoretical chemistry [17, 22, 23] and their values, products or differences appear in several bounds on combinatorial graph parameters [24, 34]. There exists close connections to graph representations, see, *e. g.*, the Lovász ϑ function [14, 21, 28, 29, 31, 36] and the Sigma Function [5, 6]. An overview over geometric representations of graphs is given in [30].

This work aims at furthering the understanding of the connections between structural properties of a graph and the eigenvector and eigenvalues of its Laplacian by investigating spectral properties of optimized extremal eigenvalues. It builds on [19, 20] and [18] where the second smallest and the largest eigenvalue of the Laplacian were (separately) optimized over all nonnegative weight distributions summing up to a given total edge weight. Reformulating such an eigenvalue optimization problem as a (primal) semidefinite program gives rise to a corresponding dual program, whose optimal solutions lie in the eigenspace of the optimized eigenvalue and may be interpreted as a realization of the graph in $\mathbb{R}^n$. Such optimal realizations and the relation of their properties to the separator structure of the underlying graph were the main object of interest in [18, 19]. In [20] the problem was generalized by introducing positive node parameters $s \in \mathbb{R}^n_{++}$ and nonnegative edge parameters $l \in \mathbb{R}^E_+$, that act as node weights and edge lengths in the corresponding graph realization. The semidefinite primal and dual problems, and the realizations (embeddings) are listed in Table 1. They differ slightly from the originals in [19, 20] and [18] in that they are not scaled by the optimal value λ_2 (λ_n) so as to highlight their connection to the problems investigated here. The aim of this paper is to study the combined problem of minimizing the difference between the maximum and the second smallest eigenvalue of the weighted Laplacian scaled by the node parameters via $D = \mathrm{Diag}(s_1^{-1/2}, \ldots, s_n^{-1/2})$,

$$\min\{\lambda_{\max}(DL_wD) - \lambda_2(DL_wD) : \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \ w \geq 0\}. \tag{1}$$

The dual of its formulation as a primal semidefinite program may again be interpreted as, in this case, finding two optimal graph realizations $U = [u_1, \ldots, u_n] \in \mathbb{R}^{n \times n}$ and

	second smallest eigenvalue [19, 20]	maximum eigenvalue [18]
	Given: graph $G = (N, E)$, $s_i > 0$ $(i \in N)$, $l_{ij} \geq 0$ $(ij \in E)$, $l \neq 0$. $D = \mathrm{Diag}(s_1^{-1/2}, \ldots, s_n^{-1/2})$	
Primal	$\min \ -\lambda_2$ subject to $\sum_{ij \in E} w_{ij} D E_{ij} D + \mu D^{-1} \mathbf{1}\mathbf{1}^\top D^{-1} - \lambda_2 I \succeq 0,$ $\sum_{ij \in E} l_{ij}^2 w_{ij} = 1,$ $\lambda_2, \mu \in \mathbb{R}, w \geq 0.$ (P_{λ_2})	$\min \ \lambda_n$ subject to $\lambda_n I - \sum_{ij \in E} w_{ij} D E_{ij} D \succeq 0, \quad (\mathrm{P}_{\lambda_n})$ $\sum_{ij \in E} l_{ij}^2 w_{ij} = 1,$ $\lambda_n, \ w \geq 0.$
Dual	$\max \ \xi$ subject to $\langle I, X \rangle = 1,$ $\langle D^{-1} \mathbf{1}\mathbf{1}^\top D^{-1}, X \rangle = 0,$ $-\langle D E_{ij} D, X \rangle - l_{ij}^2 \xi \geq 0 \ (ij \in E),$ $\xi \in \mathbb{R}, X \succeq 0.$ (D_{λ_2})	$\max \ \xi$ subject to $\langle I, Y \rangle = 1,$ $\langle D E_{ij} D, Y \rangle - l_{ij}^2 \xi \geq 0 \quad (ij \in E),$ $\xi \in \mathbb{R}, \ Y \succeq 0.$ (D_{λ_n})
Embedding	$U = [u_1, \ldots, u_n] \in \mathbb{R}^{n \times n},$ $DXD = U^\top U$ $\max \ \xi$ subject to $\sum_{i \in N} s_i \|u_i\|^2 = 1,$ $\sum_{i \in N} s_i u_i = 0,$ $-\|u_i - u_j\|^2 - l_{ij}^2 \xi \geq 0 \ (ij \in E),$ $\xi \in \mathbb{R}, u_i \in \mathbb{R}^n \ (i \in N).$ (E_{λ_2})	$V = [v_1, \ldots, v_n] \in \mathbb{R}^{n \times n},$ $DYD = V^\top V$ $\max \ \xi$ subject to $\sum_{i=1}^n s_i \|v_i\|^2 = 1,$ $\|v_i - v_j\|^2 - l_{ij}^2 \xi \geq 0 \quad (ij \in E),$ $\xi \in \mathbb{R}, \ v_i \in \mathbb{R}^n \ (i \in N).$ (E_{λ_n})

Table 1: Problems of maximizing the second smallest and minimizing the maximum eigenvalue of the weighted Laplacians (see [19, 20] and [18]).

$V = [v_1, \ldots, v_n] \in \mathbb{R}^{n \times n}$, one for λ_2 and one for $\lambda_{\max}$, that assign to node $i \in N$ the points u_i and v_i subject to constraints on the relative positions of nodes connected by edges,

$$
\begin{aligned}
\max \quad & \xi \\
\text{subject to} \quad & \sum_{i \in N} s_i \|u_i\|^2 = 1, \\
& \sum_{i \in N} s_i \|v_i\|^2 = 1, \\
& \| \sum_{i \in N} s_i u_i \|^2 = 0, \\
& \|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \xi \in \mathbb{R}, \ u_i, v_i \in \mathbb{R}^n \ (i \in N).
\end{aligned} \qquad (\mathrm{E}_{\lambda_n - \lambda_2})
$$

Optimal graph realizations U and V provide a geometric interpretation of extremal eigenvectors of $DL_w D$ for optimal w, because for any $h \in \mathbb{R}$ the vector $D^{-1} U^T h$ $(D^{-1} V^T h)$ is an eigenvector to $\lambda_2(DL_w D)$ $(\lambda_{\max}(DL_w D))$, see Rem. 2.

The optimization problems above form the main object of study here. Besides numerous properties of optimal primal and optimal dual solutions, our main results state connections between feasible (optimal) realizations of the single problems of Table 1 and feasible (optimal) realizations of the coupled problem. In particular, we show that the respective realization of any feasible solution (U, V) of $(\mathrm{E}_{\lambda_n - \lambda_2})$ is also feasible for the single problems (E_{λ_2}) and (E_{λ_n}) and *vice versa* (for a precise statement see Theorem 14). For optimal V of $(\mathrm{E}_{\lambda_n - \lambda_2})$ there exists appropriate data $\bar{s}$ and $\bar{l}$ such that V is also optimal in (E_{λ_n}) (Theorem 15). An almost identical result holds for optimal U of $(\mathrm{E}_{\lambda_n - \lambda_2})$ if some special graphs are excluded (Theorem 18). The last two theorems allow to transfer the structural results of [19, 20, 18] linking optimal graph realizations to the separator structure of the graph: optimal realizations V fold inwards along separators (Theorem 16), optimal realizations U fold outwards along separators (Theorem 19), and for both there exist optimal realizations whose dimension is bounded by the tree-width of the graph plus one (corollaries 17 and 20). Like in [25], the realization interpretation can be carried over to the eigenvectors of the unweighted Laplacian by optimizing over the edge parameters l, (theorems 39 and 40).

The paper is organized as follows. In Section 2 we formulate the primal and dual semidefinite programs to (1) and give the connection to $(\mathrm{E}_{\lambda_n - \lambda_2})$. This is followed by basic properties of optimal solutions and first examples in Section 3. Section 4 presents our main results, namely the comparison of solutions of the single and coupled problems and the results exhibiting the connections to the separator structure and the tree-width of the graph. It also includes a discussion on graphs that have isolated nodes or that result in optimal weighted Laplacians having more connected components than the graph. Bipartite graphs and graphs with some symmetries are analyzed in Section 5. At the end, in Section 6, we offer a geometric interpretation of the eigenspaces of the second smallest and the maximum eigenvalue of the unweighted Laplacian as optimal solutions to a graph realization problem.

Our notation is quite standard. We use $\| \cdot \|$ for the Euclidean norm. The inner product of matrices $A, \ B \in \mathbb{R}^{n \times n}$ 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 $A = [a_1, \ldots, a_m] \in \mathbb{R}^{n \times m}$ we denote by A_I the set $\{a_i : i \in I\}$.

2 Primal-dual formulation

Let $s_i > 0$ $(i \in N)$ be *node weights*, let $l_{ij} \geq 0$ $(ij \in E)$ specify *edge lengths* and put $D = \mathrm{Diag}(s_1^{-1/2}, \ldots, s_n^{-1/2})$. The following primal semidefinite program is a formulation of (1),

$$
\begin{aligned}
\min \quad & \lambda_n - \lambda_2 \\
\text{subject to} \quad & \sum_{ij \in E} w_{ij} D E_{ij} D + \mu D^{-1} \mathbf{1}\mathbf{1}^\top D^{-1} - \lambda_2 I \succeq 0, \\
& \lambda_n I - \sum_{ij \in E} w_{ij} D E_{ij} D \succeq 0, \qquad\qquad (\mathrm{P}_{\lambda_n - \lambda_2}) \\
& \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \\
& \lambda_2, \lambda_n, \mu \in \mathbb{R}, \ w \geq 0.
\end{aligned}
$$

Note that, in consequence of the third constraint, problem $(\mathrm{P}_{\lambda_n - \lambda_2})$ is infeasible if and only if $E = \emptyset$ or all $l_{ij} = 0$, so we will always assume $E \neq \emptyset$ and $l_{\overline{ij}} > 0$ for some $\overline{ij} \in E$. It is, however, no problem if some of the l_{ij} are zero, as we prove next.

Observation 1 *For $G = (N, E)$ with $E \neq \emptyset$ and data $s > 0$, $0 \neq l \geq 0$, problem $(\mathrm{P}_{\lambda_n - \lambda_2})$ is strictly feasible, the optimal value is attained and the set of optimal vectors w is compact.*

Proof. Choosing λ_n sufficiently positive and λ_2 negative for any feasible w reveals that $(\mathrm{P}_{\lambda_n - \lambda_2})$ is strictly feasible. Because the dual program

$$
\begin{aligned}
\max \quad & \xi \\
\text{subject to} \quad & \langle I, X \rangle = 1, \\
& \langle I, Y \rangle = 1, \\
& \langle D^{-1} \mathbf{1}\mathbf{1}^\top D^{-1}, X \rangle = 0, \qquad\qquad (\mathrm{D}_{\lambda_n - \lambda_2}) \\
& \langle D E_{ij} D, Y \rangle - \langle D E_{ij} D, X \rangle - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \xi \in \mathbb{R}, \ X, Y \succeq 0.
\end{aligned}
$$

has feasible solutions, semidefinite duality theory [44] asserts that both programs have a common finite optimal value that is attained in $(\mathrm{D}_{\lambda_n - \lambda_2})$. In order to show primal attainment, we prove that for any fixed $\delta > 0$ the assumption $\lambda_{\max}(L_w) - \lambda_2(L_w) < \delta$ implies the boundedness of w, which establishes the observation by standard compactness arguments (the scaling by $D \succ 0$ may be neglected in these considerations).

For $i, j \in N$, $i < j$, define vectors $q_{ij} = (e_i - e_j)/\sqrt{2}$, weighted degrees $d_w^i = \sum_{ik \in E} w_{ik}$ and values $\gamma_w^{ij} = q_{ij}^T L_w q_{ij} = (d_w^i + d_w^j + 2w_{ij})/2$ (setting $w_{ij} = 0$ for $ij \notin E$). Note that each q_{ij} is orthogonal to $\mathbf{1}$, so by Courant-Fischer $\lambda_{\max}(L_w) \geq \max_{ij} \gamma_w^{ij} \geq \min_{ij} \gamma_w^{ij} \geq \lambda_2(L_w)$. By $\lambda_{\max}(L_w) - \lambda_2(L_w) < \delta$ we obtain $|\gamma_w^{ij} - \gamma_w^{kh}| < \delta$ for any choice of $i, j, k, h \in N$ with

$i \neq j$, $k \neq h$. This allows to conclude $|d_w^i - d_w^j| \leq 4\delta$ for any $i < j$ as we prove next. For $k \in N \setminus \{i, j\}$,

$$|\gamma_w^{ki} - \gamma_w^{ij}| < \delta \Rightarrow |d_w^k - (d_w^j + 2w_{ij} - 2w_{ik})| \leq 2\delta,$$
$$|\gamma_w^{kj} - \gamma_w^{ij}| < \delta \Rightarrow |d_w^k - (d_w^i + 2w_{ij} - 2w_{jk})| \leq 2\delta$$
$$\Rightarrow |(d_w^i - d_w^j) - 2(w_{jk} - w_{ik})| \leq 4\delta.$$

Using this, $d_w^i > d_w^j + 4\delta$ would imply $w_{jk} > w_{ik}$ for all $k \in N \setminus \{i, j\}$ giving rise to the contradicting relation $d_w^j = \sum_{jk \in E} w_{jk} > \sum_{ik \in E} w_{ik} = d_w^i$, so we obtain $|d_w^i - d_w^j| \leq 4\delta$ as claimed. Thus, the inequality $|\gamma_w^{ij} - \gamma_w^{kh}| < \delta$ yields

$$|w_{ij} - w_{kh}| \leq 5\delta \quad \text{for } i, j, k, h \in N \text{ with } i \neq j, k \neq h.$$

Because of $l \neq 0$ there is an $ij \in E$ with $l_{ij} > 0$ and $w_{ij} \leq 1/l_{ij}^2$ by feasibility, so all w_{hk} remain bounded whenever $\lambda_n(L_w) - \lambda_2(L_w) \leq \delta$ for some fixed $\delta > 0$. $\blacksquare$

Expressing in $(D_{\lambda_n - \lambda_2})$ the semidefinite variables X and Y by Gram representations $DXD = U^\top U$, $U = [u_1, \ldots, u_n] \in \mathbb{R}^{n \times n}$ and $DYD = V^\top V$, $V = [v_1, \ldots, v_n] \in \mathbb{R}^{n \times n}$, we obtain $(E_{\lambda_n - \lambda_2})$ as an equivalent nonconvex quadratic program.

Interpreting the vectors u_i and v_i $(i \in N)$ of any feasible solution of $(E_{\lambda_n - \lambda_2})$ as vector labelings of the nodes $i \in N$, we get two realizations/embeddings U and V of the graph in $\mathbb{R}^n$. For these, the node weighted square norms sum up to one (we call this the *normalization constraints*), the weighted barycenter of U is at the origin (*equilibrium constraint*; it is convenient to keep the square in view of the KKT conditions (4) below) and the difference between the squared edge lengths of the two realizations is bounded below by the weighted variable ξ (*distance constraints*). In optimal solutions the minimal weighted difference of the distances over all $ij \in E$ with $l_{ij} > 0$ is as large as possible.

One might wonder, whether requiring $l > 0$ would not lead to more elegant formulations, after all the effect on the optimal value is small by Observation 1. However, we will see in Observation 4 below that $\xi = 0$ in $(E_{\lambda_n - \lambda_2})$ if and only if G is complete. In consequence, if $l > 0$ and G is not complete we might loose characteristic optimal solutions in $(E_{\lambda_n - \lambda_2})$, because if G is not complete the distance constraint would not allow $v_i = v_j$ for any $ij \in E$.

For optimal primal and dual solutions, semidefinite complementarity conditions imply

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

and

$$\langle Y, \lambda_n I - DL_wD \rangle = \lambda_n - \sum_{ij \in E} w_{ij}\|v_i - v_j\|^2 = 0. \tag{3}$$

Remark 2 *One may view optimal embeddings as a map of eigenvectors of λ_2 and $\lambda_{\max}$ of an optimal DL_wD. Indeed, for any $h \in \mathbb{R}^n$ and optimal embeddings $U = [u_1, \ldots, u_n]$ and $V = [v_1, \ldots, v_n]$ the scaled projections $\xi_2 = D^{-1}U^T h$ and $\xi_n = D^{-1}V^T h$ onto the one dimensional subspace spanned by h yield eigenvectors to $\lambda_2(DL_wD)$ and $\lambda_{\max}(DL_wD)$, respectively, by complementarity conditions* (2) *and* (3).

In order to analyze properties of optimal solutions it is sometimes helpful to view optimality conditions from the perspective of the embedding problem $(\mathrm{E}_{\lambda_n - \lambda_2})$. Without feasibility and using the Lagrange multipliers λ_2, λ_n, μ, and $w_{ij} \geq 0$ of $(\mathrm{P}_{\lambda_n - \lambda_2})$, its Karush-Kuhn-Tucker conditions read

$$\lambda_2 s_i u_i = \sum_{ij \in E} w_{ij}(u_i - u_j) - \mu s_i \sum_{j=1}^{n} s_j u_j \qquad (i \in N), \tag{4}$$

$$\lambda_n s_i v_i = \sum_{ij \in E} w_{ij}(v_i - v_j) \qquad (i \in N), \tag{5}$$

$$w_{ij}(\|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi) = 0 \qquad (ij \in E). \tag{6}$$

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

Definition 3 *Given a graph $G = (N, E)$ and data $s > 0$, $0 \neq l \geq 0$, let $U = [u_1, \ldots, u_n]$, $V = [v_1, \ldots, v_n]$ and ξ be an optimal solution of $(\mathrm{E}_{\lambda_n - \lambda_2})$ and let w be a corresponding optimal solution of $(\mathrm{P}_{\lambda_n - \lambda_2})$. The edge set $E_{U,V,\xi,l} = \{ij \in E : \|v_i - v_j\|^2 - \|u_i - u_j\|^2 = l_{ij}^2 \xi\}$ gives rise to the* active subgraph $G_{U,V,\xi,l} = (N, E_{U,V,\xi,l})$ *of G with respect to U, V and ξ. The* strictly active subgraph $G_w = (N, E_w)$ *of G with respect to w has edge set $E_w = \{ij \in E : w_{ij} > 0\}$.*

3   Basic Properties and Examples

We start by discussing the special case of optimal solution value 0.

Observation 4 *For any data $s > 0$, $0 \neq l \geq 0$, problem $(\mathrm{P}_{\lambda_n - \lambda_2})$ has optimal value 0 if and only if $G = K_n$. In this case, $w_{ij} = s_i s_j / \sum_{k<h} l_{kh}^2 s_k s_h$, $1 \leq i < j \leq n$, is optimal.*

Proof. Any feasible solution w with $\lambda_n = \lambda_2 =: \lambda$ satisfies $w \neq 0$ and $\lambda > 0$. Because μ only serves to shift the trivial eigenvalue 0 of the Laplacian, there is also a solution with $\mu = \lambda/\|D^{-1}\mathbf{1}\|^2 = \lambda/\sum s_i$ and we use this solution in the following. Then

$$\lambda I \preceq DL_w D + \mu D^{-1}\mathbf{1}\mathbf{1}^T D^{-1} \preceq \lambda I \quad \Leftrightarrow \quad L_w + \mu D^{-2}\mathbf{1}\mathbf{1}^T D^{-2} = \lambda D^{-2}.$$

For $i < j$ this forces $w_{ij} = \mu s_i s_j \neq 0$, therefore the graph must be complete. These values also satisfy the requirements of the i-th diagonal element, $\sum_{j \in N, j \neq i} w_{ij} + \mu s_i^2 = \mu s_i \sum_{j \in N} s_j = \lambda s_i$. The constraint $1 = \sum_{i<j} l_{ij}^2 w_{ij} = \mu \sum_{i<j} l_{ij}^2 s_i s_j$ determines μ and λ. ∎

Next we describe some optimal dual realizations for $G = K_n$. In this and in the sequel it will be convenient to abbreviate the sum of the node weights for some subset $N' \subseteq N$ by $\bar{s}(N') = \sum_{i \in N'} s_i$.

Example 5 (complete graphs) *Let G be the complete graph K_n with given data $s > 0$ and $0 \neq l \geq 0$. By Observation 4 and strong duality, any optimal solution ξ, $U = [u_1, \ldots, u_n]$ and $V = [v_1, \ldots, v_n]$ of $(\mathrm{E}_{\lambda_n - \lambda_2})$ fulfills $\xi = 0$. Because all w_{ij} are positive, complementarity implies $\|u_i - u_j\| = \|v_i - v_j\|$ for all $i, j \in N$.*

An optimal d-dimensional realization of $(\mathrm{D}_{\lambda_n - \lambda_2})$ $(1 \leq d \leq n - 1)$ is given by taking $M \subseteq N$, where $|M| = d + 1$ and

$$\xi = 0, \quad X_{kl} = Y_{kl} = \frac{1}{d\bar{s}(M)} \begin{cases} \bar{s}(M \setminus \{k\}) & \text{for } k, l \in M, \ k = l, \\ -\sqrt{s_k s_l} & \text{for } k, l \in M, \ k \neq l, \\ 0 & \text{otherwise.} \end{cases}$$

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

If the strictly active subgraph is not connected, the problem almost decomposes into subproblems (P_{λ_n}) on the components. More precisely, the value of λ_2 is zero and the minimization of the maximum eigenvalue leads to an identical maximum eigenvalue on each component consisting of at least two nodes. In order to state and prove this result in detail, we denote by $L_w^{N'}$ the principal submatrix of the weighted Laplacian L_w with indices $i \in N' \subseteq N$.

Observation 6 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let λ_2, λ_n, w be optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$ and let the strictly active subgraph G_w consist of k connected components $G_i = (N_i, E_i)$, $i = 1, \ldots, k$. Then*
  (i) $k > 1$ if and only if $\lambda_2 = 0$,
  (ii) for each component $i = 1, \ldots, k$, $\lambda_n = \lambda_{\max}(DL_w^{N_i}D)$ if and only if $E_i \neq \emptyset$.

Proof. (i) was already observed by Fiedler [12], but the argument is short: Suppose $k \geq 2$, then $q = D^{-1}(\frac{1}{\bar{s}(N_1)} \sum_{i \in N_1} e_i - \frac{1}{\bar{s}(N_2)} \sum_{i \in N_2} e_i)$ is an eigenvector to $\lambda_2 = 0$, because $DL_w Dq = 0$ and $\mathbf{1}^T D^{-1}q = 0$. The other direction follows, *e. g.*, by applying Perron-Frobenius to $(1 + \max\{L_w^{\{i\}} : i \in N\})I - L_w$.

For (ii), we know $\lambda_n > 0$ by Obs. 4. Because L_w consists of independent principal submatrices corresponding to the connected components, there is at least one block N_i with $\lambda_n = D^{V_i}L_w^{V_i}D^{V_i}$. Suppose $E_{\bar{k}} = \emptyset$ for some $\bar{k}$, then the component is an isolated node, $|N_{\bar{k}}| = 1$, and $0 = L_w^{N_{\bar{k}}}$, so $\lambda_n > \lambda_{\max}(D^{N_{\bar{k}}}L_w^{N_{\bar{k}}}D^{N_{\bar{k}}})$. If there is a connected component $(N_{\bar{k}}, E_{\bar{k}} \neq \emptyset)$ with $\lambda_n > \lambda_{\max}(D^{N_{\bar{k}}}L_w^{N_{\bar{k}}}D^{N_{\bar{k}}})$, then slightly increasing the weights w_{ij} for $ij \in E_{\bar{k}}$ and decreasing the weights of all components with $\lambda_n = \lambda_{\max}(D^{N_i}L_w^{N_i}D^{N_i})$ allows to preserve feasibility and to improve the solution at the same time, so this contradicts optimality. ∎

Remark 7 *By Observation 6 and its proof, the number of components of the strictly active subgraph with at least one edge is a lower bound on the dimension of the eigenspace corresponding to the maximum eigenvalue λ_n of $DL_w D$.*

By summing the KKT conditions (5) over all nodes of the graph, or alternatively over the nodes of each connected component, it follows that with respect to optimal V the equilibrium constraint holds automatically for each connected component.

Observation 8 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let ξ, U, $V = [v_1, \ldots, v_n]$ be optimal for $(\mathrm{E}_{\lambda_n - \lambda_2})$ and λ_2, λ_n, w be optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$. For any connected component (N_i, E_i) of the strictly active subgraph, of the active subgraph, or of the graph itself, the weighted barycenter with respect to V is in the origin,* i. e., $\sum_{i \in N_i} s_i v_i = 0$.

Considering the U-embedding, the barycenter of the entire graph is explicitly constrained to lie in the origin. This, however, does not extend to the connected components. In fact, whenever the strictly active subgraph is not connected, the optimal U-embeddings of each component collapse to single points.

Observation 9 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let $U = [u_1, \ldots, u_n]$ be optimal for $(\mathrm{E}_{\lambda_n - \lambda_2})$ and λ_2, w be optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$. The strictly active subgraph $G_w = (N, E_w)$ is not connected if and only if $u_i = u_j$ for $ij \in E_w$ if and only if $\lambda_2 = 0$.*

Proof. The claim follows from semidefinite complementarity (see (2)) and Obs. 6(i), *i. e.,* $\lambda_2 = 0$ if and only if G_w is not connected. ∎

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

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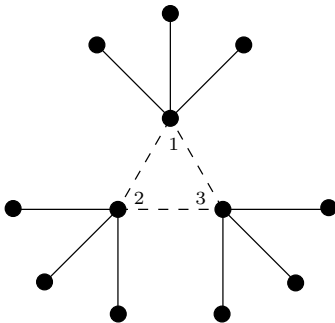

Figure 1: There may be no one-dimensional embedding U even if G_w is not connected.

Example 10 *Consider the graph of Figure 1 with data $s = 1$ and $l = 1$. The edges in the dashed triangle have optimal weight zero and the strictly active subgraph is not connected. In an optimal embedding U, each component is mapped onto one point. Computing an*

optimal V one obtains an optimal solution with $\|v_i - v_j\|^2 \approx 0.7140$ $(ij \in \{12, 23, 13\})$ and optimal $\xi \approx 4/9$. Hence, $\|u_i - u_j\|^2 \leq 0.7410 - 4/9 \approx 0.2965$ $(ij \in \{12, 23, 13\})$. There is no optimal one-dimensional embedding $u_i = x_i h$ $(i \in N)$ with $h \in \mathbb{R}^n$, $\|h\| = 1$ and $x_i \in \mathbb{R}$ $(i \in N)$, because it would have to satisfy the following infeasible system,

$$\begin{array}{ll} \text{equilibrium constraint} & 4x_1 + 4x_2 + 4x_3 = 0, \\ \text{normalization constraint} & 4x_1^2 + 4x_2^2 + 4x_3^2 = 1, \\ \text{distance constraints} & (x_i - x_j)^2 \leq 0.2965 \quad (ij \in \{12, 23, 13\}). \end{array}$$

The next observation provides a bound on the length of vectors of optimal realizations of $(\mathrm{E}_{\lambda_n - \lambda_2})$.

Observation 11 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let ξ, $U = [u_1, \ldots, u_n]$, $V = [v_1, \ldots, v_n]$ be optimal for $(\mathrm{E}_{\lambda_n - \lambda_2})$ and put $\hat{l} = (\max\{\|u_i - u_j\|^2 + l_{ij}^2 \xi : ij \in E\})^{1/2}$. Then $\|u_i\| < s_i^{-1/2}$ and $\|v_i\| < \min\{s_i^{-1/2}, \hat{l}\}$ for $i \in N$.*

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

The proof for $\hat{l}$ is as follows: Suppose, for contradiction, that there is a node $k \in N$ with $\|v_k\| = \hat{l} + \epsilon \geq \hat{l}$. Then we show that there is another feasible realization V' (and U) with no smaller objective value having the barycenter of V_N' outside the origin, which contradicts the optimality of V by Obs. 8.

Note that $\hat{l} > 0$ because $l \neq 0$ and, by Obs. 4 and Ex. 5, $\xi > 0$ or $\|u_i - u_j\|^2 > 0$ for at least one $ij \in E$. By the first part, *i.e.*, $s_k \|v_k\|^2 < 1$, the bounds $0 \leq s_k(2\hat{l}\epsilon + \epsilon^2) < 1$ hold. Because of Obs. 8 there is a vector $h \in \mathbb{R}^n$, with $\|h\| = 1$, that is orthogonal to V_N. Thus a new realization V' may be defined by

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

In words, we first embed the vector v_k in the new direction h and if $\epsilon > 0$ we shorten it. Then, if $\epsilon > 0$, we lengthen all the vectors, such that the weighted square norms sum up to one again.

In consequence, the lengths of edges not including k do not decrease. For $ik \in E$ we have

$$\|v_i' - v_k'\|^2 \geq \|v_i - \hat{l}h\|^2 = \|v_i\|^2 + \hat{l}^2 \geq \hat{l}^2 \geq \|u_i - u_k\|^2 + l_{ik}^2 \xi.$$

Thus ξ, U and V' is a feasible and optimal solution of $(\mathrm{E}_{\lambda_n - \lambda_2})$. But the barycenter of V_N' is not in the origin as only node k has a nonzero contribution in direction h. This contradicts Obs. 8. ∎

The following example illustrates that the bounds of Observation 11 cannot be improved.

Example 12 *Let $s = c\mathbf{1}$ with $c > 0$, $l = \mathbf{1}$. For $n > 2$ consider the graph $G = (N, E) = (\{1, \ldots, n\}, \{2k : k \in N \setminus \{1, 2\}\})$, i.e., it consists of two components: an isolated node and a star. Let $h \in \mathbb{R}^n$, $\|h\| = 1$. Optimal realizations of $(\mathrm{P}_{\lambda_n - \lambda_2})$ and $(\mathrm{E}_{\lambda_n - \lambda_2})$ are given by*

$$\lambda_2 = 0, \ \lambda_n = \frac{n-1}{c(n-2)}, \ \mu = 0, \ w_{ij} = \frac{1}{n-2} \ (ij \in E)$$

and

$$\xi = \frac{n-1}{c(n-2)}, \ u_i = \begin{cases} \sqrt{\frac{n-1}{cn}} h & \text{for } i = 1, \\ -\sqrt{\frac{1}{cn(n-1)}} h & \text{otherwise,} \end{cases} \quad v_i = \begin{cases} 0 & \text{for } i = 1, \\ \sqrt{\frac{n-2}{c(n-1)}} h & \text{for } i = 2, \\ -\sqrt{\frac{1}{c(n-2)(n-1)}} h & \text{otherwise.} \end{cases}$$

Because $u_i = u_j$ $(ij \in E)$ the bounds are $\hat{l} = \sqrt{\xi} > c^{-1/2} = s_i^{-1/2}$ $(i \in N)$.

For $n \to \infty$ we obtain $\hat{l} \to c^{-1/2} = s_i^{-1/2}$ $(i \in N)$, $\|u_1\|^2 \to c^{-1/2}$ and $\|v_2\|^2 \to c^{-1/2}$. Thus, the bounds cannot be improved.

Remark 13 *The embeddings of complete graphs described in Example 5 allow to construct a sequence of problems and solutions with the property that $\hat{l} \to 0$ in Observation 11. Indeed, the analysis of the embedding yields $\|v_i\|^2 = \|u_i\|^2 = d^{-1}(s_i^{-1} - \bar{s}(M)^{-1})$ and $d^{-1}(s_i^{-1} - \bar{s}(M)^{-1}) < s_i^{-1}$ for $i \in M$. In addition,*

$$\hat{l}^2 = \max\{0, \ \|u_i\|^2 \ (i \in M), \ \|u_i - u_j\|^2 = d^{-1}(s_i^{-1} + s_j^{-1}) \ (i, j \in M)\}$$
$$= \max\{d^{-1}(s_i^{-1} + s_j^{-1}) : i, j \in M\}.$$

For $s = c\mathbf{1}$, $c > 0$ and $d > 2$ we have $s_i^{-1} = c^{-1} > \hat{l}^2 = 2(dc)^{-1}$ $(i \in N)$ and for, e.g., $d = n - 1$ and $n \to \infty$ we obtain $\hat{l} \to 0$.

4 Properties common to $(\mathrm{E}_{\lambda_n - \lambda_2})$ and (E_{λ_2}) or (E_{λ_n})

Graph realizations induced by optimal solutions of (E_{λ_2}) and (E_{λ_n}) are tightly linked to the separator structure of the graph, see [20] and [18]. The aim of this section is to investigate which of the properties of the single problems can be saved for the combined problem $(\mathrm{E}_{\lambda_n - \lambda_2})$. The first theorem states that for appropriate choices of ξ feasible solutions remain feasible. While feasibility is preserved, optimality may be lost.

Theorem 14 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, there exist appropriate values for the respective ξ variables so that feasible realizations U of (E_{λ_2}) and V of (E_{λ_n}) are feasible realizations (U, V) of $(\mathrm{E}_{\lambda_n - \lambda_2})$ and vice versa.*

Proof. For feasible solutions ξ_2, U of (E_{λ_2}) (ξ_2 may be negative) and ξ_n, V of (E_{λ_n}) the normalization constraints and the equilibrium constraint are satisfied. As $\xi = \xi_n + \xi_2$ fulfills the distance constraints, ξ, U, V is feasible for $(\mathrm{E}_{\lambda_n - \lambda_2})$ with data s and l.

On the other hand let ξ, U, V be feasible for $(E_{\lambda_n - \lambda_2})$. By choosing

$$\xi_2 = \max_{l_{ij} \neq 0} \left\{ \xi - \frac{\|v_i - v_j\|^2}{l_{ij}^2} \right\} \text{ and } \xi_n = \min_{l_{ij} \neq 0} \left\{ \frac{\|u_i - u_j\|^2}{l_{ij}^2} + \xi \right\}$$

U, ξ_2 is feasible for (E_{λ_2}) and V, ξ_n is feasible for (E_{λ_n}). ∎

Next we consider optimal realizations. It turns out that optimal realizations V of $(E_{\lambda_n - \lambda_2})$ for data $s > 0$ and $0 \neq l \geq 0$ are optimal for (E_{λ_n}) for data that are adapted appropriately.

Theorem 15 (Optimal V) *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let V be an optimal realization of $(E_{\lambda_n - \lambda_2})$. There exist data $0 \neq \bar{l} \geq 0$ so that V is optimal for (E_{λ_n}) with data s and $\bar{l}$. Furthermore, if G is not complete and $l > 0$, also $\bar{l} > 0$.*

Proof. Let U, V and ξ be an optimal solution of $(E_{\lambda_n - \lambda_2})$ and w an optimal solution of $(P_{\lambda_n - \lambda_2})$. Set $\bar{l}_{ij}^2 = \|v_i - v_j\|^2 \geq 0$ $(ij \in E)$. The proof is given in three steps: first we show $\bar{l} \neq 0$, then feasibility and third optimality of V in (E_{λ_n}) with data s and $\bar{l}$.

In the first step we have to consider two cases: G is not complete and G is complete. Let G be not complete then $\xi > 0$ by Obs. 4. For each edge $ij \in E$ with $l_{ij} > 0$ (there is at least one by $0 \neq l$) the distance constraint yields $\bar{l}_{ij}^2 = \|v_i - v_j\|^2 \geq l_{ij}^2 \xi > 0$. Thus, if $l > 0$, also $\bar{l} > 0$. If G is complete, $\bar{l} = 0$ is equivalent to $v_i = v_j$ $(i, j \in N)$. The latter, however, is impossible, because the normalization constraint requires $v_i \neq 0$ for some $i \in N$ and by optimality and Obs. 8 the barycenter lies in the origin. Hence $0 \neq \bar{l} \geq 0$.

V, $\hat{\xi} = 1$ is feasible for (E_{λ_n}) with data s and $\bar{l}$ because of the feasibility of V for $(E_{\lambda_n - \lambda_2})$ and the special choice of $\bar{l}$ and $\hat{\xi}$.

In the last step assume, for contradiction, that V and $\hat{\xi}$ is not optimal in (E_{λ_n}) with data s and $\bar{l}$, i. e., there exist feasible V' and $\xi' = 1 + \epsilon > \hat{\xi}$. Then for $ij \in E$ the distance constraints read $\|v_i' - v_j'\|^2 \geq \bar{l}_{ij}^2 \xi' = \|v_i - v_j\|^2 (1 + \epsilon) \geq \|v_i - v_j\|^2$. Therefore V', U and ξ is also feasible and optimal for $(E_{\lambda_n - \lambda_2})$ with data l. Note that $\|v_i' - v_j'\|^2 > \|v_i - v_j\|^2$ whenever $v_i \neq v_j$. In consequence, for V' and $ij \in E$ with $v_i \neq v_j$, the corresponding distance constraint of $(E_{\lambda_n - \lambda_2})$ is inactive and has, by complementarity, a zero multiplier $w_{ij} = 0$. Thus, for $ij \in E$ we have $v_i = v_j$ or $w_{ij} = 0$. The contradiction now follows from semidefinite complementarity (3), because $\lambda_n > 0$. ∎

An immediate consequence is that all structural properties observed in [18] for optimal solutions of (E_{λ_n}) also hold for optimal V of $(E_{\lambda_n - \lambda_2})$ whenever these do not depend on certain constraints being active or strictly active. In particular, we obtain the following two corollaries.

Corollary 16 (Sunny Side) *Given a graph $G = (N, E \neq 0)$ and data $s > 0$, $0 \neq l \geq 0$, let U, $V = [v_1, \ldots, v_n]$ be an optimal solution of $(E_{\lambda_n - \lambda_2})$. For any two disjoint nonempty subsets A and S of N such that each edge of the corresponding active subgraph $G_{U,V,\xi,l}$ leaving A ends in S, the barycenter $\bar{v}(A) = \frac{1}{s(A)} \sum_{i \in A} s_i v_i$ is contained in $\mathcal{S} = \text{aff}(V_S) - \text{cone}(V_S)$.*

Proof. Th. 15 above and [18](Th. 9). ∎

Corollary 17 *Given a graph $G = (N, E \neq 0)$ and data $s > 0$, $0 \neq l \geq 0$, let U, V be an optimal solution of $(\mathrm{E}_{\lambda_n - \lambda_2})$. There exists, for the same U, an optimal solution V' of $(\mathrm{E}_{\lambda_n - \lambda_2})$ of dimension at most 1 if the tree-width of G is one and of dimension tree-width of G plus one otherwise.*

Proof. Th. 15 above and [18](Th. 12; note, in its proof the transformations preserve all distances $\|v_i - v_j\|$ for $ij \in E$). ∎

There is an almost analogue result for (E_{λ_2}) and optimal U whenever the strictly active subgraph is connected, *i. e.*, whenever $\lambda_2(L_w) > 0$ for some optimal w of $(\mathrm{P}_{\lambda_n - \lambda_2})$. The proof is almost identical to that of Theorem 15, so we refrain from repeating it here.

Theorem 18 (Optimal U) *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let U be an optimal realization of $(\mathrm{E}_{\lambda_n - \lambda_2})$ and suppose there is an optimal w for $(\mathrm{P}_{\lambda_n - \lambda_2})$ resulting in a connected strictly active subgraph G_w. There exist data $0 \neq \bar{l} \geq 0$ such that U is optimal for (E_{λ_2}) with data s and $\bar{l}$.*

Again, we obtain two corollaries for structural properties observed in [20].

Corollary 19 (Separator-Shadow) *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let U be an optimal realization of $(\mathrm{E}_{\lambda_n - \lambda_2})$ and suppose there is an optimal w for $(\mathrm{P}_{\lambda_n - \lambda_2})$ resulting in a connected strictly active subgraph G_w. Let S be a separator in G_w giving rise to a partition $N = S \cup C_1 \cup C_2$ where there is no edge in E_w between C_1 and C_2. For at least one C_j with $j \in \{1, 2\}$*

$$\mathrm{conv}\{0, u_i\} \cap \mathrm{conv}\{u_s : s \in S\} \neq \emptyset \qquad \forall i \in C_j. \tag{7}$$

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

Proof. Th. 18 above and [20](Th. 1.4; note, its proof in [20] also works for $l \geq 0$). ∎

Corollary 20 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, suppose there is an optimal w for $(\mathrm{P}_{\lambda_n - \lambda_2})$ resulting in a connected strictly active subgraph G_w. There exists an optimal embedding U of $(\mathrm{E}_{\lambda_n - \lambda_2})$ of dimension at most the tree-width of G plus one.*

Proof. Th. 18 above and [20](Th. 1.5; note, in its proof the transformations preserve all distances $\|u_i - u_j\|$ for $ij \in E$). ∎

The condition of an optimal w giving rise to a connected strictly active subgraph in Theorem 18 is essential. The following example provides an instance of $(\mathrm{E}_{\lambda_n - \lambda_2})$ with an optimal U so that U is not the optimal solution of (E_{λ_2}) for any choice of $s > 0$ and $l \geq 0$.
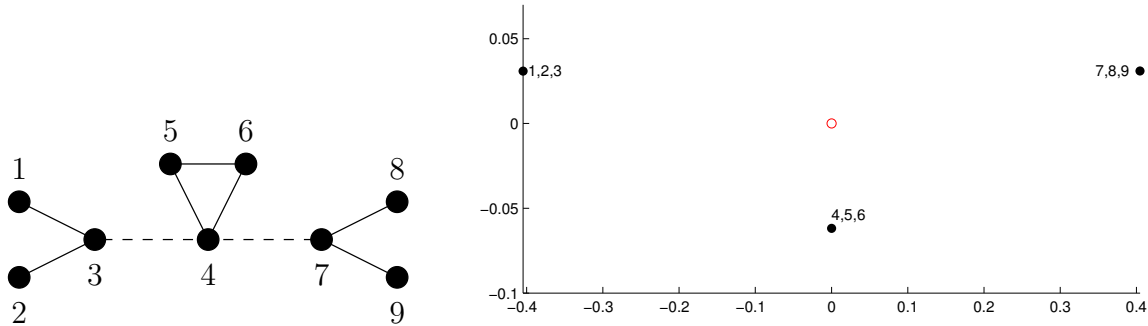
Figure 2: Graph G and optimal embedding U for $(E_{\lambda_n - \lambda_2})$ with data $s = \mathbf{1}$ and $l = \mathbf{1}$, the strictly active subgraph is not connected.

Example 21 *Consider the graph G of Figure 2 and let $s = \mathbf{1}$ and $l = \mathbf{1}$ be given data. The strictly active subgraph G_w is not connected, because dashed edges 34 and 47 have optimal weight zero. The plot on the right hand side of Figure 2 depicts a two-dimensional optimal embedding $U = [u_1, \ldots, u_9]$ of G for $(E_{\lambda_n - \lambda_2})$. There, each component is embedded into a separate point, i.e., $u_1 = u_2 = u_3 =: u_1'$, $u_4 = u_5 = u_6 =: u_s'$ and $u_7 = u_8 = u_9 =: u_2'$ with $u_s' \notin \operatorname{conv}\{0, u_1'\}$ and $u_s' \notin \operatorname{conv}\{0, u_2'\}$. For (E_{λ_2}) the Separator Shadow Theorem 1.5 of [20] holds, as noted above, for all connected graphs with data $s > 0$ and $l \geq 0$. Because $S = \{4, 5, 6\}$ is a separator in G separating $C_1 = \{1, 2, 3\}$ from $C_2 = \{7, 8, 9\}$, it requires $\operatorname{conv}\{0, u_i\} \cap \operatorname{conv}\{u_s : s \in S\} \neq \emptyset$ for all $i \in C_j$ for at least one $j \in \{1, 2\}$. So there are no choices of data $s > 0$ and $l \geq 0$ rendering U optimal for (E_{λ_2}).*

As an immediate consequence of Observation 9, optimal solutions of $(P_{\lambda_n - \lambda_2})$ are also optimal for (P_{λ_n}) whenever the strictly active subgraph is not connected.

Observation 22 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let ξ, U, V be optimal for $(E_{\lambda_n - \lambda_2})$ and λ_2, λ_n, μ and w be optimal for $(P_{\lambda_n - \lambda_2})$. If the strictly active subgraph G_w is not connected then ξ, V is optimal for (E_{λ_n}) and λ_n, w is optimal for (P_{λ_n}) with data s and l.*

Remark 23 *If for a graph $G = (V, E \neq \emptyset)$ whose strictly active subgraph is not connected, the connected components can be identified in advance, problem (P_{λ_n}) ((E_{λ_n}) respectively) can be solved by first computing the solution for each single component with the same data (disregarding isolated nodes) and by then combining these to an optimal solution of G via scaling, see Observation 6.*

Isolated nodes are a special case when considering connected components. In [18] it is shown, that in (E_{λ_n}) with data $s > 0$ and $l = \mathbf{1}$ a node is embedded in the origin if and only if it is isolated in the strictly active subgraph. It is no problem to generalize this for data $l = c\mathbf{1}$ by scaling. This is summarized together with another characterization in the next result.

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Observation 24 *Let $s > 0$ and $l = c\mathbf{1}$ with $c > 0$ be given data for a graph G with at least one edge. For $k \in N$ and optimal solutions w of (P_{λ_n}) and V of (E_{λ_n}) the following are equivalent,*

  (i) $v_k = 0$,

  (ii) k is an isolated node of G,

  (iii) k is an isolated node of the strictly active subgraph G_w.

Proof. (i) $\Rightarrow$ (ii): Let $v_k = 0$ then k is isolated because of the analogous result in [18] for $c = 1$ with an additional scaling argument.

(ii) $\Rightarrow$ (iii): If k is isolated in G, it is also isolated in the strictly active subgraph by definition.

(iii) $\Rightarrow$ (i): Let k be an isolated node in the strictly active subgraph and first suppose it is not isolated in G. Then $v_k = 0$ follows from the KKT condition for (E_{λ_n}) corresponding to (5), because $\lambda_n v_k = \sum_{ik \in E} w_{ik}(v_k - v_i)$, $w_{ik} = 0$ for $ik \in E$, and $\lambda_n \neq 0$ (because $E \neq \emptyset$).

It remains to consider the case of an isolated node k in the strictly active subgraph, that is also isolated in G. Assume for contradiction, that $v_k \neq 0$. Then we construct another feasible solution V' by setting $v_k' = 0$ and inflating the remaining graph such that the normalization constraint is satisfied again. Hence, all edge lengths are increased and we can improve the objective value which contradicts optimality of V. ∎

Almost the same results hold for $(\mathrm{E}_{\lambda_n - \lambda_2})$.

Observation 25 (isolated nodes - dual) *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let ξ, U and $V = [v_1, \ldots, v_n]$ be an optimal solution of $(\mathrm{E}_{\lambda_n - \lambda_2})$ and let w be optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$. A node $k \in N$ that is isolated in the strictly active subgraph G_w is embedded in the origin.*

Proof. If $v_k \neq 0$, shift it into the origin and inflate the remaining graph such that the normalization constraint is satisfied. The distances between all nodes in $N \setminus \{k\}$ increase, thus all the edge lengths increase and we may increase ξ without changing U. ∎

The converse implication is not true in general, see the complete graph of Example 5. On the other hand one can find graphs $G \neq K_n$ and data $0 \neq l \geq 0$, such that a node $k \in N$ that is not isolated in the strictly active subgraph is forced to the origin in V. Because of Observation 24 we conjecture that this is not possible whenever $l = c\mathbf{1}$ for some $c > 0$ and $G \neq K_n$. For bipartite graphs we are able to prove this, see Observation 31.

Observation 26 (isolated nodes - primal) *Let $s > 0$ and $l = c\mathbf{1}$, $c > 0$ be given data for a graph G with at least one edge and let w be optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$. A node $k \in N$ is isolated in G if and only if k is isolated in the strictly active subgraph G_w.*

Proof. Because $E_w \subseteq E$ a node k is isolated in G_w if it is isolated in G. It remains to consider the case of k being isolated in G_w. Because G_w is not connected, it suffices to invoke Obs. 22 and 24 to complete the proof. ∎

Again, Observation 26 does not hold for arbitrary $0 \neq l \geq 0$, in general. If we choose appropriate l, nodes that are not isolated in G may be isolated in G_w.

If G is connected, any optimal solution of (P_{λ_2}) yields a connected strictly active subgraph. So for connected graphs, a non connected strictly active subgraph indicates a dominance of (P_{λ_n}) over (P_{λ_2}). While the optimal value of (P_{λ_2}) is related to the connectivity of the graph — it is referred to as absolute algebraic connectivity of G in [12, 13] — k-connectivity cannot ensure connectedness of the strictly active subgraph in ($P_{\lambda_n - \lambda_2}$).

Example 27 (k-edge-connected graphs) *For $k \geq 1$, $s = \mathbf{1}$ and $l = \mathbf{1}$ let G be a graph on $12k$ nodes with edge set $E = \{ij : i, j \in \{1, \ldots, 3k\}, i \neq j\} \cup \{ij : i \in \{1 + rk, \ldots, k + rk\}, j \in \{1 + 3k(r+1), \ldots, 3k + 3k(r+1)\}, r \in \{0, 1, 2\}\}$. So the core of G consists of a complete graph on $3k$ nodes and for each of the core's three node disjoint subgraphs K_k further $3k$ independent nodes are fully linked to it (see Figure 3). Because there are k edge*
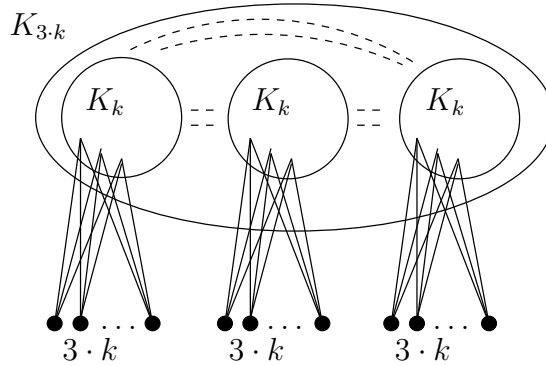

Figure 3: A k-edge-connected graph may have a disconnected strictly active subgraph (see Example 27).

disjoint paths between any two nodes $i, j \in V$, G is k-edge-connected.

Put $\omega = \frac{2}{3(7k^2 - k)}$. We prove in the following that an optimal solution with $\lambda_2 = 0$, $\mu = 0$ and $\lambda_n = 4k\omega$ is obtained by setting $w_{ij} = 0$ for edges ij that connect the three K_k (the dashed edges in Figure 3) and $w_{ij} = \omega$ for the other edges (ω normalizes the sum of these weights to 1). Note that the strictly active subgraph (V, E_w) consists of three connected components, so $\lambda_2 = 0$ by Observation 6. In order to see that indeed $\lambda_{\max}(L_w) = 4k\omega$ it suffices to consider the Laplacian block $\bar{L}_w \in \mathbb{R}^{4k \times 4k}$ of a single component. Let the first k columns and rows belong to the complete subgraph K_k. Then

$$x^\top(\lambda_n I - \bar{L}_w)x = \omega x^\top(4kI - \bar{L})x = \omega\left(\left(\sum_{i=1}^{4k} x_i\right)^2 + \sum_{k+1 \leq i < j \leq 4k}(x_i - x_j)^2\right) \geq 0 \quad \forall x \in \mathbb{R}^{4k}$$

and $\bar{L}_w \succeq 0$ yields feasibility. To show optimality it suffices to construct a feasible dual solution with identical objective value.

By Observation 9, in any optimal U of $(\mathrm{D}_{\lambda_n - \lambda_2})$ the nodes of each of the three components are mapped onto a single point. Because of the equilibrium constraint the three points form a regular triangle having its barycenter in the origin. Together with the normalization constraint this yields

$$\|u_i\|^2 = \frac{1}{12k}, \quad \|u_i - u_j\|^2 = \begin{cases} 0 & ij \in E \setminus E_w, \\ \frac{1}{4k} & ij \in E_w. \end{cases}$$

In an optimal V of $(\mathrm{D}_{\lambda_n - \lambda_2})$ each component results in a regular $(k+1)$-simplex where the $3k$ independent nodes are mapped onto a common vertex. We call the straight line segment connecting this special vertex to the barycenter of the remaining k vertices the height *of the simplex. Observe that — due to the $3k$ nodes assigned to the special vertex — the barycenter of the vertex weighted simplex splits the height into segments of relative length $1 : 3$. The requirement of identical primal and dual objective values forces the squared distances of the vertices to $\xi = \lambda_n = 4k\omega$. The length h of the height satisfies $h^2 = \frac{k+1}{2k}\xi$. By Obs. 8 the barycenter must coincide with the origin, resulting in the distances*

$$\|v_i\|^2 = \begin{cases} \frac{25k-7}{8}\omega & i \in \{1, \ldots, 3k\} \\ \frac{k+1}{8}\omega & i \in \{3k+1, \ldots, 12k\} \end{cases}, \quad \|v_i - v_j\|^2 = 4k\omega \ (ij \in E_w).$$

Finally, the distance constraints also need to hold for the zero-weighted-edges $ij \in E \setminus E_w$, so the corresponding distances should be as long as possible. For this, arrange the components heights in a common plane (they intersect in the components barycenters, which is in the origin) so that pairwise they enclose an angle of $2\pi/3$ and rotate the components around this height such that the affine subspaces spanned by the K_k are pairwise perpendicular and also perpendicular to the plane spanned by the heights (this is possible, because we do not restrict the dimension of the realization). Then for all edges in $E \setminus E_w$ one obtains the same length,

$$\|v_i - v_j\|^2 = \frac{59k - 5}{8}\omega > \xi \quad \text{for } ij \in E \setminus E_w.$$

Therefore these realizations are feasible and optimality is proven. Note, that the above construction yields a $(3k - 1)$-dimensional realization.

For $k = 2$ Figure 4 shows the graph, an optimal U and a three dimensional projection of an optimal V.

It seems unlikely that there is a simple structural property characterizing connected graphs whose strictly active subgraph is not connected for $(\mathrm{P}_{\lambda_n - \lambda_2})$ or even (P_{λ_n}). In order to shed some light on the embedding properties underlying the loss of connectedness, consider for
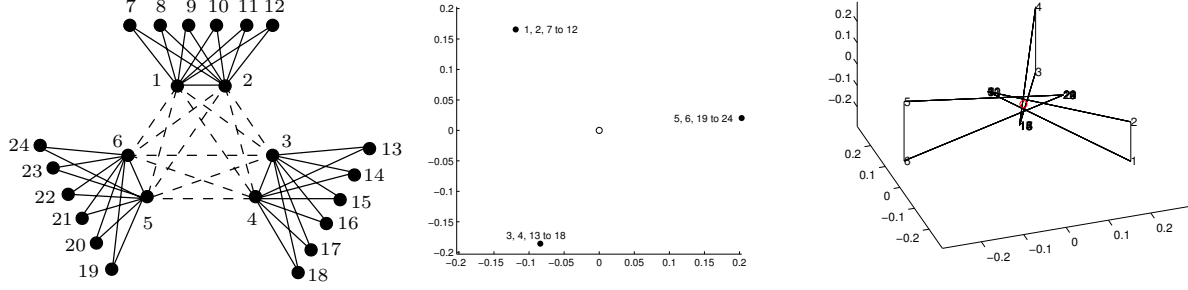
Figure 4: A 2-connected graph whose strictly active subgraph is disconnected (left), a corresponding optimal U (center) and a projection of an optimal V (right).

some given $\gamma \geq 0$ the primal dual pair of programs

$$
\begin{aligned}
\min \quad & \lambda_n - \gamma \lambda_2 \\
\text{subject to} \quad & \sum_{ij \in E} w_{ij} D E_{ij} D + \mu D^{-1} \mathbf{1} \mathbf{1}^\top D^{-1} - \lambda_2 I \succeq 0, \\
& \lambda_n I - \sum_{ij \in E} w_{ij} D E_{ij} D \succeq 0, \\
& \sum_{ij \in E} l_{ij}^2 w_{ij} = 1, \\
& \lambda_2, \lambda_n, \mu \in \mathbb{R}, \ w \geq 0.
\end{aligned} \tag{$\mathrm{P}_{\lambda_n - \gamma \lambda_2}$}
$$

$$
\begin{aligned}
\max \quad & \xi \\
\text{subject to} \quad & \sum_{i \in N} s_i \|u_i\|^2 = \gamma, \\
& \sum_{i \in N} s_i \|v_i\|^2 = 1, \\
& \| \sum_{i \in N} s_i u_i \|^2 = 0, \\
& \|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \xi \in \mathbb{R}, \ u_i, v_i \in \mathbb{R}^n \ (i \in N).
\end{aligned} \tag{$\mathrm{E}_{\lambda_n - \gamma \lambda_2}$}
$$

Note that the set of optimal solutions w to $(\mathrm{P}_{\lambda_n - \gamma \lambda_2})$ is compact by the same arguments leading to Observation 1. Given a connected graph G, whose strictly active subgraph is not connected for $\gamma = 0$, consider the development of optimal U in $(\mathrm{E}_{\lambda_n - \gamma \lambda_2})$ while increasing γ until the strictly active subgraph $G_{w,\gamma}$ becomes connected. At first $G_{w,\gamma}$ consists of components $G_{w,\gamma}^h = (N_{w,\gamma}^h, E_{w,\gamma}^h)$ and, by Observation 9, each node i of component h is embedded in a point $\bar{u}_h$, i.e., $u_i = \bar{u}_h$ for $i \in N_{w,\gamma}^h$. As γ is increased, the values $\|\bar{u}_h\|$ have to increase due to the normalization constraint for U. By the equilibrium constraints the distances $\|\bar{u}_h - \bar{u}_{h'}\|$ have to increase for at least two distinct components h and h' that are connected in G, so the distance constraint corresponding to an edge connecting the two components will become strictly active eventually, thereby reducing the number of components in the strictly active subgraph until only one connected component remains.

This intuitive explanation provides a geometric interpretation for the next result, whose proof is actually much simpler.

Observation 28 *For any connected graph $G = (N, E)$ and data $s > 0$, $0 \neq l \geq 0$ there is a $\underline{\gamma} \geq 0$ so that for all optimal w of $(\mathrm{P}_{\lambda_n - \gamma \lambda_2})$ with $\gamma > \underline{\gamma}$ the strictly active subgraph G_w is connected.*

Proof. Take some $\bar{w} > 0$ with $\sum_{ij \in E} l_{ij}^2 \bar{w}_{ij} = 1$, then $\lambda_2(L_{\bar{w}}) > 0$ (see the proof of Obs. 6(i)) and put $\underline{\gamma} = \lambda_{\max}(L_{\bar{w}})/\lambda_2(L_{\bar{w}})$. For $\gamma > \underline{\gamma}$ the value of $(\mathrm{P}_{\lambda_n - \gamma \lambda_2})$ is negative for this feasible $\bar{w}$, and because $\lambda_n > 0$ for all feasible w we must have $\lambda_2 > 0$ for all optimal w of $(\mathrm{P}_{\lambda_n - \gamma \lambda_2})$. The result now follows from Obs. 6 (i). ∎

The size of the smallest such $\underline{\gamma}(s, l)$ may be interpreted as representing the dominance of λ_n over λ_2 for data s and l. Again, it does not seem easy to determine this value on basis of structural properties of the graph.

At the end of this section we give some examples where optimal solutions of the coupled problem $(\mathrm{P}_{\lambda_n - \lambda_2})$ coincide with optimal solutions of just one, of both or of none of the single problems (P_{λ_2}) and (P_{λ_n}).

Example 29 *Let G be a graph consisting of two cycles of length n and additional edges $\{ij : j = n + i, \ j = n + 1 + ((i + 2) \mod n), \ i = 1, \ldots, n\}$ among them (see Figure 5). Let $s = \mathbf{1}$ and $l = \mathbf{1}$. Let $\lambda_2, \lambda_n, \mu, w_{ij} \ (ij \in E)$ be optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$. For*

- *$n = 5$ an optimal solution of $(\mathrm{P}_{\lambda_n - \lambda_2})$ is optimal for (P_{λ_2}) and optimal for (P_{λ_n}) for the same data s and l,*

- *$n = 6$ none of the single problems dominate the solution of $(\mathrm{P}_{\lambda_n - \lambda_2})$, i.e., $\lambda_2, \mu, w_{ij} \ (ij \in E)$ is not optimal for (P_{λ_2}) and $\lambda_n, w_{ij} \ (ij \in E)$ is not optimal for (P_{λ_n}) for the same data s and l,*

- *$n = 7$ an optimal solution of (P_{λ_2}) dominates that of $(\mathrm{P}_{\lambda_n - \lambda_2})$, i.e., $\lambda_2, \mu, w_{ij} \ (ij \in E)$ is optimal for (P_{λ_2}) and $\lambda_n, w_{ij} \ (ij \in E)$ is not optimal for (P_{λ_n}) for the same data s and l,*

- *$n = 9$ an optimal solution of (P_{λ_n}) dominates that of $(\mathrm{P}_{\lambda_n - \lambda_2})$, i.e., $\lambda_2, \mu, w_{ij} \ (ij \in E)$ is not optimal for (P_{λ_2}) and $\lambda_n, w_{ij} \ (ij \in E)$ is optimal for (P_{λ_n}) for the same data s and l.*

5 Special graph classes

In [18] bipartite graphs turned out to play a special role because for these graphs there always exist one-dimensional optimal realizations. It is therefore natural to look at optimal realizations V of $(\mathrm{E}_{\lambda_n - \lambda_2})$ for bipartite graphs first. Indeed, the existence of an optimal one-dimensional V-embedding for bipartite graphs is a direct consequence of Theorem 15 above and Theorem 12 in [18].
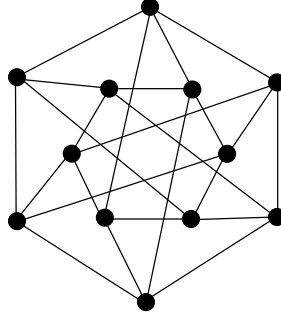
Figure 5: Graph G of Example 29 for $n = 6$.

Observation 30 *Let $s > 0$ and $0 \neq l \geq 0$ be given data and G a bipartite graph with at least one edge. There is a one-dimensional optimal realization V of $(\mathrm{E}_{\lambda_n - \lambda_2})$.*

Let $G = (N_1 \cup N_2, E \subseteq \{ij : i \in N_1, j \in N_2\})$ be bipartite with at least one edge, $s > 0$, $0 \neq l \geq 0$ be given data and $V = [v_1, \ldots, v_n]$ an optimal embedding of $(\mathrm{E}_{\lambda_n - \lambda_2})$. A one-dimensional optimal embedding corresponding to Observation 30 may be constructed via

$$v_i' = \begin{cases} \|v_i\| h & \text{for } i \in N_1, \\ -\|v_i\| h & \text{for } i \in N_2 \end{cases} \tag{8}$$

with $h \in \mathbb{R}^n$ and $\|h\| = 1$. This is used in the next observation, which is closely related to Observation 25.

Observation 31 *Let G be a bipartite graph with at least one edge and given data $s > 0$ and $l > 0$. In an optimal realization V of $(\mathrm{E}_{\lambda_n - \lambda_2})$ a node is embedded in the origin if and only if it is isolated in the strictly active subgraph.*

Proof. Because of Obs. 25 it remains to show that for the optimal one-dimensional realization $V = [v_1, \ldots, v_n] \in \mathbb{R}^{1 \times N}$ of $(\mathrm{E}_{\lambda_n - \lambda_2})$ constructed by (8) with $h = e_1$ any node $k \in N$ with $v_k = 0$ is isolated in the strictly active subgraph. It suffices to consider, w.l.o.g., $k \in N_2$ with at least one neighbor in G. For this k the KKT condition (5) reads $0 = \sum_{kj \in E} w_{kj} v_j$. By construction $v_j \geq 0$ ($kj \in E$) thus the condition requires every single summand to be zero. Suppose, for contradiction, that there is a neighbor j of k in the strictly active subgraph. Then also $v_j = 0$ and, by complementarity, the distance constraint corresponding to jk is active and reads $-\|u_j - u_k\|^2 - l_{jk}^2(\lambda_n - \lambda_2) = 0$, thus $\lambda_2 = \lambda_n + l_{ij}^{-2}\|u_j - u_k\|^2$. But $\lambda_2 \geq \lambda_n$ is possible only for complete graphs. The only complete graph that is bipartite is K_2 and $v_1 = v_2 = 0$ contradicts the normalization constraint. Thus, k is isolated in the strictly active subgraph. $\blacksquare$

Note that the restriction concerning data l cannot be dropped. If zero values are allowed there exist bipartite graph instances having a node embedded in the origin without the node being isolated in the strictly active subgraph.

For $l > 0$ the only reason for the existence of higher dimensional realizations V are the possibilities to rotate the connected components of the strictly active subgraph.

Observation 32 *Let G be a bipartite graph with at least one edge and given data $s > 0$ and $l > 0$. In an optimal realization V of $(\mathrm{E}_{\lambda_n - \lambda_2})$ each connected component of the strictly active subgraph is one-dimensional.*

Proof. Consider an arbitrary optimal solution U, V, ξ of $(\mathrm{E}_{\lambda_n - \lambda_2})$, a corresponding (optimal) one-dimensional realization V' as defined in (8) and an optimal solution λ_2, λ_n, w of $(\mathrm{P}_{\lambda_n - \lambda_2})$. For $ij \in E_w$ complementarity implies $\|u_i - u_j\|^2 + l_{ij}^2 \xi = \|v_i - v_j\|^2 = \|v_i' - v_j'\|^2 = (\|v_i'\| - \|v_j'\|)^2 = (\|v_i\| - \|v_j\|)^2$. Together with Obs. 31 this asserts that $v_i \neq 0$ and $v_j \neq 0$ are linearly dependent. Because a component is connected, all corresponding nodes are linearly dependent. Hence any component of G_w is one-dimensional. ■

In the remainder of this section we consider properties of optimal solutions connected to the symmetry of the underlying graph. Considering symmetry in semidefinite programming is profitable in general (see, *e. g.*, [3, 4, 8, 9, 10, 15, 26, 27, 40]) and much of the following is directly implied by the more general theory. Still it seems to be worth to highlight a few basic properties in a short and self contained exposition.

An *automorphism* φ of a graph $G = (N, E)$ is a permutation of the vertices N that leaves the edge set E invariant, *i. e.*, $\varphi : N \to N$ and $ij \in E$ if and only if $\varphi(i)\varphi(j) \in E$. For simplicity, we write $\varphi(ij)$ instead of $\varphi(i)\varphi(j)$. If there are given node weights s_i ($i \in N$) and edge weights l_{ij} ($ij \in E$) then we extend the definition by requiring that $\varphi : N \to N$ is an automorphism of G with weights s and l if $ij \in E$ if and only if $\varphi(ij) \in E$, $s_k = s_{\varphi(k)}$ ($k \in \{i, j\}$), and $l_{ij} = l_{\varphi(ij)}$ (see also [4]). It is well known that the set of all automorphisms of G forms the automorphism group $\mathrm{Aut}(G)$. The same holds for the automorphisms of G with weights s and l. We denote this group by $\mathrm{Aut}(G, s, l)$. Note that $\mathrm{Aut}(G, s, l) \subseteq \mathrm{Aut}(G)$ and $\mathrm{Aut}(G, c_s \mathbf{1}, c_l \mathbf{1}) = \mathrm{Aut}(G)$ for $c_s, c_l \in \mathbb{R}$. The orbits $E_1, \ldots, E_k$ of the edge set E under the action of $\mathrm{Aut}(G, s, l)$ give rise to a partition of E. Furthermore if the edges e_1, e_2, e_3, e_4 (not necessarily different) lie in the same orbit, then $|\{\varphi \in \mathrm{Aut}(G, s, l) : \varphi(e_1) = e_2\}| = |\{\varphi \in \mathrm{Aut}(G, s, l) : \varphi(e_3) = e_4\}| \neq 0$. We assign to each orbit E_r ($r = 1, \ldots, k$) the number of automorphisms $a_r = |\{\varphi \in \mathrm{Aut}(G, s, l) : \varphi(e) = e'\}|$ with $e, e' \in E_r$. This leads to the following observation (which may also be seen as a direct consequence of Lagrange's theorem in group theory).

Observation 33 *Let G be a graph with weights s and l, $\mathrm{Aut}(G, s, l)$ its automorphism group and $E_1, \ldots, E_k$ the orbits of the edge set E. Then $|\mathrm{Aut}(G, s, l)| = a_r \cdot |E_r|$ for $r = 1, \ldots, k$.*

Proof. Enumerate the edges, $E = \{e_1, \ldots, e_m\}$, and let $e_1 \in E_r$ for some $r \in \{1, \ldots, k\}$.
$$|\mathrm{Aut}(G, s, l)| = \sum_{\varphi \in \mathrm{Aut}(G, s, l)} 1 = \sum_{e_i \in E} \sum_{\substack{\varphi \in \mathrm{Aut}(G, s, l) \\ \varphi(e_1) = e_i}} 1 = \sum_{e_i \in E_r} \sum_{\substack{\varphi \in \mathrm{Aut}(G, s, l) \\ \varphi(e_1) = e_i}} 1 = \sum_{e_i \in E_r} a_r = a_r \cdot |E_r|. \blacksquare$$

An automorphism of a graph does not change the graph's structure, so the next observation about optimal primal solutions of $(\mathrm{P}_{\lambda_n - \lambda_2})$ follows immediately.

Observation 34 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let $\varphi \in \mathrm{Aut}(G, s, l)$ and let λ_2, λ_n, μ and w_{ij} $(ij \in E)$ be optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$. Then λ_2, λ_n, μ and $w_{\varphi(ij)}$ $(ij \in E)$ is also optimal for $(\mathrm{P}_{\lambda_n - \lambda_2})$.*

Because any convex combination of optimal solutions is again optimal, there is a special primal optimal solution with the property that all edges within the same orbit of the automorphism group have the same weight. So this solution is invariant under the group action (see, *e. g.*, [10, 15, 40]).

Observation 35 *Given $G = (N, E \neq \emptyset)$ and data $s > 0$, $0 \neq l \geq 0$, let $E_1, \ldots, E_k$ be the orbits of the edge set E under the action of the automorphism group $\mathrm{Aut}(G, s, l)$. There exists an optimal solution of $(\mathrm{P}_{\lambda_n - \lambda_2})$ with $w_{ij} = c_r \geq 0$ for $ij \in E_r$ $(r = 1, \ldots, k)$.*

Proof. Let λ_2, λ_n, μ and w_{ij} $(ij \in E)$ be optimal in $(\mathrm{P}_{\lambda_n - \lambda_2})$. For $\varphi \in \mathrm{Aut}(G, s, l)$ the solution λ_2, λ_n, μ and $w_{\varphi(ij)}$ $(ij \in E)$ is optimal by Obs. 34. Using Obs. 33 define new weights $\hat{w}_{ij}$ for $ij \in E_r$ $(r \in \{1, \ldots, k\})$ via

$$|\mathrm{Aut}(G, s, l)|\hat{w}_{ij} = \sum_{\varphi} w_{\varphi(ij)} = \sum_{xy \in E} \sum_{\varphi(ij) = xy} w_{\varphi(ij)} = \sum_{xy \in E_r} \sum_{\varphi(ij) = xy} w_{xy} = a_r \cdot \sum_{xy \in E_r} w_{xy}. \quad (9)$$

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

Remark 36 *The same arguments yield analogous results for (P_{λ_n}) and (P_{λ_2}).*

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

Observation 37 (edge transitive graphs, see also [3]) *Let $G = (N, E)$ be edge transitive with at least one edge and $s = c_s \mathbf{1} > 0$, $l = c_l \mathbf{1} > 0$ be given data. There is an optimal solution of $(\mathrm{P}_{\lambda_n - \lambda_2})$, of (P_{λ_n}) and of (P_{λ_2}) with edge weights $w_{ij} = \frac{1}{|E|c_l^2}$ $(ij \in E)$.*

Proof. Because $\mathrm{Aut}(G) = \mathrm{Aut}(G, c_s\mathbf{1}, c_l\mathbf{1})$ and because the single orbit is the entire edge set E, Obs. 33 asserts $|\mathrm{Aut}(G)| = a_1 \cdot |E|$. With this, (9) of Obs. 35 yields the result. ∎

Observation 38 *Let $G = (N, E)$ be edge transitive, $s = c_s\mathbf{1} > 0$ and $l = c_l\mathbf{1} > 0$ given data. Then optimal λ_2 of (P_{λ_2}) and optimal λ_n of (P_{λ_n}) are also optimal in $(\mathrm{P}_{\lambda_n - \lambda_2})$.*

6   Variable edge length parameters

In order to interpret the eigenvectors of the unweighted Laplace matrix of a graph in terms of the graph realization results, it is helpful to consider $(\mathrm{E}_{\lambda_n - \lambda_2})$ with $s = \mathbf{1}$ but with variable edge length parameters l_{ij}^2 $(ij \in E)$ subject to a normalization constraint

$\sum_{ij \in E} l_{ij}^2 \geq 1$. Some normalization is needed, because otherwise the problem would be unbounded.

$$
\begin{aligned}
\xi_* = \quad & \max \quad \xi \\
& \text{subject to} \quad \sum_{i \in N} \|u_i\|^2 = 1, \\
& \qquad \qquad \quad \sum_{i \in N} \|v_i\|^2 = 1, \\
& \qquad \qquad \quad \|\sum_{i \in N} u_i\|^2 = 0, \qquad \qquad \qquad \qquad (\text{E}_{\lambda_n - \lambda_2, l}) \\
& \qquad \qquad \quad \sum_{ij \in E} l_{ij}^2 \geq 1, \\
& \qquad \qquad \quad \|v_i - v_j\|^2 - \|u_i - u_j\|^2 - l_{ij}^2 \xi \geq 0 \quad (ij \in E), \\
& \qquad \qquad \quad \xi \in \mathbb{R}, \ u_i, v_i \in \mathbb{R}^n \ (i \in N), \ l_{ij}^2 \geq 0 \ (ij \in E).
\end{aligned}
$$

The l_{ij}^2 may be viewed as simple nonnegative variables, so $(\text{E}_{\lambda_n - \lambda_2, l})$ is again a nonconvex quadratic program. By exploiting the fact that $\xi_* > 0$ whenever $G \neq K_n$, the bilinear terms $l_{ij}^2 \xi$ can be eliminated by dividing all constraints by ξ so as to obtain an equivalent semidefinite problem in analogy to $(\text{D}_{\lambda_n - \lambda_2})$. Using the scaled variables $\bar{X} = X/\xi$ and $\bar{Y} = Y/\xi$, the maximization of ξ then corresponds to minimizing $\langle I, \bar{X} \rangle$. For $G \neq K_n$, this results in the semidefinite program

$$
\begin{aligned}
\tfrac{1}{\xi_*} = \quad & \min \quad \langle I, \bar{X} \rangle, \\
& \text{subject to} \quad \langle I, \bar{X} \rangle - \langle I, \bar{Y} \rangle = 0, \\
& \qquad \qquad \quad \langle \mathbf{1}\mathbf{1}^\top, \bar{X} \rangle = 0, \\
& \qquad \qquad \quad \langle E_{ij}, \bar{Y} \rangle - \langle E_{ij}, \bar{X} \rangle - l_{ij}^2 \geq 0 \quad (ij \in E), \qquad (\text{D}_{\lambda_n - \lambda_2, l}) \\
& \qquad \qquad \quad \sum_{ij \in E} l_{ij}^2 \geq 1, \\
& \qquad \qquad \quad \bar{X}, \ \bar{Y} \succeq 0, \ l_{ij}^2 \geq 0 \ (ij \in E).
\end{aligned}
$$

Its dual, $i.\,e.$, the problem corresponding to the primal $(\text{P}_{\lambda_n - \lambda_2})$, reads

$$
\begin{aligned}
& \max \quad \rho \\
& \text{subject to} \quad (1 - \lambda)I - \mu \mathbf{1}\mathbf{1}^\top + \sum_{ij \in E} w_{ij} E_{ij} \succeq 0, \\
& \qquad \qquad \quad \lambda I - \sum_{ij \in E} w_{ij} E_{ij} \succeq 0, \qquad \qquad \qquad \qquad (\text{P}_{\lambda_n - \lambda_2, l}) \\
& \qquad \qquad \quad \rho - w_{ij} = 0 \quad (ij \in E), \\
& \qquad \qquad \quad \lambda, \ \mu \in \mathbb{R}, \ w \geq 0, \ \rho \geq 0.
\end{aligned}
$$

Due to the constraints $\rho = w_{ij}$ for $ij \in E$ this problem reduces to finding λ and μ so as to maximize ρ with

$$
(\lambda - 1)I \preceq \rho L(G) - \mu \mathbf{1}\mathbf{1}^\top \preceq \lambda I.
$$

Like in [25] we obtain the following theorems exhibiting the direct relation between optimal solutions of $(\text{E}_{\lambda_n - \lambda_2, l})$ and the eigenvectors of $\lambda_2(L(G))$ and $\lambda_{\max}(L(G))$ whenever G is not complete. The proofs are almost identical to those in [25] and are therefore omitted.

Theorem 39 *Given a graph $G = (N, E)$ that is not complete, let $U = [u_1, \ldots, u_n]$, $V = [v_1, \ldots, v_n]$ be an optimal solution of $(\mathrm{E}_{\lambda_n - \lambda_2, l})$. Then $\xi_* = \lambda_{\max}(L(G)) - \lambda_2(L(G))$ and for $h \in \mathbb{R}^n$ the vector $U^\top h$ is an eigenvector of $\lambda_2(L(G))$ and the vector $V^\top h$ is an eigenvector of $\lambda_{\max}(L(G))$.*

Theorem 40 *Given a graph $G = (N, E)$ that is not complete, let $u \in \mathbb{R}^n$, $\|u\| = 1$, be an eigenvector of $\lambda_2(L(G))$ and let $v \in \mathbb{R}^n$, $\|v\| = 1$ be an eigenvector of $\lambda_{\max}(L(G))$. An optimal solution of $(\mathrm{D}_{\lambda_n - \lambda_2, l})$ is $\bar{X} = \frac{1}{\lambda_{\max}(L(G)) - \lambda_2(L(G))} u u^\top$, $\bar{Y} = \frac{1}{\lambda_{\max}(L(G)) - \lambda_2(L(G))} v v^\top$ and $l_{ij}^2 = \frac{(v_i - v_j)^2 - (u_i - u_j)^2}{\lambda_{\max}(L(G)) - \lambda_2(L(G))}$, $ij \in E$.*

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