Embedding optimization problems for a graph related to Laplacian eigenvalue maximization (ラプラシアン固有値の最大化に関連するグラフ の埋め込み最適化問題)

Takumi Gomyou

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Introduction

We study graph embedding problems that are related to an optimization problem maximizing the first nonzero eigenvalue of the graph Laplacian.

An embedding of a finite graph associates a point in a Euclidean space to each vertex of the graph. Then the whole geometric graph, in which all pairs of adjacent vertices are joined by arcs, is realized in the same Euclidean space by joining the image points of adjacent vertices by straight line segments. (Notice that though we use the terminology "embedding", we allow different vertices are associated with a common point of the Euclidean space.) In the graph embedding problem introduced by Göring-Helmberg-Wappler [10, 11], one looks for a graph embedding such that the image points of all vertices are located in the Euclidean space as far apart to each other as possible, while keeping their affine barycenter at the origin and the distances of adjacent vertices equal to or less than 1 (or length parameters in the generalized problem).

If a semidefinite programming problem, referred to as a primal problem, is given, a new semidefinite programming problem is derived from it as a dual problem by appropriately defining a Lagrange function. Interpreting an eigenvalue maximization problem as a semidefinite programming problem, Göring-Helmberg-Wappler [10] derived the embedding optimization problem mentioned above as a dual problem. For a finite weighted graph G = (V, E, w), where $w \in (\mathbb{R}_{\geq 0})^{|E|}$ is an edge weight, let L(G, w) be the graph Laplacian with respect to w. The first eigenvalue of L(G, w) is zero and the second eigenvalue is positive, when the graph G is connected. Fiedler [7] focused on the second eigenvalue $\lambda_2(G, w)$, which is related to graph connectivity, and introduced the following optimization problem:

Problem 0.1.

$$\begin{aligned} \text{maximize} \quad & \lambda_2(G, w) \\ \text{subject to} \quad & \sum_{ij \in E} w_{ij} = |E|, \\ & w \in (\mathbb{R}_{\geq 0})^{|E|}. \end{aligned}$$

Let $\hat{a}(G)$ be the optimal value of this problem.

Fiedler called the optimal value $\hat{a}(G)$ the absolute algebraic connectivity of G [7]. This problem is associated with the following embedding problem via Lagrange primal-dual approach to semidefinite programming problems by Göring et al. as mentioned above.

Problem 0.2 (Problem 4.3).

$$\begin{split} \text{maximize} \quad & \sum_{i \in V} ||v_i||^2 \\ \text{subject to} \quad & || \sum_{i \in V} v_i||^2 = 0, \\ & \quad & ||v_i - v_j|| \leq 1, \quad \forall ij \in E, \\ & \quad & v_i \in \mathbb{R}^n, \quad \forall i \in V. \end{split}$$

Example 1. For a complete graph, a regular simplex with side length one is an optimal solution for Problem 0.2. This embedding is a unique optimal solution by regarding the embeddings which differ by a rotation around the origin as essentially the same embeddings.

Let $s = {}^{t}(\cdots, s_{i}, \cdots) \in (\mathbb{R}_{\geq 0})^{n}$ be a vertex weight vector and $l = {}^{t}(\cdots, l_{ij}, \cdots) \in (\mathbb{R}_{\geq 0})^{|E|}$ be an edge length vector. When defining a Laplacian, we assume that the components of the vertex weight vector s are all positive. The following is the generalized embedding problem.

Problem 0.3 (Problem 9.1).

$$\begin{aligned} \text{maximize} \quad & \sum_{i \in V} s_i ||v_i||^2 \\ \text{subject to} \quad & ||\sum_{i \in V} s_i v_i||^2 = 0, \\ & ||v_i - v_j|| \leq l_{ij}, \quad \forall ij \in E, \\ & v_i \in \mathbb{R}^n, \quad \forall i \in V. \end{aligned}$$

The rotational dimension is defined by maximizing, over all s and l, the minimum dimension of an optimal embedding.

Definition 0.4 (rotational dimension, Göring-Helmberg-Wappler [11]).

$$\operatorname{rotdim}_G(s,l) := \min \{ \dim \operatorname{span} \{ v_i \mid i \in V \} \mid \\ (v_i)_{i \in V} \text{ is an optimal solution for Problem 0.3} \},$$
$$\operatorname{rotdim}_G(s,l) \mid s \in (\mathbb{N} \cup \{0\})^{|V|}, l \in (\mathbb{N} \cup \{0\})^{|E|} \}.$$

Here dim span $\{v_i \mid i \in V\}$ is the dimension of the linear subspace spanned by $(v_i)_{i \in V}$. The value rotdim(G) is called the *rotational dimension* of G.

The rotational dimension is a minor-monotone graph invariant. Several other minor-monotone invariants or optimal embeddings related to the multiplicity of the second Laplacian eigenvalue are also known, such as the Colin de Verdière number and the valid representation. Van der Holst-Lovász-Schrijver present a survey on the Colin de Verdière number in [22]. The valid representation is the graph embedding introduced by Van der Holst-Laurent-Schrijver in [21].

The rotational dimension is bounded by other graph invariants. For any graph G

$$\omega(G) - 1 \le \operatorname{rotdim}(G) \le \operatorname{tw}(G) + 1 \tag{0.1}$$

holds [11], where $\omega(G)$ is the clique number of G and $\mathrm{tw}(G)$ is the tree-width of G.

In this thesis, we mainly study the following two problems.

(i): The rotational dimension of a graph containing a large complete graph.

The rotational dimension of the complete graph on n vertices is n-1. Since the rotational dimension is a minor-monotone graph invariant, for any n vertices graph G we have $\operatorname{rotdim}(G) \leq n-1$. One of the main results is the characterization of the complete graph by its rotational dimension.

Theorem 0.5 (Theorem 6.3). If G is a graph on n vertices, then

$$\operatorname{rotdim}(G) = n - 1$$
 if and only if $G = K_n$.

For the valid representation invariant $\lambda(G)$ a similar result is known [21]. Let $K_n \setminus \{e\}$ be a graph obtained by removing one edge e from the complete graph K_n . Since an arbitrary graph on n vertices which is not complete is a minor of $K_n \setminus \{e\}$, Theorem 0.5 is proved by showing that the rotational dimension of $K_n \setminus \{e\}$ equals to n-2.

Theorem 0.6 (Theorem 6.5).

$$\operatorname{rotdim}(K_n \setminus \{e\}) = n - 2.$$

For this graph the optimal embedding for Problem 0.2 is found uniquely, and the vertices of a complete subgraph K_m are located at the vertices of an (m-1)-regular simplex. In general, for an optimal embedding of an arbitrary graph its complete subgraph K_m is not embedded as an (m-1)-regular simplex, but this statement is true under a certain natural assumption.

We study rotational dimensions of graphs including large cliques such as $K_n \setminus \{e\}$. We consider a chordal graph. For a chordal graph the bounds of the rotational dimension (0.1) are tight. In fact, if G is a chordal graph, then we have

$$\omega(G) - 1 \le \operatorname{rotdim}(G) \le \omega(G).$$

Applying the properties of a chordal graph, we may make a chordal graph larger while keeping the rotational dimension constant. For example, we can determine the rotational dimension of the graph of order n + k in which n vertices form K_n and each of the remaining k vertices is adjacent to all the vertices of K_n . Note that this graph generalizes $K_{n-2} \setminus \{e\}$.

(ii): Another embedding problem.

In [9], we introduced an embedding optimization problem which is different from that introduced by Göring-Helmberg-Wappler.

Problem 0.7 (Problem 8.1).

minimize
$$\left\| \frac{1}{\sum_{i \in V} s_i} \sum_{i \in V} s_i v_i \right\|^2$$
subject to
$$\frac{1}{\sum_{i \in V} s_i} \sum_{i \in V} s_i ||v_i||^2 = 1,$$
$$||v_i - v_j|| \le l_{ij}, \quad \forall i j \in E,$$
$$v_i \in \mathbb{R}^n, \quad \forall i \in V.$$

This problem is also related to an optimization problem concerning the smallest nonzero eigenvalue of the graph Laplacian. We establish a relation between the optimal values of Problems 0.3 and 0.7. It then follows that the optimal value of Problem 0.7 can be computed explicitly in terms of the optimal value of the eigenvalue optimization problem. Further, we show that our embedding problem is also dual to the eigenvalue optimization problem.

Theorem 0.8. Problem 0.7 is dual to the eigenvalue optimization problem via the Lagrange approach to semidefinite programming problems.

We present examples of graphs isomorphic to the 1-skeletons of regular and semiregular polyhedra. These polyhedra arise as optimal embeddings of the 1-skeleton graphs for Problem 0.2. The fullerene graph C_{60} that is isomorphic to the 1-skeleton of a truncated icosahedron is one example. The graph C_{60} has 60 vertices and 90 edges, 60 of which are pentagonal edges and the remaining 30 of which are hexagonal ones. For the parameter $l \equiv 1$, the truncated icosahedron with side length one is obtained as an optimal embedding of C_{60} . Further, if we consider the case that the parameter l is given by

$$l_{ij} = \begin{cases} a & \text{if } ij \text{ is a pentagonal edge,} \\ b & \text{if } ij \text{ is a hexagonal edge,} \end{cases}$$

then the truncated icosahedron in which the ratio of the length of a pentagonal edge to that of a hexagonal edge is a:b is obtained as an optimal embedding for Problem 0.3.

About this thesis

This thesis is organized as follows. In Part 1 we introduce the basic notions and results. In Part 2 we recall the work on the optimal dimensions of graphs by Göring-Helmberg-Wappler. We derive the embedding problem dual to the optimization problem whose optimal value is the absolute algebraic connectivity. In addition we describe the properties of the optimal dimensions of graphs. In Part 3 we consider a graph obtained by removing one edge from a complete graph, and find the optimal embedding and the optimal dimension of this graph. We study the rotational dimension of a chordal graph. With a given chordal graph G, we present a way to construct a larger chordal graph containing G as a minor without changing the rotational dimension. In the final part, we define a new embedding problem which is different from the problem introduced by Göring et al. We study the relation between the two embedding problems, and show that our embedding problem is also dual to the eigenvalue optimization problem. We present examples of graphs for which these optimization problems can be explicitly solved.

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Part I

Preliminaries

This part provides basic concepts and results used in this thesis.

1 Linear Algebra

For $m \times n$ matrices $A = (a_{ij})$ and $B = (b_{ij})$, let $\langle \cdot, \cdot \rangle$ be an inner product given by

$$\langle A, B \rangle = \operatorname{tr}({}^{t}BA) = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}b_{ij}.$$

 Sym_n denotes the set of all $n \times n$ symmetric matrices. If a symmetric matrix X is positive semidefinite, this is denoted by $X \succeq 0$. All eigenvalues of a semidefinite matrix are nonnegative.

Proposition 1.1. For a symmetric matrix X, the following are equivalent.

(i)
$$X \succeq 0$$
,

(ii)
$$\langle X, Y \rangle > 0$$
, $\forall Y \succ 0$.

Proof. See, e.g. Corollary 7.5.4 in [20].

Proposition 1.2. For $A, B \in Sym_n$, let $\lambda_i(A)$, $\lambda_i(B)$ and $\lambda_i(A+B)$ be the eigenvalues of A, B and A+B, respectively, where they are ordered as $\lambda_1 \leq \cdots \leq \lambda_n$. Then for $i=1,\cdots,n$,

$$\lambda_1(A) + \lambda_i(B) \le \lambda_i(A+B) \le \lambda_n(A) + \lambda_i(B).$$

Proof. See, e.g. Corollary 4.3.7 in [20].

If X is represented as $X = {}^tVV$ by using a square matrix V, then X is called a Gram matrix.

Proposition 1.3. A matrix is positive semidefinite if and only if it is a Gram matrix.

Proof. For an $n \times n$ matrix X let $\{\lambda_i \mid i = 1, \dots, n\}$ be the set of its eigenvalues. We assume $X \succeq 0$. Then $\lambda_i \geq 0$ for $i = 1, \dots, n$ and X is represented by a diagonal matrix and an orthogonal matrix P as follows:

$$X = P \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} {}^t P.$$

Now by letting

$$V = \begin{pmatrix} \sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n} \end{pmatrix} {}^t P,$$

it follows that $X = {}^{t}VV$, that is, X is a Gram matrix.

On the other hand, let X be a Gram matrix of the form $X = {}^t AA$, where A is some $n \times n$ matrix. For an arbitrary $x \in \mathbb{R}^n$ we obtain

$${}^{t}xXx = {}^{t}x {}^{t}AAx = \langle Ax, Ax \rangle \ge 0.$$

Thus X is positive semidefinite.

Proposition 1.4. For $X, Y \succeq 0$, the equation $\langle X, Y \rangle = 0$ holds if and only if XY is the zero matrix.

Proof. It is clear that $\langle X, Y \rangle = 0$ holds when XY = 0. For the converse, if X and Y are positive semidefinite matrices, then they can be represented by $X = {}^tVV$ and $Y = {}^tUU$ using some square matrices V and U. Thus we have

$$\langle X, Y \rangle = \operatorname{tr}(XY) = \operatorname{tr}({}^tV(V{}^tUU)) = \operatorname{tr}((V{}^tUU){}^tV) = \operatorname{tr}(V{}^tU{}^t(V{}^tU)).$$

If $\langle X, Y \rangle = 0$, then V^tU is the zero matrix. Then $XY = {}^tVV^tUU = 0$.

2 Graph Theory

Unless otherwise noted, we deal with undirected and simple graphs. Let G = (V, E, w) be a finite graph, where $V = \{1, \dots, n\}$ is the vertex set, $E = \{ij \mid i, j \in V, i \text{ is adjacent to } j\}$ is the edge set, $w = {}^t(\dots w_{ij} \dots) \in (\mathbb{R}_{\geq 0})^{|E|}$ is an edge weight vector. Let E_{ij} be a symmetric $n \times n$ matrix whose ii and jj components are 1, ij and ji components are -1, and all other components are zero. The Laplacian matrix of G with an edge weight w is defined by

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

The Laplacian L(G, w) is positive semidefinite, because for $x = {}^{t}(x_1, \dots, x_n)$, a quadratic form is

$${}^{t}xL(G,w)x = \frac{1}{2}\sum_{i,j}w_{ij}(x_i - x_j)^2.$$
(2.1)

The Laplacian L(G, w) of G has the eigenvalue 0 with the eigenvector e in which all components are 1. Thus eigenvalues of L(G, w) are ordered as $0 = \lambda_1(L(G, w)) \le \lambda_2(L(G, w)) \le \cdots \le \lambda_n(L(G, w))$. The eigenvalues of the Laplacian have information about the connectivity of a graph.

Proposition 2.1. If G is a connected graph, then the geometric multiplicity of eigenvalue 0 is one.

Proof. Let $x \in \text{Ker}(L(G, w))$. Then the right-hand side of the equation (2.1) equals zero and so

$$x_i = x_j, \quad \forall ij \in E.$$

This means that all x_i are equal, because G is connected. Then the dimension of $\operatorname{Ker}(L(G,w))$ is one.

Corollary 2.2. The number of components of a graph is equal to the geometric multiplicity of eigenvalue 0 of the Laplacian.

Minors of graphs are also important in our discussion.

Definition 2.3 (minor). A graph G' obtained from a graph G by repeating three operations (i) deletion of an isolated vertex in G, (ii) deletion of an edge in G, is called a *minor* of G. We write $G \succeq G'$.

The graph minor theory began with Wagner's theorem that characterizes a planar graph by using graph minor.

Definition 2.4 (planar graph). A *planar graph* is a graph that can be drawn on a plane in such a way that no edges cross each other.

Theorem 2.5 (Wagner [23]). A graph G is planar if and only if G does not contain the complete graph K_5 or the complete bipartite graph $K_{3,3}$ as a minor.

For outer planar graphs we have a similar characterization.

Definition 2.6 (outer planar graph). An *outer planar graph* is a graph that can be drawn on a plane such that every vertex lies on the outer face.

Theorem 2.7 (Chartrand and Harary [3]). A graph G is outer planar if and only if G does not contain the complete graph K_4 or the complete bipartite graph $K_{2,3}$ as a minor.

There is a survey on the graph minor theory in [16].

Definition 2.8. A tree-decomposition of a graph G = (V, E) is a tree T whose vertex set V(T) is a family of subsets of V, satisfying the following properties.

- (i) $V = \bigcup_{U \in V(T)} U$,
- (ii) for any edge $e \in E$ there exists $U \in V(T)$ such that $e \subset U$,
- (iii) If $U_1, U_2, U_3 \in V(T)$ and the path between U_1 and U_2 contains U_3 , then $U_3 \supset U_1 \cap U_2$.

The width of a tree-decomposition T is the cardinality of the largest size subset $U \in V(T)$ of V minus 1, and the tree-width $\operatorname{tw}(G)$ of a graph G is the minimum width of a tree-decomposition of G.

Example 2. The tree-width of the complete graph on n vertices is n-1.

The tree-width is a minor-monotone graph invariant.

Proposition 2.9. If G' is a minor of G, then $tw(G') \le tw(G)$.

Proof. If H is subgraph of G, then clearly $\operatorname{tw}(H) \leq \operatorname{tw}(G)$. Let G' be a graph obtained by contracting an edge ij to a vertex i' from G. For a tree-decomposition T of G we replace every $\{i,j\}(\in U \in V(T))$ with i'. Then the resulting graph T' is a tree-decomposition of G', and the width of T' is smaller than the width of T. Therefore we obtain $\operatorname{tw}(G') \leq \operatorname{tw}(G)$.

The tree-width is bounded below by the clique number.

Definition 2.10. The *clique number* $\omega(G)$ of a graph G is the number of vertices of a largest complete subgraph in G.

Proposition 2.11. We have

$$tw(G) \ge \omega(G) - 1.$$

Proof. By Example 2 and Proposition 2.9 this proof is completed.

See, e.g. [1] for details about tree-decompositions and the tree-width.

3 Duality of semidefinite programming problems and KKT-conditions

A semidefinite programming problem is a mathematical optimization problem over the cone of positive semidefinite matrices. A semidefinite programming problem minimizes or maximizes a linear function subject to linear equality and inequality constraints, and additionally, positive semidefinite constraints. Although semidefinite programming problems generalize linear programming problems which have only linear constraints, they are not much harder to solve. Most interior-point methods for linear programming problems are generalized to semidefinite programming problems. Semidefinite programming problems are studied in a wide range of fields. There are details, applications and computational methods of semidefinite programming problems in [13].

In this section we will study the dual problem of a semidefinite programming problem and the gap between the primal and dual problems.

For $X \in \operatorname{Sym}_n$ we define a linear operator $\mathcal{A} : \operatorname{Sym}_n \to \mathbb{R}^m$ as

$$\mathcal{A}X = \begin{pmatrix} \langle A_1, X \rangle \\ \vdots \\ \langle A_m, X \rangle \end{pmatrix},$$

where $A_1, \dots, A_m \in \operatorname{Sym}_n$. Also let ${}^t\mathcal{A} : \mathbb{R}^m \to \operatorname{Sym}_n$ be a linear operator that satisfies

$$\langle \mathcal{A}X, y \rangle = \langle X, {}^t \mathcal{A}y \rangle, \quad \forall X \in \operatorname{Sym}_n, \forall y \in \mathbb{R}^m.$$

Then

$${}^{t}\mathcal{A}y = \sum_{i=1}^{m} y_i A_i$$

holds. A semidefinite programming problem is an optimization problem that minimizes $\langle C, X \rangle$ subject to $\mathcal{A}X = b$ for $X \succeq 0$, where $C \in \operatorname{Sym}_n$ and $b \in \mathbb{R}^m$ are constant. This is expressed in the following form:

minimize
$$\langle C, X \rangle$$

subject to $\mathcal{A}X = b$, (3.1)
 $X \succeq 0$.

In addition to this form, various variations of semidefinite programming problems that have constraints including inequalities are also formulated.

Let $X \in \operatorname{Sym}_n$ and $y \in \mathbb{R}^m$. We define the Lagrange function as follows:

$$L(X, y) = \langle C, X \rangle + \langle b - AX, y \rangle.$$

It is easy to see that the following inequality holds.

$$\inf_{X \succeq 0} \sup_{y \in \mathbb{R}^m} L(X, y) \ge \sup_{y \in \mathbb{R}^m} \inf_{X \succeq 0} L(X, y). \tag{3.2}$$

The left-hand side of (3.2) is exactly the problem (3.1).

Proposition 3.1. The problem (3.1) is expressed as $\inf_{X\succeq 0} \sup_{y\in\mathbb{R}^m} L(X,y)$.

Proof. Since $L(X,y) = \langle C, X \rangle + \langle b - AX, y \rangle$, observe that

$$\sup_{y \in \mathbb{R}^m} L(X, y) = \begin{cases} \langle C, X \rangle & \text{if } \mathcal{A}X = b, \\ \infty & \text{if } \mathcal{A}X \neq b. \end{cases}$$

Thus

$$\inf_{\substack{\mathcal{A}X=b,\\X\succeq 0}}\langle C,X\rangle=\inf_{X\succeq 0}\sup_{y\in\mathbb{R}^m}L(X,y).$$

The right-hand side of the inequality (3.2) is the *dual problem*, which we will closely look at now. First, L(X, y) is organized in terms of X as follows:

$$L(X,y) = \langle b, y \rangle + \langle C - {}^{t} \mathcal{A} y, X \rangle.$$

The infimum of L(X,y) with respect to $X \succeq 0$ is therefore

$$\inf_{X \succeq 0} L(X, y) = \langle b, y \rangle + \inf_{X \succeq 0} \langle C - {}^{t} \mathcal{A} y, X \rangle.$$

We show that

$$\inf_{X\succeq 0} L(X,y) = \begin{cases} \langle b,y \rangle & \text{if } 0 \leq C - {}^t \mathcal{A}y, \\ -\infty & \text{otherwise.} \end{cases}$$

We consider the following two cases.

Case (i) : $0 \leq C - {}^{t}Ay$. By Proposition 1.1,

$$\langle C - {}^t \mathcal{A} y, X \rangle \ge 0$$

for $X \succeq 0$. Furthermore, the equality holds when X = 0. Hence, we obtain

$$\inf_{X \succeq 0} L(X, y) = \langle b, y \rangle.$$

Case (ii) : $0 \npreceq C - {}^t Ay$. By Proposition 1.1 there exists $\widetilde{X} \succeq 0$ such that

$$\langle C - {}^t \mathcal{A}y, \widetilde{X} \rangle < 0.$$

For a positive number a, the matrix $a\widetilde{X}$ is positive semidefinite and

$$0 > a\langle C - {}^{t}\mathcal{A}y, \widetilde{X}\rangle = \langle C - {}^{t}\mathcal{A}y, a\widetilde{X}\rangle.$$

If a increases to infinity, then $\langle C - {}^t \mathcal{A}y, a\widetilde{X} \rangle$ diverges to negative infinity. Thus we have

$$\inf_{X \succeq 0} L(X, y) = -\infty.$$

As a result, the right-hand side of the inequality (3.2) boils down to

$$\sup_{y \in \mathbb{R}^m} \inf_{X \succeq 0} L(X, y) = \sup_{\substack{0 \preceq C - {}^t \mathcal{A}y, \\ y \in \mathbb{R}^m}} \langle b, y \rangle,$$

and the optimization is now

maximize
$$\langle b, y \rangle$$

subject to $0 \leq C - {}^{t}\mathcal{A}y$, $y \in \mathbb{R}^{m}$.

Let p^* be an optimal value of the primal problem and d^* be an optimal value of the dual problem. The inequality (3.2) is written as

$$p^* \geq d^*$$
.

This property is called a *weak duality*. In general, the equality does not necessarily hold for a semidefinite programming problem. The situation where the equality holds is called a *strong duality*, or is said that there is no *duality gap*. The conditions for the equality to occur are discussed in [13].

The Karush-Kuhn-Tucker(KKT)-conditions can be used to determine optimal solutions. See [2] for the details of KKT-conditions. Now let $X \in \operatorname{Sym}_n$ and $y \in \mathbb{R}^m$ be feasible solutions, that is, these solutions satisfy the constraints. Objective values of primal and dual problem satisfy

$$\langle C, X \rangle \ge \langle b, y \rangle$$
.

By the Lagrange function the inequality becomes

$$\langle C - {}^t \mathcal{A}y, X \rangle - \langle b - \mathcal{A}X, y \rangle \ge 0.$$

When there is no duality gap, feasible solutions X, y satisfy

$$\langle C - {}^{t} \mathcal{A} y, X \rangle = 0,$$

 $\langle b - \mathcal{A} X, y \rangle = 0$

if and only if these feasible solutions are optimal. These formulae are called KKT-conditions. If there is no duality gap and one optimal solution is obtained, then for the other unresolved problem a feasible solution that satisfies the KKT-conditions is optimal.

Part II

Second eigenvalue optimization and graph embedding problem

4 Duality of the embedding problem of Göring-Helmberg-Wappler

In this section we sketch the procedure deriving the dual problem from the Problem 0.1. First, Problem 0.1 is rewritten in a standard form of a semidefinite programming problem. To see this we consider a new constraint $L(G, w) + \mu e^t e - \lambda I \succeq 0$, where $\mu \in \mathbb{R}$ and e is an n-column vector in which all components are 1. In this constraint μ shifts the eigenvalue 0 to a sufficiently large value. Thus λ attains the second eigenvalue of L(G, w). Then Problem 0.1 is rewritten as follows.

maximize
$$\lambda$$
 subject to $L(G, w) + \mu e^{t} e - \lambda I \succeq 0$,
$$\sum_{ij \in E} w_{ij} = |E|,$$

$$w \in (\mathbb{R}_{\geq 0})^{|E|},$$

$$\lambda, \mu \in \mathbb{R}.$$

The optimal value of this problem is equal to $\hat{a}(G)$. Next we regard this problem as a minimization of $1/\lambda$. Let $\widetilde{w}_{ij} = w_{ij}/\lambda$ and $\widetilde{\mu} = \mu/\lambda$. We are led to the following problem.

Problem 4.1.

(P): minimize
$$\sum_{ij\in E} \widetilde{w}_{ij}$$
 subject to
$$\sum_{ij\in E} \widetilde{w}_{ij} E_{ij} + \widetilde{\mu} e^{t} e - I \succeq 0,$$

$$\widetilde{w} \in (\mathbb{R}_{\geq 0})^{|E|},$$

$$\widetilde{\mu} \in \mathbb{R}.$$

The optimal value of this problem is equal to $|E|/\hat{a}(G)$. We define the Lagrange function with $\widetilde{w} \in (\mathbb{R}_{\geq 0})^{|E|}$, $\widetilde{\mu} \in \mathbb{R}$ and $X \succeq 0$ as follows.

$$L(\widetilde{w}, \widetilde{\mu}, X) := \sum_{ij \in E} \widetilde{w}_{ij} - \langle \sum_{ij \in E} \widetilde{w}_{ij} E_{ij} + \widetilde{\mu} e^{t} e - I, X \rangle$$
$$= \sum_{ij \in E} \widetilde{w}_{ij} (1 - \langle E_{ij}, X \rangle) - \widetilde{\mu} \langle e^{t} e, X \rangle + \langle I, X \rangle.$$

It is straightforward to see that the following inequality holds.

$$\frac{|E|}{\hat{a}(G)} = \inf_{\substack{\widetilde{w} \in (\mathbb{R}_{\geq 0})^{|E|}, \ \widetilde{\mu} \in \mathbb{R}}} \sup_{X \succeq 0} L(\widetilde{w}, \widetilde{\mu}, X) \ge \sup_{\substack{X \succeq 0 \ \widetilde{\mu} \in \mathbb{R}}} \inf_{\substack{\widetilde{w} \in (\mathbb{R}_{\geq 0})^{|E|}, \ \widetilde{\mu} \in \mathbb{R}}} L(\widetilde{w}, \widetilde{\mu}, X). \tag{4.1}$$

The left-hand side is equal to the optimal value of the primal problem (P). The right-hand side is the dual problem:

Problem 4.2.

(D): maximize
$$\langle I, X \rangle$$

subject to $\langle e^t e, X \rangle = 0$,
 $\langle E_{ij}, X \rangle \leq 1$, $\forall ij \in E$,
 $X \succeq 0$.

By the constraint $X \succeq 0$, Proposition 1.3 implies that $X = {}^tVV$ using an $n \times n$ matrix $V = (v_1 \cdots v_n)$. Then we can rewrite Problem 4.2 as a problem on v_i 's:

Problem 4.3 (Problem 0.2).

$$\begin{aligned} & \text{maximize} & & \sum_{i \in V} ||v_i||^2 \\ & \text{subject to} & & ||\sum_{i \in V} v_i||^2 = 0, \\ & & & ||v_i - v_j|| \leq 1, \quad \forall ij \in E, \\ & & v_i \in \mathbb{R}^n, \quad \forall i \in V. \end{aligned}$$

Since v_i 's are regarded as position vectors of points in a Euclidean space, indexed by the vertices of the graph, they can be identified with a mapping from the vertex set of the graph into a Euclidean space.

Definition 4.4 (graph embedding). For a graph G = (V, E) on n vertices. A mapping $v: V \to \mathbb{R}^n$ is called an *embedding* of the graph G. If $v(i) = v_i$ for $i \in V$, the collection of points $(v_i)_{i \in V}$ is also called an embedding of G.

As mentioned in the introduction, it is not assumed that the mapping v is injective. We determine optimal embeddings, that is, optimal solutions of Problem 4.3 for a star graph.

Example 3 ([10]). $K_{1,m}$ denotes a complete bipartite graph with the vertex set $V = \{0\} \cup \{1, \dots, m\}$ and the edge set $E = \{0i \mid i = 1, \dots, m\}$ for $m \geq 2$. $K_{1,m}$ is called a star graph. We have one optimal embedding that the center vertex 0 is placed at the origin and the others $\{1, \dots, m\}$ are arranged in the vertices of an (m-1)-regular simplex whose circumscribed sphere has radius one. The objective value of this embedding is m.

However, there are other solutions that are realized in lower dimensional space and have the same objective value.

For even $m \geq 2$ an optimal embedding in \mathbb{R}^1 is obtained by arranging the center vertex 0 at the origin, half of the other vertices at +1 and the other half at -1. The objective value of this embedding is also m. For odd $m \geq 3$ the following solution $(v_i)_{i \in V}$ is an optimal embedding in \mathbb{R}^2 with the objective value m.

$$v_{0} = 0,$$

$$v_{i} = \begin{cases} \left(-\frac{1}{n-1}, \sqrt{1 - \left(\frac{1}{n-1}\right)^{2}} \right) & \text{if } i \geq 2 \text{ is even,} \\ \left(-\frac{1}{n-1}, -\sqrt{1 - \left(\frac{1}{n-1}\right)^{2}} \right) & \text{if } i \text{ is odd.} \end{cases}$$

In [10], the authors show that there is no duality gap for Problems 4.1 and 4.2, that is, the equality holds in the inequality (4.1). Thus the optimal value of Problem 4.2 is equal to $|E|/\hat{a}(G)$.

For any parameters $s \in (\mathbb{R}_{>0})^n$ and $l \in (\mathbb{R}_{\geq 0})^{|E|}$, the following problem is derived as a dual problem of Problem 0.3 by similar discussion, and there is no duality gap.

Problem 4.5 (Problem 8.2).

maximize
$$\lambda_2(G, (s, w))$$

subject to $\sum_{ij \in E} w_{ij} l_{ij}^2 = \sum_{ij \in E} l_{ij}^2$, $w \in (\mathbb{R}_{>0})^{|E|}$,

Here $\lambda_2(G,(s,w))$ is the first nonzero eigenvalue of the Laplacian DL(G,w)D, where $D = \operatorname{diag}(s_1^{-1/2}, \dots, s_n^{-1/2})$.

In general, when there is no duality gap, both feasible solutions satisfy the KKT-conditions if and only if these feasible solutions are optimal. In the present case, for optimal \widetilde{w} and v_i 's they are expressed as follows.

$$\begin{cases}
(i) & \widetilde{w}_{ij}(1 - \langle E_{ij}, X \rangle) = 0, \quad \forall ij \in E, \\
(ii) & \langle \sum_{ij \in E} \widetilde{w}_{ij} E_{ij} - I, X \rangle = 0.
\end{cases}$$
(4.2)

Conversely, if feasible solutions satisfy these conditions, then these solutions are optimal and there is no duality gap.

In (i) when $\widetilde{w}_{ij} > 0$, $||(v_i - v_j)||^2 = 1$ should holds. This means that the distance of v_i and v_j is maximized in the optimal embedding.

The formula (ii) gives

$$v_i = \sum_{ij \in E} \widetilde{w}_{ij}(v_i - v_j), \quad \forall i \in V.$$
(4.3)

These are equivalent to

$$\begin{pmatrix} {}^t v_1 \\ \vdots \\ {}^t v_n \end{pmatrix} = L(G, \widetilde{w}) \begin{pmatrix} {}^t v_1 \\ \vdots \\ {}^t v_n \end{pmatrix}.$$

This gives that v_i 's are the eigenfunctions of the first nonzero eigenvalue of the Laplacian L(G, w). Thus, the dimension of the linear subspace spanned by the optimal v_i 's are less than the multiplicity of the first nonzero eigenvalue of L(G, w).

5 Graph embedding problem and rotational dimension

In the previous section we showed that the dimension of the optimal embedding is bounded by the multiplicity of the second eigenvalue. However, this bound is not necessarily optimal, and better bounds were studied by Göring et al. [10].

A *separator* is a vertex subset whose removal divides a graph into two or more components. The Separator-Shadow theorem is one of the ingredients that give a better bound.

Theorem 5.1 (Separator-Shadow [10]). Let S be a separator that divides G = (V, E, w) into two components C_1 and $C_2 \subset V$, and let $(v_i)_{i \in V}$ be an optimal solution for Problem 0.3. Then at least one of C_1 and C_2 , say C_1 , satisfies

$$\operatorname{conv}\{0, v_i\} \cap \operatorname{conv}\{v_s \mid s \in S\} \neq \emptyset, \quad \forall i \in C_1.$$

Here, $\operatorname{conv}\{0, v_i\}$ is a line segment connecting the origin and v_i , and $\operatorname{conv}\{v_s \mid s \in S\}$ is the convex hull of the set $\{v_s \mid s \in S\}$.

If we regard the origin as a light source and the convex hull of the separator's points as a solid body, then all the vertices of either components are in the shadow of the separator. By the Separator-Shadow theorem, the dimension of the subspace spanned by S and one component which is not contained in the shadow of S attains the optimal dimension for G. In the case when the convex hull of the separator contains the origin, this theorem is not very effective, but even in that situation the dimension can still be bounded [10].

Göring-Helmberg-Wappler gave the tree-width bound of the minimum dimension of an optimal embedding.

Theorem 5.2 ([10], [11]). For any graph G and any parameters s and l, there exists an optimal embedding whose dimension is less than or equal to tw(G) + 1.

Note that the rotational dimension has the same bound. Next we describe some facts about the rotational dimension.

Theorem 5.3 (minor monotonicity of rotational dimension [11]). If G' is a minor of G, then

$$\operatorname{rotdim}(G) \ge \operatorname{rotdim}(G')$$
.

In the definition of the rotational dimension we can replace $s \in (\mathbb{N} \cup \{0\})^{|V|}, l \in (\mathbb{N} \cup \{0\})^{|E|}$ by $s \in (\mathbb{R}_{\geq 0})^{|V|}, l \in (\mathbb{R}_{\geq 0})^{|E|}$ or $s \in (\mathbb{R}_{> 0})^{|V|}, l \in (\mathbb{R}_{> 0})^{|E|}$ [11]. When a graph G is disconnected, the rotational dimension of G is defined as

$$rotdim(G) := max\{rotdim(C) \mid C \text{ is a component of } G\}.$$

Graphs having low rotational dimensions are classified as follows.

Theorem 5.4 ([11]).

- $\operatorname{rotdim}(G) = 0$ if and only if G does not have edges.
- $\operatorname{rotdim}(G) \leq 1$ if and only if G is a union of paths.
- $\operatorname{rotdim}(G) \leq 2$ if and only if G is outer planar.

Part III

The rotational dimension of a graph containing a large complete graph

In this part, we study rotational dimensions of graphs containing a large complete subgraph. These are the main results of [8].

6 Rotational dimension of a complete graph

In this section we prove that the rotational dimension of graph on n vertices is bounded above by n-1 and the complete graph is the only n vertices graph whose rotational dimension attains this upper bound.

Proposition 6.1. If G is a graph on n vertices, then

$$\operatorname{rotdim}(G) \leq n - 1.$$

Proof. For any parameters s, l and optimal solution $(v_i)_{i \in V}$ we have dim span $\{v_i \mid i \in V\} \leq n-1$, because the vectors v_i 's are not linearly independent by the constraint $||\sum_{i \in V} s_i v_i||^2 = 0$. Therefore $\operatorname{rotdim}(G) \leq n-1$.

When each entry in the parameters s, l is one, a regular simplex is a unique optimal solution of a complete graph. Here we regard the embeddings which differ by a rotation around the origin as the same embeddings. Then $\operatorname{rotdim}_{K_n}(1,1) = n-1$ (see Example 7 in [10]).

Proposition 6.2.

$$\operatorname{rotdim}(K_n) = n - 1.$$

Proof. Since $\operatorname{rotdim}(K_n) \geq \operatorname{rotdim}_{K_n}(1,1) = n-1$, we obtain $\operatorname{rotdim}(K_n) = n-1$ by Proposition 6.1.

We can immediately see that $\operatorname{rotdim}(G) \geq \omega(G) - 1$ by this proposition and Theorem 5.3, where $\omega(G)$ is the clique number of G.

The following theorem is the main result in this section. We characterize the complete graph by its rotational dimension.

Theorem 6.3 (Theorem 0.5). If G is a graph on n vertices, then

$$\operatorname{rotdim}(G) = n - 1$$
 if and only if $G = K_n$.

A similar property for the valid representation invariant $\lambda(G)$ is obtained by Van der Holst-Laurent-Schrijver in [21]. In order to prove Theorem 6.3, we consider a graph obtained by connecting complete graphs.

Definition 6.4. Let G_1 and G_2 be graphs with cliques of the same size. Let G be the graph obtained by identifying the respective cliques in the disjoint union of G_1 and G_2 . This G is called the *clique sum* and denoted by $G = G_1 \oplus G_2$.

A graph obtained by removing one edge from the complete graph K_n is the clique sum of two K_{n-1} 's. The rotational dimension of that graph is calculated as follows.

Theorem 6.5 (Theorem 0.6). Let $e \in E$. Then

$$\operatorname{rotdim}(K_n \setminus \{e\}) = n - 2.$$

Proof. The fact $\operatorname{rotdim}(K_n \setminus \{e\}) \geq n-2$ holds by Theorem 5.3 because $K_n \setminus \{e\}$ contains K_{n-1} as a minor. Therefore we prove the other inequality. Let V be the vertex set of $K_n \setminus \{e\}$, and s, l be parameters all of whose components are positive. If $\operatorname{rotdim}_{K_n \setminus \{e\}}(s, l) \leq n-2$ is shown for such parameters, then we can obtain the same inequality for parameters whose components are nonnegative. Let $(v_i)_{i \in V}$ be an optimal solution for Problem 0.3 that attains $\operatorname{rotdim}_{K_n \setminus \{e\}}(s, l)$. We regard $K_n \setminus \{e\}$ as $K_{n-1} \oplus K_{n-1}$ with a common clique K_{n-2} and let S be this common clique K_{n-2} . Without loss of generality, let $S = V \setminus \{1, 2\}$.

Case (i): $0 \notin \text{conv}(S)$. Note that the dimension of the linear subspace span(S) is n-2 or less. By Theorem 5.1 we see that $v_1 \in \text{span}(S)$ or $v_2 \in \text{span}(S)$, say the former. We also have $v_2 \in \text{span}(S)$ by the equilibrium constraint $||\sum_{i \in V} s_i v_i||^2 = 0$. Thus span(V) $\subset \text{span}(S)$, and dim span(V) $\leq n-2$.

Case (ii): $0 \in \text{conv}(S)$. Let v_1 and v_2 be vectors which are not included in the common clique. Since $0 \in \text{aff-span}(S \cup \{v_1\})$ holds, we also have dim $\text{span}(S \cup \{v_1\}) \leq n-2$. By the equilibrium constraint we also have $v_2 \in \text{span}(S \cup \{v_1\})$, and dim $\text{span}(V) \leq n-2$.

Proof of Theorem 6.3. Since $\operatorname{rotdim}(K_n) = n - 1$, it remains to verify that if $G \neq K_n$, then $\operatorname{rotdim}(G) \leq n - 2$. If G is an arbitrary graph on n vertices which is not complete, then $K_n \setminus \{e\} \succeq G$. By Theorems 5.3 and 6.5, we have $n - 2 = \operatorname{rotdim}(K_n \setminus \{e\}) \geq \operatorname{rotdim}(G)$.

Even if an optimal dimension can be calculated, it is generally difficult to find an optimal embedding that attains the optimal dimension. However, for example, when all

parameters are one, this is possible for K_n and $K_n \setminus \{e\}$. The regular simplex is the only optimal embedding of the complete graph. For a general graph its complete subgraph may be embedded similarly.

Proposition 6.6. Let G = (V, E) be an n vertices graph. For a complete subgraph K_m of G and an optimal embedding $(v_i)_{i\in V}$ of Problem 0.2, if $||v_i-v_j||=1$ holds for every $ij \in E(K_m)$, then the vectors corresponding to the vertices of K_m form an (m-1)regular simplex with side length 1.

Proof. It is clear when m is 1 or 2. Assuming that the claim is satisfied up to $m \geq 2$ vertices, we consider where a new vertex can be added. This new vertex may be placed on a straight line which is orthogonal to the given (m-1)-regular simplex with side length 1 and passes through the center of mass of the simplex. Thus we obtain an m-regular simplex with side length 1.

If we apply Proposition 6.6 to $K_n \setminus \{e\}$, the configuration of an optimal embedding can be found.

Proposition 6.7. When $s \equiv 1$ and $l \equiv 1$, we have

$$\operatorname{rotdim}_{K_n \setminus \{e\}}(1,1) = n - 2.$$

The optimal embedding that gives this dimension exists uniquely.

Proof. Let $m = n - 2, \{1, \dots, m\}$ be the vertex set of the common clique K_m when considered as $K_n \setminus \{e\} = K_{n-1} \oplus K_{n-1}$, and let m+1, m+2 be the other vertices. We will prove that the following embedding (6.1) is the only optimal embedding of $K_n \setminus \{e\}$.

Let $(\widetilde{v}_i)_{i\in V}$ be the embedding described above. Note that the second property implies that $||\widetilde{v}_{m+1}||=||\widetilde{v}_{m+2}||=\sqrt{(m+1)/2m}$ since $||\widetilde{v}_i-\widetilde{v}_j||=1$ for $i=1,\cdots,m$ and j = m + 1, m + 2.

First we verify that $(\tilde{v}_i)_{i \in V}$ is optimal. This embedding is obviously feasible, and the objective value is $(m^2 + m + 2)/2m$. On the other hand,

$$\widetilde{w}_{ij} = \begin{cases} \frac{1}{m} - \frac{2}{m^2} & \text{if } 1 \le i, j \le m, \\ \frac{1}{m} & \text{if } 1 \le i \le m, \ j = m + 1 \text{ or } m + 2 \end{cases}$$
(6.2)

is feasible solution for Problem 4.1, because

$$L(G, \widetilde{w}) + \widetilde{\mu}e^{t}e - I = \left(\begin{array}{c|c} 2/m^{2} & 0 \\ \hline 0 & 1/m \end{array}\right) \succeq 0$$

is satisfied where $\tilde{\mu} = 1/m$. This solution is found as follows. Let

$$\widetilde{w}_{ij} = \begin{cases} a & \text{if } 1 \le i, j \le m, \\ b & \text{if } 1 \le i \le m, \ j = m+1 \text{ or } m+2 \end{cases}$$

by taking the symmetry of the graph into account. By inserting this \widetilde{w} and $(\widetilde{v}_i)_{i \in V}$ into the KKT-condition (4.3)

$$\widetilde{v}_i = \sum_{ij \in E} \widetilde{w}_{ij} (\widetilde{v}_i - \widetilde{v}_j), \quad \forall i \in V,$$

we obtain (6.2). For this edge weight the objective value is also $(m^2 + m + 2)/2m$. Since both objective values are equal, \widetilde{w} and $(\widetilde{v_i})_{i \in V}$ are both optimal.

Next, we give an arbitrary optimal embedding $(v_i)_{i \in V}$. By inserting \widetilde{w} and $(v_i)_{i \in V}$ into the KKT-conditions (4.2), we obtain

$$||v_i - v_j|| = 1, \quad \forall ij \in E,$$

$$\sum_{1 \le i \le m} v_i = 0,$$

$$v_{m+1} + v_{m+2} = 0.$$

Thus, by Proposition 6.6 this embedding is exactly (6.1).

7 Rotational dimension of a chordal graph

In the Separator-Shadow Theorem the upper bound for the optimal dimension becomes tight if the chosen separator has strong connectivity close to that of a clique. A chordal graph has the required structure. A chordal graph is a graph in which all cycles of length 4 or more have a chord that is an edge connecting two nonadjacent vertices of this cycle. The inequality $\operatorname{tw}(G) \geq \omega(G) - 1$ holds for a general graph G by Proposition 2.11. In fact, the equality holds for a chordal graph (see, e.g. [12]). For any graph G

$$\omega(G) - 1 \le \operatorname{rotdim}(G) \le \operatorname{tw}(G) + 1$$
 (7.1)

holds by Theorems 5.2, 5.3 and Proposition 6.2. It turns out that those bounds are tight for a chordal graph. In fact, if G is a chordal graph, then $\operatorname{tw}(G) \ge \omega(G) - 1$ holds and so (7.1) becomes

$$\omega(G) - 1 \le \operatorname{rotdim}(G) \le \omega(G)$$
.

Example 4. Let $G(n) = K_{n+1} \oplus K_{n+1} \oplus K_{n+1}$ with the common clique K_n , that is, G(n) is the graph of order n+3 in which n vertices form K_n and each of the remaining 3 vertices is adjacent to all the vertices of K_n . Then for $n \geq 4$ we have

$$\operatorname{rotdim}_{G(n)}(1,1) = n + 1.$$

Detailed calculation is given in [10].

Since G(n) is a chordal graph and $\omega(G(n)) = n + 1$, we conclude

$$\operatorname{rotdim}(G(n)) = n + 1, \quad n > 4.$$

Using this fact, we can calculate the rotational dimension of the graph $G(n,k) = K_{n+1} \oplus K_{n+1} \oplus \cdots \oplus K_{n+1}$ which is the k-clique sum with the common clique K_n for $n \geq 4$ and $k \geq 3$. Note that $G(n,1) = K_{n+1}$, $G(n,2) = K_{n+2} \setminus \{e\}$ and G(n,3) = G(n). By $G(n) \leq G(n,k)$ and the evaluation by the clique number, we obtain

$$\operatorname{rotdim}(G(n,k)) = n + 1.$$

Rotational dimensions of G(n, k) for $n \ge 4$ and $k \ge 1$ are as follows.

$$\operatorname{rotdim}(G(n,k)) = \begin{cases} n & \text{if } k = 1, 2, \\ n+1 & \text{if } k \ge 3. \end{cases}$$

Applying the properties of a chordal graph, we calculate the rotational dimension of some large graphs.

Theorem 7.1. Let G be a chordal graph that satisfies $\operatorname{rotdim}(G) = \omega(G)$. Also, let \widehat{G} be a chordal graph containing G as a subgraph. If $\omega(\widehat{G}) = \omega(G)$, then

$$\operatorname{rotdim}(\widehat{G}) = \operatorname{rotdim}(G).$$

Proof. Since $\operatorname{tw}(\widehat{G}) = \omega(\widehat{G}) - 1 = \omega(G) - 1$, we obtain $\operatorname{rotdim}(\widehat{G}) \leq \operatorname{tw}(\widehat{G}) + 1 = \omega(G) = \operatorname{rotdim}(G)$. On the other hand, $\operatorname{rotdim}(G) \leq \operatorname{rotdim}(\widehat{G})$ by Theorem 5.3.

The technique in this theorem is used to obtain $\operatorname{rotdim}(G(n,k)) = n+1$ for $k \geq 4$.

Part IV

Another embedding problem and spectral gap of a finite graph

In this part, we study an embedding problem which is different from the problem derived by Göring-Helmberg-Wappler. In [9], we introduced this embedding problem.

8 Another embedding problem

Set $M := \sum_{i \in V} s_i$ and $L^2 := \sum_{ij \in E} l_{ij}^2$, where $s \in (\mathbb{R}_{>0})^n$ and $l \in (\mathbb{R}_{\geq 0})^{|E|}$. The affine barycenter of $\mathbf{v} := (v_i)_{i \in V}$, where $v_i \in \mathbb{R}^n$, is denoted by $\operatorname{bar}(\mathbf{v}) = \frac{1}{M} \sum_{i \in V} s_i v_i$. We consider the following optimization problem.

Problem 8.1 (Problem 0.7).

minimize
$$\| \operatorname{bar}(\boldsymbol{v}) \|^2$$

subject to $\frac{1}{M} \sum_{i \in V} s_i ||v_i||^2 = 1$,
 $||v_i - v_j|| \le l_{ij}$, $\forall ij \in E$,
 $v_i \in \mathbb{R}^n$, $\forall i \in V$.

Let $\delta(G, s, l)$ be the optimal value of this problem.

The first nonzero eigenvalue of the Laplacian is called the *spectral gap*. Our first observation is that this problem is related to an optimization problem regarding the spectral gap of the Laplacian, which we now review. First, we reiterate the following problem.

Problem 8.2 (Problem 4.5).

maximize
$$\lambda_2(G, (s, w))$$

subject to $\sum_{ij \in E} w_{ij} l_{ij}^2 = L^2,$
 $w \in (\mathbb{R}_{>0})^{|E|}.$

Here $\lambda_2(G,(s,w))$ is the first nonzero eigenvalue of the Laplacian $\Delta_{(s,w)} := DL(G,w)D$, where $D = \operatorname{diag}(s_1^{-1/2}, \dots, s_n^{-1/2})$. Let $\sigma(G,s,l)$ be the optimal value of this problem.

Remark 1. $\lambda_2(G,(s,w))$ is characterized variationally as

$$\lambda_2(G, (s, w)) = \inf \frac{\sum_{ij \in E} w_{ij} ||v_i - v_j||^2}{\sum_{i \in V} s_i ||v_i - \text{bar}(\boldsymbol{v})||^2},$$

where the infimum is taken over all non-constant maps $v: V \ni i \mapsto v_i \in \mathbb{R}^n$.

Remark 2. When $s \equiv 1$ and $l \equiv 1$, note that the optimal value $\sigma(G, s, l)$ is exactly $\hat{a}(G)$, the absolute algebraic connectivity of G, studied by Fiedler [7] (discussed in Introduction).

The following proposition is the key to relate the two optimization problems.

Proposition 8.3. Let G = (V, E) be a finite connected graph equipped with a vertex weight s and a length parameter l. For an edge weight w satisfying

$$\sum_{ij\in E} w_{ij} l_{ij}^2 = L^2, \tag{8.1}$$

we have

$$\delta(G, s, l) \ge 1 - \frac{L^2/M}{\lambda_2(G, (s, w))}.$$
 (8.2)

In (8.2), the equality holds if and only if there exists v satisfying

$$\frac{1}{M} \sum_{i \in V} s_i ||v_i||^2 = 1,
||v_i - v_j|| \le l_{ij}, \quad \forall ij \in E,$$
(8.3)

such that

(i)
$$w_{ij}(l_{ij}^2 - ||v_i - v_j||^2) = 0, \forall ij \in E,$$

(ii) $\Delta_{(s,w)}v_i = \lambda_2(G,(s,w))(v_i - \text{bar}(\boldsymbol{v}))$, that is, each component of the map $v_i - \text{bar}(\boldsymbol{v})$ is an eigenvector of the eigenvalue $\lambda_2(G,(s,w))$ of the Laplacian $\Delta_{(s,w)}$.

Proof. Observe that

$$\| \operatorname{bar}(\boldsymbol{v}) \|^{2} = \frac{1}{M} \sum_{i \in V} s_{i} \|v_{i}\|^{2} - \frac{1}{M} \sum_{i \in V} s_{i} \|v_{i} - \operatorname{bar}(\boldsymbol{v})\|^{2}$$

$$\geq \frac{1}{M} \sum_{i \in V} s_{i} \|v_{i}\|^{2}$$

$$- \frac{1}{M} \frac{1}{\lambda_{2}(G, (s, w))} \sum_{ij \in E} w_{ij} \|v_{i} - v_{j}\|^{2}$$

$$\geq 1 - \frac{1}{M} \frac{1}{\lambda_{2}(G, (s, w))} \sum_{ij \in E} w_{ij} l_{ij}^{2}$$

$$= 1 - \frac{1}{M} \frac{L^{2}}{\lambda_{2}(G, (s, w))}.$$

The assertion on the equality case is clear.

Since the left-hand side of (8.2) does not depend on w, we obtain the following.

Corollary 8.4. Let G = (V, E) be a finite connected graph equipped with a vertex weight s and a length parameter l. Then we have

$$\delta(G, s, l) \ge 1 - \frac{L^2/M}{\sigma(G, s, l)}.$$
(8.4)

In (8.4), the equality holds if and only if there exist an edge weight w and v satisfying (8.3) and the two conditions (i) and (ii) in Proposition 8.3.

Remark 3. The conditions for the equality case in Proposition 8.3 and Corollary 8.4 coincide with the so-called KTT-conditions associated with Problems 8.1 and 8.2 which are shown to be dual to each other in Section 11.

Example 5. Let G_p be the incidence graph of the projective plane $\mathbf{P}^2(\mathbb{F}_p)$ over the field $\mathbb{F}_p = \mathbb{Z}/p\mathbb{Z}$, where p is a prime number. Since $\mathbf{P}^2(\mathbb{F}_p)$ has $p^2 + p + 1$ lines and $p^2 + p + 1$ points with p + 1 points on every line and p + 1 lines through every point, G_p is a (p+1)-regular bipartite graph with $2(p^2 + p + 1)$ vertices. Define weights s, w and a length parameter l by

$$s_i = p + 1, \quad \forall i \in V,$$

 $w_{ij} = 1, l_{ij} = 1, \quad \forall ij \in E,$

so that the normalization (8.1) is satisfied and $L^2/M = 1/2$. By a result of Feit and Higman [6], we have $\lambda_2(G_p,(s,w)) = 1 - \frac{\sqrt{p}}{p+1}$, and therefore

$$1 - \frac{L^2/M}{\lambda_2(G_p, (s, w))} = \frac{p + 1 - 2\sqrt{p}}{2(p + 1 - \sqrt{p})}.$$

On the other hand, Problem 8.1 for G_p is solved in [14], and the solution v satisfies

$$\langle v_i, v_j \rangle = \begin{cases} \frac{\frac{1}{2}}{2} & \text{if } d_{G_p}(u, v) = 1, \\ \frac{p - 1 - \sqrt{p}}{2p} & \text{if } d_{G_p}(u, v) = 2, \\ \frac{p^2 - p - (p + 1)\sqrt{p}}{2p^2} & \text{if } d_{G_p}(u, v) = 3, \end{cases}$$

where d_{G_p} is the standard graph distance on V in the graph G_p . It follows that

$$\delta(G, s, l) = \left\| \frac{1}{M} \sum_{i \in V} s_i v_i \right\|^2 = \frac{p^2 + 1 - (p+1)\sqrt{p}}{2(p^2 + p + 1)} = \frac{p + 1 - 2\sqrt{p}}{2(p + 1 - \sqrt{p})}.$$

Thus the equality holds in (8.2) (and hence in (8.4)). In particular, when the vertex weight $s \equiv p+1$ and the parameter $l \equiv 1$ are fixed, the choice of edge weight $w \equiv 1$ maximizes the spectral gap $\lambda_2(G_p,(s,w))$ over all edge weights subject to the normalization (8.1), and $\sigma(G,s,l) = 1 - \frac{\sqrt{p}}{p+1}$.

9 Relation between optimization problems

In [10, 11] optimization problems similar to those in Section 8 are considered. Again, the problems are concerned with graph embeddings and the spectral gap of the Laplacian, and very importantly they are dual to each other. In this section, after reviewing this duality, we discuss how our problems are related to those in [10, 11]. (In fact, our problems 8.1 and 8.2 are also dual to each other. This will be discussed in Section 11.)

We first reiterate the embedding problem of Göring-Helmberg-Wappler.

Problem 9.1 (Problem 0.3).

maximize
$$\frac{1}{M} \sum_{i \in V} s_i ||v_i||^2$$
subject to
$$||\sum_{i \in V} s_i v_i||^2 = 0,$$
$$||v_i - v_j|| \le l_{ij}, \quad \forall ij \in E,$$
$$v_i \in \mathbb{R}^n, \quad \forall i \in V.$$

Let $\nu(G, s, l)$ be the optimal value of this problem.

It is shown in [11] that Problem 9.1 is dual to Problem 8.2. By semidefinite duality theory together with strict feasibility, they deduce that the optimal values of the two problems (are attained and) coincide. We record this fact as follows.

Theorem 9.2 ([11]). For any finite connected graph G = (V, E) equipped with a vertex weight s and a length parameter l, we have

$$\nu(G, s, l) = \frac{L^2/M}{\sigma(G, s, l)}.$$
(9.1)

Remark 4. The inequality

$$\nu(G, s, l) \le \frac{L^2/M}{\sigma(G, s, l)} \tag{9.2}$$

is an analogue of (8.4) and can be proved by a similar argument. Indeed, if \boldsymbol{v} satisfies the constraints

$$\left\| \sum_{i \in V} s_i v_i \right\|^2 = 0,$$

$$||v_i - v_j|| \le l_{ij}, \quad \forall ij \in E,$$

$$(9.3)$$

then

$$\sum_{i \in V} s_i \|v_i\|^2 = \sum_{i \in V} s_i \|v_i - \text{bar}(\boldsymbol{v})\|^2
\leq \frac{1}{\lambda_2(G, (s, w))} \sum_{ij \in E} w_{ij} \|v_i - v_j\|^2
\leq \frac{L^2}{\lambda_2(G, (s, w))}.$$
(9.4)

Therefore, (9.2) follows.

Let w and v be optimal solutions for Problems 8.2 and 9.1, respectively. Then the inequalities in (9.4) become equalities, and hence each component of v has to be an eigenvector of the eigenvalue $\lambda_2(G,(s,w))$ of $\Delta_{(s,w)}$.

By combining (8.4) and (9.1), we obtain

$$\delta(G, s, l) \ge 1 - \frac{L^2/M}{\sigma(G, s, l)} = 1 - \nu(G, s, l).$$

The following proposition gives a more precise relation between Problems 8.1 and 9.1 concerning optimal embeddings.

Proposition 9.3. For any finite connected graph G = (V, E) equipped with a vertex weight s, we have

$$\delta(G, s, l) = \max\{1 - \nu(G, s, l), 0\}. \tag{9.5}$$

Proof. Let $\mathbf{v} = (v_i)_{i \in V}$ be an optimal solution for Problem 8.1. Then $(u_i := v_i - \text{bar}(\mathbf{v}))_{i \in V}$ satisfies the constraints (9.3) of Problem 9.1. Since

$$\sum_{i \in V} s_i ||u_i||^2 = \sum_{i \in V} s_i ||v_i||^2 - M ||\operatorname{bar}(\boldsymbol{v})||^2$$
$$= M(1 - \delta(G, s, l)),$$

we obtain

$$\nu(G, s, l) \ge 1 - \delta(G, s, l), \text{ or } \delta(G, s, l) \ge 1 - \nu(G, s, l).$$

The other way around, let v be an optimal solution for Problem 9.1. We treat the following two cases separately: (i) $\nu(G, s, l) > 1$, (ii) $\nu(G, s, l) \leq 1$. In case (i),

$$(u := \sqrt{1/\nu(G, s, l)} \, v)_{i \in V}$$

satisfies the constraints (8.3) of Problem 8.1. Since

$$\left\| \frac{1}{M} \sum_{i \in V} s_i u_i \right\|^2 = \frac{1}{M^2 \nu(G, s, l)} \left\| \sum_{i \in V} s_i v_i \right\|^2 = 0,$$

we obtain $\delta(G, s, l) = 0$. In case (ii), define u_i 's by

$$u_i = v_i + \sqrt{1 - \nu(G, s, l)} e, \quad i \in V,$$

where e is any unit vector in $\mathbb{R}^{|V|}$. Then u_i 's satisfy the constraints (8.3) of Problem 8.1, and

$$\left\| \frac{1}{M} \sum_{i \in V} s_i u_i \right\|^2 = 1 - \nu(G, s, l).$$

Therefore,

$$\delta(G, s, l) \le 1 - \nu(G, s, l).$$

We may now conclude (9.5).

Remark 5. Combining Proposition 9.3 with Theorem 9.2, we obtain

$$\delta(G, s, l) = \max \left\{ 1 - \frac{L^2/M}{\sigma(G, s, l)}, 0 \right\}.$$

This improves the inequality (8.4) of Corollary 8.4.

10 Optimal embeddings of polyhedra

In this section, we consider highly-symmetric graphs isomorphic to the 1-skeletons of regular and semi-regular polyhedra, and decide their optimal embeddings for Problem 9.1. For such a graph equipped with the parameters $w \equiv 1$, $s \equiv 1$ and $l \equiv 1$, Padrol-Sureda and Pfeifle discuss in [18] that the arrangement of the vertices by the eigenfunctions of the non-weighted Laplacian reproduces the polyhedron. For Problem 9.1, when the edge parameter l is not uniform but has symmetry, a polyhedron whose edge set has similar symmetry arises as an optimal solution. We confirm this for the fullerene graph C_{60} .

10.1 Platonic solids

The Platonic solids are the five regular convex polyhedra: the regular tetrahedron, the regular hexahedron, the regular octahedron, the regular dodecahedron and the regular icosahedron. Let parameters s, l be uniform ones: $s \equiv 1$, $l \equiv 1$.

We discuss the dodecahedron in detail. The other polyhedra can be similarly handled. Let $C_{20} = (V, E)$ a graph isomorphic to the 1-skeleton of the dodecahedron which has 20 vertices and 30 edges. We verify that the optimal embedding of C_{20} realizes it as the 1-skeleton of the regular dodecahedron. In fact, if we choose w uniform, that is, $w \equiv 1$, then the first nonzero eigenvalue of the corresponding Laplacian is computed as $\lambda_2(C_{20}, (s, w)) = 3 - \sqrt{5}$.

On the other hand, for the regular dodecahedron with edge length one, the radius of its circumscribed sphere is $(\sqrt{15} + \sqrt{3})/4$. Therefore, this feasible solution has $30/[20((\sqrt{15} + \sqrt{3})/4)^2] = 3 - \sqrt{5}$, the same as above, as the objective value of the embedding problem. Thus we conclude that the optimal embedding of C_{20} gives the 1-skeleton of the regular dodecahedron.

Similar results are obtained for the other four regular polyhedra. The optimal values of Problem 8.2 for these polyhedra with the same choices of parameters are listed in Table 1.

Table 1: Maximum spectral gaps for the Platonic solids

Regular polyhedron	Maximum spectral gap
Tetrahedron	4
Hexahedron	2
Octahedron	4
Dodecahedron	$3-\sqrt{5}$
Icosahedron	$5-\sqrt{5}$

10.2 Fullerene C_{60}

Let $C_{60} = (V, E)$ denote the graph isomorphic to the 1-skeleton of a truncated icosahedron, also called a buckyball. The graph C_{60} has 60 vertices and 90 edges, 60 of which are pentagonal edges and the remaining 30 of which are hexagonal ones. Here, an edge is called *pentagonal* if it is on the boundary of a pentagonal face; otherwise, it is called *hexagonal*. Let the vertex weight s be the uniform one: $s \equiv 1$. Choose the edge weight s as

$$w_{ij} = \begin{cases} x & \text{if } ij \text{ is a pentagonal edge,} \\ y & \text{if } ij \text{ is a hexagonal edge.} \end{cases}$$

Then by a result of [4], the first nonzero eigenvalue of the Laplacian for the above vertex and edge weights is

$$\lambda_2(G, (s, w)) = (2x + y) - \frac{x}{4} \left(3 + \sqrt{5} + \sqrt{2} \sqrt{15 - 5\sqrt{5} - 4t + 4\sqrt{5}t + 8t^2} \right) \Big|_{t = \frac{y}{x}}.$$

We begin with the case that the edge parameter l is uniform: $l \equiv 1$. The circumscribed sphere of the truncated icosahedron with edge length one has radius $\sqrt{58 + 18\sqrt{5}}/4$. Therefore, the objective value of Problem 9.1 for this embedding is

$$60\left(\frac{\sqrt{58+18\sqrt{5}}}{4}\right)^2 = \frac{15}{2}(29+9\sqrt{5}).$$

On the other hand, the choice of w with

$$x = \frac{1}{218}(189 + 9\sqrt{5}), \quad y = \frac{1}{109}(138 - 9\sqrt{5})$$

satisfies the constraint of the eigenvalue optimization problem Problem 8.2. The objective value for this feasible solution is $(87 - 27\sqrt{5})/109$, and

$$\frac{L^2/M}{(87 - 27\sqrt{5})/109} = \frac{90}{(87 - 27\sqrt{5})/109} = \frac{15}{2}(29 + 9\sqrt{5}).$$

Therefore, the 1-skeleton of the truncated icosahedron is realized by an optimal embedding.

We now consider the case that the parameter l is given by

$$l_{ij} = \begin{cases} a & \text{if } ij \text{ is a pentagonal edge,} \\ b & \text{if } ij \text{ is a hexagonal edge.} \end{cases}$$

It is reasonable to expect that the truncated icosahedron in which the ratio of the length of a pentagonal edge to that of a hexagonal edge is a:b is obtained as an optimal embedding. The barycenter of this truncated icosahedron is at the origin again, and the objective value for this feasible solution is

$$\frac{15}{2}a^2\left\{(5+\sqrt{5})s^2+(4\sqrt{5}+12)(s+1)\right\},\,$$

where s = b/a. (Note that this value coincides with the one in the previous case when a = b = 1.)

A feasible solution for Problem 8.2 with the symmetric parameter l is found as

$$x = \frac{(2a^2 + b^2) \left((6 + 2\sqrt{5})a + (3 + \sqrt{5})b \right)}{a \left(\left(12 + 4\sqrt{5} \right) a^2 + \left(12 + 4\sqrt{5} \right) ab + \left(5 + \sqrt{5} \right) b^2 \right)},$$
$$y = \frac{(2a^2 + b^2) \left((6 + 2\sqrt{5})a + (5 + \sqrt{5})b \right)}{b \left(\left(12 + 4\sqrt{5} \right) a^2 + \left(12 + 4\sqrt{5} \right) ab + \left(5 + \sqrt{5} \right) b^2 \right)}.$$

The objective value for this feasible solution is

$$A := \frac{4(2a^2 + b^2)}{(12 + 4\sqrt{5}) a^2 + (12 + 4\sqrt{5}) ab + (5 + \sqrt{5}) b^2},$$

and

$$\frac{L^2/M}{A} = \frac{15}{2}a^2 \left\{ (5 + \sqrt{5})s^2 + (4\sqrt{5} + 12)(s+1) \right\}.$$

Since the objective values are equal, we get the expected result.

10.3 Other Archimedean solids

Archimedean solids are convex polyhedra all of whose faces are regular polygons, and which have a symmetry group acting transitively on the vertices. (Note, however, that the prisms, antiprisms and five Platonic solids are excluded.) Archimedean solids are classified and identified by the vertex configuration which refers to polygons that meet at any vertex. For example, a truncated icosahedron is denoted by (5,6,6).

Let G be the 1-skeleton of a truncated icosidodecahedron (4,6,10), with an edge weight w given by

$$w_{ij} = \begin{cases} x & \text{if } ij \text{ separates 4-gon and 6-gon,} \\ y & \text{if } ij \text{ separates 4-gon and 10-gon,} \\ z & \text{if } ij \text{ separates 6-gon and 10-gon,} \end{cases}$$

where x, y, z satisfy x + y + z = 1. In [15] the optimization problem minimizing the second largest eigenvalue of the adjacency matrix over all edge weights w of the above form is solved, and $(179 + 24\sqrt{5})/241$ is obtained as the optimal value. By choosing parameters $s \equiv 1$ and $l \equiv \sqrt{3}$, the edge weight w satisfies the constraint in Problem 8.2. Then we have

$$\frac{|E|}{\sigma(G, s, l)} \le \frac{180}{1 - (179 + 24\sqrt{5})/241} = 90(31 + 12\sqrt{5}).$$

For the truncated icosidodecahedron with side length $\sqrt{3}$ the radius of its circumscribed sphere is $\sqrt{93+36\sqrt{5}}/2$, and thus the objective value is $120\times(93+36\sqrt{5})/4=90(31+12\sqrt{5})$. Therefore, the 1-skeleton of the truncated icosidodecahedron is realized by an optimal embedding.

In the same way, the 1-skeletons of the truncated cuboctahedron (4, 6, 8) and the truncated octahedron (4, 6, 6) are also realized by optimal embeddings of the corresponding graphs.

11 Duality of our embedding problem

In [11] it is shown by using the Lagrange approach that Problem 8.2 is dual to Problem 9.1. In this section, we prove Theorem 0.8, namely, we show that Problem 8.2 is also dual to Problem 8.1.

Let $\mathbf{v} = (v_i)_{i \in V}$ be an arbitrary collection of vectors $v_i \in \mathbb{R}^n$ which are unconstrained, and let $\widetilde{w} \in (\mathbb{R}_{\geq 0})^{|E|}$ and $\mu \in \mathbb{R}$ be new variables. We define the Lagrange function by

$$L(\widetilde{w}, \mu, \mathbf{v}) = \sum_{ij \in E} \widetilde{w}_{ij} \left(||v_i - v_j||^2 - l_{ij}^2 \right) + \mu \sum_{i \in V} s_i \left(||v_i||^2 - 1 \right) + \left\| \sum_{i \in V} s_i v_i \right\|^2.$$
(11.1)

It is easy to see that the following inequality holds.

$$\inf_{\boldsymbol{v}} \sup_{\widetilde{w},\mu} L(\widetilde{w},\mu,\boldsymbol{v}) \geq \sup_{\widetilde{w},\mu} \inf_{\boldsymbol{v}} L(\widetilde{w},\mu,\boldsymbol{v}).$$

For any \boldsymbol{v} we have

$$\sup_{\substack{\widetilde{w} \in (\mathbb{R} \geq 0)^{|E|}, \\ \mu \in \mathbb{R}}} L(\widetilde{w}, \mu, \boldsymbol{v}) = \begin{cases} \left\| \sum_{i \in V} s_i v_i \right\|^2 & \text{if } ||v_i - v_j|| \leq l_{ij}, \ \forall ij \in E \\ & \text{and } \sum_{i \in V} s_i ||v_i||^2 = M, \end{cases}$$

Thus the optimization system of the left-hand side is the same as that of Problem 8.1, that is,

$$M^2\,\delta(G,s,l) = \inf_{\boldsymbol{v} \text{ satisfying (8.3)}} \,\, \sup_{\widetilde{\boldsymbol{w}},\mu} L(\widetilde{\boldsymbol{w}},\mu,\boldsymbol{v}).$$

The right-hand side gives its dual problem, which we shall identify. To do so, we rewrite the Lagrange function (11.1) as

$$L(\widetilde{w}, \mu, \mathbf{v}) = -\mu M - \sum_{ij \in E} l_{ij}^2 \widetilde{w}_{ij}$$

$$+ \left\| \sum_{i \in V} s_i v_i \right\|^2 + \mu \sum_{i \in V} s_i ||v_i||^2$$

$$+ \sum_{ij \in E} \widetilde{w}_{ij} ||v_i - v_j||^2.$$

Let $\mu \in \mathbb{R}$ and $\widetilde{w} \in (\mathbb{R}_{>0})^{|E|}$. If these parameters satisfy the inequality

$$\left\| \sum_{i \in V} s_i v_i \right\|^2 + \mu \sum_{i \in V} s_i ||v_i||^2 + \sum_{ij \in E} \widetilde{w}_{ij} ||v_i - v_j||^2 \ge 0$$
 (11.2)

for all \boldsymbol{v} , then the minimum of $L(\widetilde{w}, \mu, \boldsymbol{v})$ over \boldsymbol{v} is attained when $v_i = 0$ for all $i \in V$. Otherwise, $L(\widetilde{w}, \mu, \boldsymbol{v})$ diverges to negative infinity:

$$\inf_{\boldsymbol{v}} L(\widetilde{w}, \mu, \boldsymbol{v}) = \begin{cases} -\mu M - \sum_{ij \in E} l_{ij}^2 \widetilde{w}_{ij} & \text{if } v \text{ satisfies the inequality (11.2),} \\ -\infty & \text{otherwise.} \end{cases}$$

We derive $\lambda_2(G,(s,\widetilde{w}))$ from the inequality (11.2). If \boldsymbol{v} satisfies $v_1 = \cdots = v_n$, then the inequality (11.2) becomes

$$0 \leq \left\| \sum_{i \in V} s_i v_i \right\|^2 + \mu \sum_{i \in V} s_i ||v_i||^2$$
$$= (M + \mu) \sum_{i \in V} s_i ||v_i||^2.$$

Thus we get $M \ge -\mu$.

Next we assume v_i 's are eigenfunctions of $\lambda_2(G,(s,\widetilde{w}))$. Then the inequality (11.2) is

$$0 \leq M^{2}||\operatorname{bar}(\boldsymbol{v})||^{2} + \mu \sum_{i \in V} s_{i}||v_{i}||^{2}$$
$$+\lambda_{2}(G, (s, \widetilde{w})) \left(\sum_{i \in V} s_{i}||v_{i}||^{2} - M||\operatorname{bar}(\boldsymbol{v})||^{2}\right).$$

By using $\operatorname{bar}(\boldsymbol{v}) = 0$ we get $\lambda_2(G,(s,\widetilde{w})) \geq -\mu$. Therefore the dual problem is the problem that maximizes

$$-\mu M - \sum_{ij \in E} l_{ij}^2 \widetilde{w}_{ij}$$

over all μ and \widetilde{w} subject to the constraints $M \geq -\mu$ and $\lambda_2(G,(s,\widetilde{w})) \geq -\mu$.

 $-\mu$ can be replaced by μ . Introducing a new variable $\lambda > 0$, we may add a new constraint $\sum_{ij\in E} l_{ij}^2 \widetilde{w}_{ij} = 1/\lambda$. Then the objective function is $\mu M - 1/\lambda$, and all constraints are listed as

$$M \ge \mu,$$

$$\lambda_2(G, (s, \widetilde{w})) \ge \mu,$$

$$\sum_{ij \in E} l_{ij}^2 \widetilde{w}_{ij} = \frac{1}{\lambda}.$$

If we set $w_{ij} := L^2 \lambda \widetilde{w}_{ij}$ for $ij \in E$, then the constraints are

$$M \ge \mu,$$

$$-\frac{1}{\lambda} \le -\frac{1}{\lambda_2(G,(s,w))} \mu L^2,$$

$$\sum_{ij \in E} l_{ij}^2 w_{ij} = L^2.$$

In this optimization process, we first optimize the objective function with respect to the parameters μ and λ . Thus μ attains M and $-1/\lambda$ attains $-\mu L^2/\lambda_2(G,(s,w))$, and the problem reduces to the following.

maximize
$$M^2 - \frac{L^2 M}{\lambda_2(G, (s, w))}$$

subject to $\sum_{ij \in E} l_{ij}^2 w_{ij} = L^2$, $w \in (\mathbb{R}_{\geq 0})^{|E|}$.

This problem is nothing but Problem 8.2 and the desired duality is established. In particular, the inequality (8.4) in Corollary 8.4 is reproduced.

12 Concluding remarks

We recall the characterization of a graph having the rotational dimension less than or equal to 2:

$$\operatorname{rotdim}(G) \leq 2$$
 if and only if G is outer planar.

There is a similar characterization for the Colin de Verdière number $\mu(G)$:

$$\mu(G) \leq 2$$
 if and only if G is outer planar.

Moreover, graphs having the Colin de Verdière number less than or equal to 3 can be characterized.

$$\mu(G) \leq 3$$
 if and only if G is planar.

In the thesis by Wappler [24], the followings are conjectured.

- $\operatorname{rotdim}(G) \leq \mu(G)$.
- Graphs having these respective invariants less than or equal to 3 are characterized by different graph properties.

The complete bipartite graph $K_{3,3}$ is the minor-minimal non-planar graph, that is, this is not planar, but all of its minor graphs are planar. If the rotational dimension of $K_{3,3}$ is 4, then $\operatorname{rotdim}(G)$ is 3 or less if and only if G is planar. However, Wappler conjectures

$$\operatorname{rotdim}(K_{3,3}) = 3$$

and expects that $K_{3,3}$ supports the second conjecture above. By investigating optimal embeddings of $K_{3,3}$, we have tried to determine the desired minimum dimension, but this conjecture remains unresolved at this moment.

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